SOLMINEQ.88: A COMPUTER PROGRAM FOR GEOCHEMICAL MODELING OF WATER-ROCK INTERACTIONS

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U.S. GEOLOGICAL SURVEY

Water-Resources Investigations Report 88-4227

*Alberta Research Council

Oil Sands and Hydrocarbon Recovery Department

Edmonton, Alberta, Canada

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Columbus, Ohio

Menlo Park, California

1988

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PREFACE

This report describes the theoretical aspects, the modeling capabilities and the limitations of the geochemical computer code SOLMINEQ.88. This code is the latest version of SOLMNEQ (Kharaka and Barnes, 1973), SOLMNEQF (Aggarwal and others, 1986), and several unpublished versions of this software package. The computer program can be used to model speciation, saturation, dissolution/precipitation, ion exchange/adsorption, mixing, boiling, and gas partitioning between water, oil, and gas phases. The program is comprehensive but it is especially useful for modeling water-rock interactions in sedimentary basins where high temperatures, pressures, salinities, and dissolved organic species prevail.

The user is requested to kindly notify the originating office of any errors found in this report or in the computer program. Updates may occasionally be made to both the report and the program. Users who wish to receive a copy of the computer program and report may send a request to the following addresses:

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CONVERSION FACTORS

Metric (International System) units are used in this report. For those readers who prefer to use inch-pound units, conversion factors for the terms used in this report are listed below:

Multiply metric unit	by	To obtain inch-pound unit
micrometer (μm)	0.03937	mil
centimeter	0.3937	inch
meter (m)	3.281	foot (ft)
square centimeter (cm^2)	0.1550	square inch (in^2)
cubic centimeter (cm^3)	0.06102	cubic inch (in^3)
cubic meter (m^3)	35.31	cubic feet (ft^3)
liter (l)	0.03531	cubic feet (ft^3)
microgram (μg)	1.543×10^{-5}	grain (gr)
miligram (mg)	1.543×10^{-2}	grain (gr)
gram (g)	2.205×10^{-3}	pound (lb)
kilogram (kg)	2.205	pound (lb)
miligram/liter (mg/l)	6.243×10^{-5}	pound/cubic foot (lb/ft^3)
atmosphere (atm)	14.70	pounds per square inch (psi)
bar	14.50	pounds per square inch (psi)
kilopascal (kPa)	0.1450	pounds per square inch (psi)
degree Celcius (°C)	1.8 °C + 32	degree Fahrenheit (°F)
degree Kelvin (K)	(K - 273.15)1.8 + 32	degree Fahrenheit (°F)
calorie (cal)	3.968×10^{-3}	British thermal unit (Btu)
kilocalorie (kcal)	3.968	British thermal unit (Btu)

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ABSTRACT

Geochemical modeling based on equilibrium and irreversible thermodynamics has, in the last 20 years, become a well recognized tool for understanding the processes of water-rock interactions and predicting their consequences. SOLMINEQ.88 is the latest version of the 1973-computer program code SOLMNEQ and its various updated versions. This program is general and comprehensive, but is particularly useful for modeling geochemical interactions in sedimentary basins and petroleum reservoirs where petroleum, aqueous organic species, and subsurface pressure play an important role.

SOLMINEQ.88 is written in FORTRAN-77 and has an improved algorithm over that in previous versions for faster execution. This version has a revised thermodynamic database, more inorganic (260) and organic (80) aqueous species and minerals (220), computes the activity coefficients in brines using Pitzer equations, and computes pH and mineral solubilities at subsurface temperatures (0° to 350° C) and pressures (1 to 1,000 bars). New modeling options in SOLMINEQ.88 can be used to study the effects of boiling, mixing of solutions and partitioning of gases between water, oil and gas phases. SOLMINEQ.88 has several mass transfer options that can be used to predict the effects of ion exchange, adsorption/desorption, and dissolution/precipitation of solid phases. A user-friendly interactive code SOLINPUT is available for use to generate and update the input file for SOLMINEQ.88.

The numerous assumptions and limitations of geochemical models like SOLMINEQ.88 are described in detail because they indicate the range of conditions where the models can be used successfully. The limitations may be related to incomplete and/or unreliable chemical and mineral data as well as to uncertainties in equilibrium constants for aqueous species and minerals. The modeling capabilities and the limitations of the various options in this code are described with output from selected examples.

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INTRODUCTION

Water-rock interactions in natural systems comprise a combination of several physical and chemical processes, including (a) mineral dissolution and precipitation; (b) ion exchange and adsorption/desorption; (c) mixing of fluids; (d) gas separation by pressure-drawdown or boiling; and (e) organic/inorganic interactions. In the last 20 years, geochemical modeling based on equilibrium and irreversible thermodynamics has become a well recognized tool for understanding the processes of water-rock interaction and predicting their consequences. Numerous computer program codes are presently available for geochemical modeling of water-rock interactions (Nordstrom and others, 1979; Wolery, 1983; EPRI, 1984; Nordstrom and Munoz, 1985). The list of commonly used programs is large and expanding; it includes the following software packages:

1. PATHI and its modified versions (Helgeson and others, 1970; Perkins, 1980).
2. SOLMNEQ and its modified versions (Kharaka and Barnes, 1973; Aggarwal and others, 1986).
3. WATEQ and its modified versions (Truesdell and Jones, 1974; Plummer and others, 1984; Ball and others, 1987).
4. MINEQL (Westall and others, 1976).
5. EQ3/EQ6 (Wolery, 1979; 1983; 1984).
6. PHREEQE (Parkhurst and others, 1980).
7. GEOCHEM (Sposito and Mattigod, 1980).
8. SOLVEQ (Reed, 1982).
9. MINTEQ (Felmy and others, 1984).
10. DYNAMIX (Narasimhan and others, 1986)

The computer program code SOLMNEQ (Kharaka and Barnes, 1973) was originally written in PL/1 for the IBM 360 computers. The original program computed the equilibrium distribution of 162 inorganic aqueous species generally present in natural waters over the temperature range of 0° to 350 °C from the reported physical and chemical properties of the water and an internally consistent set of thermodynamic data. The program also computed the saturation states of 158 minerals commonly encountered in sedimentary rocks. SOLMNEQ has undergone continuous updating, additions and modifications. The additions and modifications were carried out to develop a general comprehensive computer program for geochemical modeling of water-rock interactions. This program, however, is particularly useful for modeling

interactions in sedimentary basins and in thermally stimulated oil reservoirs where petroleum and aqueous organic species play an important role.

The present version, renamed SOLMINEQ.88 (SOLution MINeral EQuilibrium, 1988), is written in FORTRAN-77 and has an improved algorithm for faster execution. This version has a revised thermodynamic data base, more inorganic (260) and organic (80) aqueous species and minerals (220), and computes pH and mineral solubilities at subsurface temperatures and pressures. New modeling options have been added to SOLMINEQ.88 that can be used to study the effects of boiling, mixing of solutions, and partitioning of gases between water, oil and gas phases. SOLMINEQ.88 has mass-transfer capabilities that can be used to study the effects of ion exchange, adsorption/desorption, and dissolution/precipitation of solid phases.

This report documents the modeling capabilities of the computer code SOLMINEQ.88. It is intended as a user's guide, describing the assumptions underlying the various options and summarizing the mathematical and numerical techniques used. The thermochemical and other data used in the computations are tabulated. The fixed and optional data used to create the input file are described in detail. An interactive input program, SOLINPUT, is available to create or modify the input file. Output from several examples has been included to illustrate various applications of this code, and for comparison by users on other computer systems to verify that the program is functioning correctly.

Acknowledgments

This code has been greatly improved because of suggestions and corrections from many users including Bob Mariner, Randy Bassett, Jim Bishoff, Sheldon Sommer, Indu Mishri, Brian Hitchon, Gordon Bird, and several scientists at Alberta Research Council, and many students at the U.S. Geological Training Center in Denver, Colorado.

Dan Specht, Bob Hull, Ming Ko, and Pat Dorherty have made important contributions to the code. We are grateful for thorough reviews of this document by our colleagues Bob Mariner, Charly Alpers, Rich Wanty and Art White. Special thanks are due Jackie Hamilton for the many typings of this bulky report.

Table 1. Glossary of Symbols Used in Text

a	Sum of the Goldschmidt radii
a	Stands for anion when used as a subscript
a,b,c,W,θ	Temperature-independent constants in eqn. 48
a_i	Activity of species i
$a_1, a_2, a_3, a_4, \Theta, w, Q$	Constants used in eqn. 55
$\bar{a}_i$	Activity of species i at equilibrium
a_i^o	Ion size parameter of species i
A,B,C	Fitted pressure constants see appendix 1
A,B,C	Meyer-Kelley heat capacity temperature fit constants.
A	Chemical affinity
A_T	Total area of the exchanging surface per kg of water
A_γ	Debye-Hückel limiting law slope.
A^ϕ	Adjusted Debye-Hückel constant used in Pitzer eqn.
AP	Ion activity product
B_γ	Extended Debye-Hückel limiting law constant.
$B^\bullet, B_u^*, B_m^*$	Activity coefficient deviation functions subscripts for univalent and multivalent species.
B_{MX}, B'_{MX}	Cation-anion interaction coefficients in pitzer eqns.
c	Represents a cation when used as a subscript.
$C_{1i}, C_{2i}, w_i, \theta_i$	Empirical constants in eqn. 47
C_p	Isobaric heat capacity
$\Delta C^o_{p,r}$	Standard state isobaric heat capacity of reaction
C_{MX}	Cation-anion interaction coefficient in pitzer eqns.
C^ϕ_{MX}	Cation-anion interaction parameter in pitzer eqns.
e	Electron charge, 1.602×10^{-19} coulomb
E	Equivalent fraction of surface sites occupied by a specific surface complex
E^o	Standard state potential

Eh	Oxidation potential referred to hydrogen half cell
$E_{\theta_{ij}}(I), E_{\theta'_{ij}}(I)$	Electrostatic effect of unsymmetrical unmixing used in Pitzer equations
F	Faraday constant, 9.648×10^4 coulomb mol^{-1}
$\mathbf{F}$	General Debye-Hückel interaction term used in Pitzer eqns.
g(x), g'(x)	Fitting functions used in Pitzer equations
ΔG_r^o	Standard state Gibbs free energy of reaction
ΔG_{diff}	Gibbs free energy difference between the actual and equilibrium states of a mineral
ΔH_f^o	Standard state enthalpy of formation
ΔH_r^o	Standard state enthalpy of reaction
I	Ionic strength
k	Henry's Law coefficient in pure water
k_m	Henry's Law coefficient in a solution of molality m
K_i	Equilibrium constant of species i
ℓ	Refers to a liquid when used as a subscript or superscript
L	Number of ligands in eqns. 51 & 52
m_i	Molality of species i
$m_{i,t}$	Total analytical molality of component i
M	Represents positively charged species as a subscript
$M_{i,t}$	Total moles of substance i
N_A	Avogadro's number, 6.022×10^{23} mol^{-1}
N_S	Number of sites per unit area of the mineral surface
N_a, N_c	Total number of the subscripted species
n	Number of electrons involved in redox reactions
$n_{i,j}$	Stoichiometric coefficient of component i in species j
p	Polarizability in eqn. 51
P	Pressure in bars
Q	Reaction quotient
R	Gas constant, 1.987 cal K^{-1} mol^{-1}

ΔS_r^o	Standard state entropy of reaction
SI	Saturation index
t	Temperature in degrees C
T	Temperature in degrees K
T_r	Reference temperature in degrees K
v	Refers to a vapor as a subscript or superscript
$\bar{V}_i$	Partial molal volume of aqueous species i
$\bar{V}_i^v$	Specific volume of gas i
ΔV_r^o	Standard state volume of reaction
W	Weight of a substance
x	Derivative of the variation of ϵ
X	Represents negatively charged ions when used as a subscript
Y_i	Tolerance factor for subscripted ion
z_i	Charge on species i
Z	Pitzer eqn. charge sum
Z	Compressibility factor
α	Charge fraction on surface sites
α_{MX}	Fitting parameter used in Pitzer equations
β	Coefficient of isothermal compressibility of water
$\beta_{MX}^{(0)}, \beta_{MX}^{(1)}, \beta_{MX}^{(2)}$	Pitzer cation-anion interaction parameters
γ_i	Activity coefficient of species i
$\gamma_{i,P}$	Activity coefficient of species i from Pitzer eqns.
ϵ	Dielectric constant of water
ϵ_o	Permittivity of the vacuum, 8.854×10^{-12} farad m^{-1}
θ_{ij}	Pitzer anion-anion/cation-cation interaction parameter
κ	Boltzman constant, 3.298×10^{-24} cal K^{-1}
ν_i	Number of moles of ions in component i
ρ	Density (g/cm^3)
σ_o, σ_d	Charge density at mineral surface (o) or diffuse layer (d)

ϕ_e	Osmotic coefficient of the subscripted electrolyte
$\Phi_{MM}, \Phi_{XX}, \Phi'_{MM}, \Phi'_{XX}$	Pitzer cation-cation/anion-anion interaction coefficients
χ	Fugacity coefficient
ψ	Surface potential
ψ_{ijk}	Pitzer cation-cation-anion/anion-anion-cation interaction parameters

METHOD OF COMPUTATION

The principal computations carried out by SOLMINEQ.88 are aqueous speciation and saturation states of minerals. This program computes the equilibrium distribution of more than 340 inorganic and organic aqueous species of major, minor and trace elements generally present in natural waters. The distribution of 54 organic species of acetate, oxalate, succinate and two user-defined (additional) organic anions has been included because organic species are important components of natural waters, especially those present in sedimentary basins (Carothers and Kharaka, 1978; Kharaka and others, 1986; MacGowan and Surdam, 1987; and many others). Although the total number of possible organic species is extremely large, the number of important anions in any given natural system in addition to acetate, oxalate and succinate is generally small (Kharaka and others, 1986; MacGowan and Surdam, 1987). Consequently, two additional user-defined organic anions together with their complexes with H^+ and 12 other cations usually are sufficient for modeling purposes. A user-defined cation together, with 13 complexes with anions, also was added to make the code of more general application.

The distribution of aqueous species for a given composition of water at specified pH and temperature (or temperatures) is computed using the same approach as in the original code (Kharaka and Barnes, 1973) by solving a set of mass-action, oxidation-reduction and mass-balance equations based on the ion-association aqueous model (Garrels and Christ, 1965; Helgeson, 1967). In this model, the dissociation reaction for each of the aqueous complexes (Table 2) has a corresponding mass-action equation. For example, the dissociation reactions for $CaHCO_3^+$ and $CaCO_3^o$ are

$$CaHCO_3^+ \rightleftarrows Ca^{++} + HCO_3^- \quad , \tag{1}$$

and

$$CaCO_3^o \rightleftarrows Ca^{++} + CO_3^{--} \quad , \tag{2}$$

for which the respective mass-action equations are:

$$K_{CaHCO_3^+} = \frac{m_{Ca^{++}} \cdot \gamma_{Ca^{++}} \cdot m_{HCO_3^-} \cdot \gamma_{HCO_3^-}}{m_{CaHCO_3^+} \cdot \gamma_{CaHCO_3^+}} \quad , \tag{1}$$

$$K_{CaCO_3^o} = \frac{m_{Ca^{++}} \cdot \gamma_{Ca^{++}} \cdot m_{CO_3^{--}} \cdot \gamma_{CO_3^{--}}}{m_{CaCO_3^o} \cdot \gamma_{CaCO_3^o}} \quad , \tag{2}$$

where m_i and γ_i are, respectively, the molality and activity coefficient of the subscripted species and K is the dissociation constant of the subscripted aqueous complex.

The mass-balance equations take the form:

$$m_{i,t} = \sum_{1}^{j} n_{i,j}\, m_j \quad , \tag{3}$$

where $m_{i,t}$, $n_{i,j}$ and m_j are, respectively, the analytical (or total) molality of the component i, the stoichiometric coefficient of component i in species j, and the computed molality of species j. For a system of i components and j species, i mass-balance and j-i mass-action equations can be written. With the additional constraints of specified pH and temperature, an iterative technique (see below) can be used to solve, simultaneously, the system of equations for the concentration of all species (Smith and Missin, 1982).

For aqueous species of Ca, for example, the mass-balance equation is

$$m_{Ca,t} = m_{Ca^{++}} + m_{CaHCO_3^+} + m_{CaCO_3^o} + \ldots \quad . \tag{4}$$

The mass-action and mass-balance equations are combined and rearranged after the activity coefficients have been computed (see below) to give the value of $m_{Ca^{++}}$ from the following:

$$m_{Ca^{++}} = \frac{m_{Ca,t}}{1 + \gamma_{Ca^{++}} \cdot \Omega} \quad , \tag{5}$$

where $$\Omega = \frac{m_{HCO_3^-} \cdot \gamma_{HCO_3^-}}{K_{CaHCO_3^+} \cdot \gamma_{CaHCO_3^+}} + \frac{m_{CO_3^{--}} \cdot \gamma_{CO_3^{--}}}{K_{CaCO_3^o} \cdot \gamma_{CaCO_3^o}} + \ldots \quad .$$

$m_{CaHCO_3^+}$ and $m_{CaCO_3^o}$ are then computed from equations (1) and (2), respectively, after substituting the computed $m_{Ca^{++}}$.

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data (see references at end of Table 3)

ID # and Name	Reaction	References
1 HCO_3^-	$HCO_3^- \rightleftarrows H^+ + CO_3^{--}$	1a, 2a
2 H_2O^0	$H_2O^0 \rightleftarrows H^+ + OH^-$	3a
3 $H_4SiO_4^0$	$H_4SiO_4^0 \rightleftarrows H^+ + H_3SiO_4^-$	4a, 24a
4 Cu^{++}	$Cu^{++} + Fe^{++} \rightleftarrows Cu^+ + Fe^{+3}$	5b
5 Fe^{+3}	$Fe^{+3} + \frac{1}{2}H_2O + \frac{1}{8}HS^- \rightleftarrows Fe^{++} + \frac{1}{8}SO_4^{--} + \frac{9}{8}H^+$	6b
6 Hg^{++}	$2Hg^{++} + 2Fe^{++} \rightleftarrows Hg_2^{++} + 2Fe^{+3}$	2c
7 Mn^{+3}	$Mn^{+3} + Fe^{++} \rightleftarrows Mn^{++} + Fe^{+3}$	2b
8 $H_2AsO_3^-$	$H_2AsO_3^- \rightleftarrows H^+ + HAsO_3^{--}$	2a
9 AlF_5^{--}	$AlF_5^{--} \rightleftarrows Al^{+3} + 5F^-$	2a
10 H_2S^0	$H_2S^0 \rightleftarrows H^+ + HS^-$	7a, 64a
11 AlF^{++}	$AlF^{++} \rightleftarrows Al^{+3} + F^-$	2a, 8a
12 AlF_2^+	$AlF_2^+ \rightleftarrows Al^{+3} + 2F^-$	2a, 8a
13 AlF_3^0	$AlF_3^0 \rightleftarrows Al^{+3} + 3F^-$	2a
14 AlF_4^-	$AlF_4^- \rightleftarrows Al^{+3} + 4F^-$	2a
15 $Al(OH)^{++}$	$Al(OH)^{++} \rightleftarrows Al^{+3} + OH^-$	9b
16 $Al(OH)_2^+$	$Al(OH)_2^+ \rightleftarrows Al^{+3} + 2OH^-$	10e
17 $Al(OH)_4^-$	$Al(OH)_4^- \rightleftarrows Al^{+3} + 4OH^-$	7a
18 $Al(SO_4)^+$	$Al(SO_4)^+ \rightleftarrows Al^{+3} + SO_4^{--}$	2a
19 $Al(SO_4)_2^-$	$Al(SO_4)_2^- \rightleftarrows Al^{+3} + 2SO_4^{--}$	2a
20 $AgCl^0$	$AgCl^0 \rightleftarrows Ag^+ + Cl^-$	11a
21 $AgCl_2^-$	$AgCl_2^- \rightleftarrows Ag^+ + 2Cl^-$	11a
22 $AgCl_3^{--}$	$AgCl_3^{--} \rightleftarrows Ag^+ + 3Cl^-$	11a
23 $AgCl_4^{-3}$	$AgCl_4^{-3} \rightleftarrows Ag^+ + 4Cl^-$	11a
24 $Ag(SO_4)^-$	$Ag(SO_4)^- \rightleftarrows Ag^+ + SO_4^{--}$	2a
25 CH_3COOH^0	$CH_3COOH^0 \rightleftarrows H^+ + CH_3COO^-$	12a
26 $BaCO_3^0$	$BaCO_3^0 \rightleftarrows Ba^{++} + CO_3^{--}$	7f
27 $Ba(HCO_3)^+$	$Ba(HCO_3)^+ \rightleftarrows Ba^{++} + HCO_3^-$	7f

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
28 $Ba(OH)^{+}$	$Ba(OH)^{+} \rightleftarrows Ba^{++} + OH^{-}$	9b
29 $BaSO_4^{0}$	$BaSO_4^{0} \rightleftarrows Ba^{++} + SO_4^{--}$	7f
30 $CaCO_3^{0}$	$CaCO_3^{0} \rightleftarrows Ca^{++} + CO_3^{--}$	1a, 7f
31 $Ca(HCO_3)^{+}$	$Ca(HCO_3)^{+} \rightleftarrows Ca^{++} + HCO_3^{-}$	1a, 13a
32 $Ca(OH)^{+}$	$Ca(OH)^{+} \rightleftarrows Ca^{++} + OH^{-}$	9b
33 $CaPO_4^{-}$	$CaPO_4^{-} \rightleftarrows Ca^{++} + PO_4^{-3}$	7a
34 $CaHPO_4^{0}$	$CaHPO_4^{0} \rightleftarrows Ca^{++} + HPO_4^{--}$	7a
35 $CaH_2PO_4^{+}$	$CaH_2PO_4^{+} \rightleftarrows Ca^{++} + H_2PO_4^{-}$	7a
36 $CaSO_4^{0}$	$CaSO_4^{0} \rightleftarrows Ca^{++} + SO_4^{--}$	14a
37 $CuCl^{0}$	$CuCl^{0} \rightleftarrows Cu^{+} + Cl^{-}$	15a, 16a
38 $CuCl_2^{-}$	$CuCl_2^{-} \rightleftarrows Cu^{+} + 2Cl^{-}$	7a
39 $CuCl_3^{--}$	$CuCl_3^{--} \rightleftarrows Cu^{+} + 3Cl^{-}$	7a
40 $CuCl^{+}$	$CuCl^{+} \rightleftarrows Cu^{++} + Cl^{-}$	7a
41 $CuCl_2^{0}$	$CuCl_2^{0} \rightleftarrows Cu^{++} + 2Cl^{-}$	7a
42 $CuCl_3^{-}$	$CuCl_3^{-} \rightleftarrows Cu^{++} + 3Cl^{-}$	7a
43 $CuCl_4^{--}$	$CuCl_4^{--} \rightleftarrows Cu^{++} + 4Cl^{-}$	7a
44 $Cu(OH)^{+}$	$Cu(OH)^{+} \rightleftarrows Cu^{++} + OH^{-}$	9a
45 $CuSO_4^{0}$	$CuSO_4^{0} \rightleftarrows Cu^{++} + SO_4^{--}$	2a
46 $FeCl^{+}$	$FeCl^{+} \rightleftarrows Fe^{++} + Cl^{-}$	17a
47 $FeCl_2^{0}$	$FeCl_2^{0} \rightleftarrows Fe^{++} + 2Cl^{-}$	17a
48 $FeHPO_4^{0}$	$FeHPO_4^{0} \rightleftarrows Fe^{++} + HPO_4^{--}$	52c
49 $H_3PO_4^{0}$	$H_3PO_4^{0} \rightleftarrows 3H^{+} + PO_4^{-3}$	24a
50 $Fe(OH)^{+}$	$Fe(OH)^{+} \rightleftarrows Fe^{++} + OH^{-}$	9b
51 $Fe(OH)_2^{0}$	$Fe(OH)_2^{0} \rightleftarrows Fe^{++} + 2OH^{-}$	9b
52 $FeOOH^{-}$	$FeOOH^{-} + 3H^{+} \rightleftarrows Fe^{++} + 2H_2O$	9b
53 $FeSO_4^{0}$	$FeSO_4^{0} \rightleftarrows Fe^{++} + SO_4^{--}$	2c
54 $FeCl^{++}$	$FeCl^{++} \rightleftarrows Fe^{+3} + Cl^{-}$	7a, 8a
55 $FeCl_2^{+}$	$FeCl_2^{+} \rightleftarrows Fe^{+3} + 2Cl^{-}$	7a, 8a

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
56 $FeCl_3^0$	$FeCl_3^0 \rightleftarrows Fe^{+3} + 3Cl^-$	7a, 8a
57 $FeCl_4^-$	$FeCl_4^- \rightleftarrows Fe^{+3} + 4Cl^-$	7a, 8a
58 $Fe(SO_4)^+$	$Fe(SO_4)^+ \rightleftarrows Fe^{+3} + SO_4^{--}$	2c
59 $Fe(SO_4)_2^-$	$Fe(SO_4)_2^- \rightleftarrows Fe^{+3} + 2SO_4^{--}$	18d
60 $Fe(OH)^{++}$	$Fe(OH)^{++} \rightleftarrows Fe^{+3} + OH^-$	9b
61 $Fe(OH)_2^+$	$Fe(OH)_2^+ \rightleftarrows Fe^{+3} + 2OH^-$	2e
62 $Fe(OH)_3^0$	$Fe(OH)_3^0 \rightleftarrows Fe^{+3} + 3OH^-$	10f, 19f
63 $Fe(OH)_4^-$	$Fe(OH)_4^- \rightleftarrows Fe^{+3} + 4OH^-$	19e
64 $B(OH)_4^-$	$B(OH)_4^- \rightleftarrows B(OH)_3^0 + OH^-$	20a
65 AlF_6^{-3}	$AlF_6^{-3} \rightleftarrows Al^{+3} + 6F^-$	2b
66 $H_3SiO_4^-$	$H_3SiO_4^- \rightleftarrows H^+ + H_2SiO_4^{--}$	2a
67 $H_3AsO_3^0$	$H_3AsO_3^0 \rightleftarrows H^+ + H_2AsO_3^-$	24a
68 $HAsO_4^{--}$	$HAsO_4^{--} \rightleftarrows H^+ + AsO_4^{-3}$	21c
69 $H_2AsO_4^-$	$H_2AsO_4^- \rightleftarrows 2H^+ + AsO_4^{-3}$	24a
70 $H_3AsO_4^0$	$H_3AsO_4^0 \rightleftarrows 3H^+ + AsO_4^{-3}$	24a
71 HF^0	$HF^0 \rightleftarrows H^+ + F^-$	7a
72 $H_2CO_3^0$	$H_2CO_3^0 \rightleftarrows H^+ + HCO_3^-$	1a, 7a
73 HPO_4^{--}	$HPO_4^{--} \rightleftarrows H^+ + PO_4^{-3}$	7a
74 $H_2PO_4^-$	$H_2PO_4^- \rightleftarrows 2H^+ + PO_4^{-3}$	24a
75 HS^-	$HS^- \rightleftarrows H^+ + S^{--}$	7a
76 HSO_4^-	$HSO_4^- \rightleftarrows H^+ + SO_4^{--}$	7a
77 HNO_3^0	$HNO_3^0 \rightleftarrows H^+ + NO_3^-$	24a
78 $HgCl^+$	$HgCl^+ \rightleftarrows Hg^{++} + Cl^-$	7c
79 $HgCl_2^0$	$HgCl_2^0 \rightleftarrows Hg^{++} + 2Cl^-$	7c
80 $HgCl_3^-$	$HgCl_3^- \rightleftarrows Hg^{++} + 3Cl^-$	7c
81 $HgCl_4^{--}$	$HgCl_4^{--} \rightleftarrows Hg^{++} + 4Cl^-$	7c
82 $HgSO_4^0$	$HgSO_4^0 \rightleftarrows Hg^{++} + SO_4^{--}$	18f, 22f

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
83 $HgS(H_2S)_2^0$	$HgS(H_2S)_2^0 + H^+ \rightleftarrows Hg^{++} + 2H_2S^0 + HS^-$	23c
84 $Hg(HS)_3^-$	$Hg(HS)_3^- \rightleftarrows Hg^{++} + 3HS^-$	17c
85 Hg^0	$Hg^0 + 2Fe^{+3} \rightleftarrows Hg^{+2} + 2Fe^{++}$	23d
86 KCl^0	$KCl^0 \rightleftarrows K^+ + Cl^-$	7a, 11a
87 KCO_3^-	$KCO_3^- \rightleftarrows K^+ + CO_3^{--}$	31f
88 $KHSO_4^0$	$KHSO_4^0 \rightleftarrows K^+ + HSO_4^-$	15c
89 KSO_4^-	$KSO_4^- \rightleftarrows K^+ + SO_4^{--}$	7a
90 $KHPO_4^-$	$KHPO_4^- \rightleftarrows K^+ + HPO_4^{--}$	7a
91 $LiOH^0$	$LiOH^0 \rightleftarrows Li^+ + OH^-$	25c
92 $LiSO_4^-$	$LiSO_4^- \rightleftarrows Li^+ + SO_4^{--}$	25
93 $MgCO_3^0$	$MgCO_3^0 \rightleftarrows Mg^{++} + CO_3^{--}$	26d
94 $MgHCO_3^+$	$MgHCO_3^+ \rightleftarrows Mg^{++} + HCO_3^-$	26d
95 MgF^+	$MgF^+ \rightleftarrows Mg^{++} + F^-$	7a
96 $MgOH^+$	$MgOH^+ \rightleftarrows Mg^{++} + OH^-$	9a
97 $MgSO_4^0$	$MgSO_4^0 \rightleftarrows Mg^{++} + SO_4^{--}$	15, 27b
98 $MgPO_4^-$	$MgPO_4^- \rightleftarrows Mg^{++} + PO_4^{-3}$	7a
99 $MgHPO_4^0$	$MgHPO_4^0 \rightleftarrows Mg^{++} + HPO_4^{--}$	7a
100 $MgH_2PO_4^+$	$MgH_2PO_4^+ \rightleftarrows Mg^{++} + H_2PO_4^-$	7a
101 $MnCl^+$	$MnCl^+ \rightleftarrows Mn^{++} + Cl^-$	28d
102 $MnCl_2^0$	$MnCl_2^0 \rightleftarrows Mn^{++} + 2Cl^-$	28d
103 $MnCl_3^-$	$MnCl_3^- \rightleftarrows Mn^{++} + 3Cl^-$	28d
104 $MnCl_4^{--}$	$MnCl_4^{--} \rightleftarrows Mn^{++} + 4Cl^-$	28d
105 $MnHCO_3^+$	$MnHCO_3^+ \rightleftarrows Mn^{++} + HCO_3^-$	29d
106 $MnSO_4^0$	$MnSO_4^0 \rightleftarrows Mn^{++} + SO_4^{--}$	25d
107 $MnCl^{++}$	$MnCl^{++} \rightleftarrows Mn^{+3} + Cl^-$	15a
108 $MnHPO_4^0$	$MnHPO_4^0 \rightleftarrows Mn^{++} + HPO_4^{--}$	52c
109 $MnOH^+$	$MnOH^+ \rightleftarrows Mn^{++} + OH^-$	9c
110 $NaCl^0$	$NaCl^0 \rightleftarrows Na^+ + Cl^-$	30a

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
111 $NaCO_3^-$	$NaCO_3^- \rightleftarrows Na^+ + CO_3^{--}$	31c
112 $NaHCO_3^0$	$NaHCO_3^0 \rightleftarrows Na^+ + HCO_3^-$	32, 22f
113 $Na_2CO_3^0$	$Na_2CO_3^0 \rightleftarrows 2Na^+ + CO_3^{--}$	32, 33f
114 $Na_2SO_4^0$	$Na_2SO_4^0 \rightleftarrows 2Na^+ + SO_4^{--}$	
115 $NaSO_4^-$	$NaSO_4^- \rightleftarrows Na^+ + SO_4^{--}$	54a
116 $NaHPO_4^-$	$NaHPO_4^- \rightleftarrows Na^+ + HPO_4^{--}$	35c
117 $HgOH^+$	$HgOH^+ \rightleftarrows Hg^{++} + OH^-$	9b
118 NH_4OH^0	$NH_4OH^0 \rightleftarrows NH_4^+ + OH^-$	7a
119 $NaHS^0$	$NaHS^0 \rightleftarrows Na^+ + HS^-$	46a
120 NaF^0	$NaF^0 \rightleftarrows Na^+ + F^-$	57c
121 $PbCl^+$	$PbCl^+ \rightleftarrows Pb^{++} + Cl^-$	36a
122 $PbCl_2^0$	$PbCl_2^0 \rightleftarrows Pb^{++} + 2Cl^-$	36a
123 $PbCl_3^-$	$PbCl_3^- \rightleftarrows Pb^{++} + 3Cl^-$	36a
124 $PbCl_4^{--}$	$PbCl_4^{--} \rightleftarrows Pb^{++} + 4Cl^-$	36a
125 $PbSO_4^0$	$PbSO_4^0 \rightleftarrows Pb^{++} + SO_4^{--}$	15
126 $Zn(CH_3COO)_2^0$	$Zn(CH_3COO)_2^0 \rightleftarrows Zn^{++} + 2CH_3COO^-$	18c, 38a
127 $SrOH^+$	$SrOH^+ \rightleftarrows Sr^{++} + OH^-$	9b
128 $SrCO_3^0$	$SrCO_3^0 \rightleftarrows Sr^{++} + CO_3^{--}$	40c
129 $SrHCO_3^+$	$SrHCO_3^+ \rightleftarrows Sr^{++} + HCO_3^-$	40c
130 $SrSO_4^0$	$SrSO_4^0 \rightleftarrows Sr^{++} + SO_4^{--}$	7a
131 $ZnCl^+$	$ZnCl^+ \rightleftarrows Zn^{++} + Cl^-$	41a
132 $ZnCl_2^0$	$ZnCl_2^0 \rightleftarrows Zn^{++} + 2Cl^-$	41a
133 $ZnCl_3^-$	$ZnCl_3^- \rightleftarrows Zn^{++} + 3Cl^-$	41a
134 $ZnCl_4^{--}$	$ZnCl_4^{--} \rightleftarrows Zn^{++} + 4Cl^-$	41a
135 $ZnSO_4^0$	$ZnSO_4^0 \rightleftarrows Zn^{++} + SO_4^{--}$	42d
136 AsO_4^{-3}	$AsO_4^{-3} + 4H^+ + 2Fe^{++} \rightleftarrows H_2AsO_3^- + 2Fe^{+3} + H_2O$	7a
137 $Hg(OH)_2^0$	$Hg(OH)_2^0 \rightleftarrows Hg^{++} + 2OH^-$	9b

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
138 Fe^{++} to Fe^{+3}	$Fe^{++} \rightleftarrows Fe^{+3} + e^-$	6b
139 Cu^{+} to Cu^{++}	$Cu^{+} \rightleftarrows Cu^{++} + e^-$	5b
140 Hg_2^{++} to Hg^{++}	$Hg_2^{++} \rightleftarrows 2Hg^{++} + 2e^-$	7c
141 Mn^{++} to Mn^{+3}	$Mn^{++} \rightleftarrows Mn^{+3} + e^-$	7c
142 U^{+4} to UO_2^{+}	$U^{+4} \quad 2H_2O \rightleftarrows UO_2^{+} + 4H^{+} + e^-$	43b
143 UO_2^{+} to UO_2^{++}	$UO_2^{+} \rightleftarrows UO_2^{++} + e^-$	43b
144 V^{+3} to VO^{++}	$V^{+3} + H_2O \rightleftarrows VO^{++} + 2H^{+} + e^-$	44b, 2b
145 VO^{++} to VO_4^{-3}	$VO^{+3} + 2H_2O \rightleftarrows VO_4^{-3} + 6H^{+} + e^-$	44c, 45c
146 $CaCl^{+}$	$CaCl^{+} \rightleftarrows Ca^{++} + Cl^-$	46a
147 $CaCl_2^{o}$	$CaCl_2^{o} \rightleftarrows Ca^{++} + 2Cl^-$	79a
148 UOH^{+3}	$UOH^{+3} \rightleftarrows U^{+4} + OH^-$	5b, 43b
149 $U(OH)_2^{++}$	$U(OH)_2^{++} \rightleftarrows U^{+4} + 2OH^-$	5b, 43b
150 $U(OH)_3^{+}$	$U(OH)_3^{+} + 3H^{+} \rightleftarrows U^{+4} + 3H_2O$	5b, 43b
151 $U(OH)_4^{o}$	$U(OH)_4^{o} + 4H^{+} \rightleftarrows U^{+4} + 4H_2O$	5b, 43b
152 $U(OH)_5^{-}$	$U(OH)_5^{-} + 5H^{+} \rightleftarrows U^{+4} + 5H_2O$	47a
153 UF^{+3}	$UF^{+3} \rightleftarrows U^{+4} + F^-$	5b, 43b
154 UF_2^{++}	$UF_2^{++} \rightleftarrows U^{+4} + 2F^-$	5b, 43b
155 UF_3^{+}	$UF_3^{+} \rightleftarrows U^{+4} + 3F^-$	5b, 43b
156 UF_4^{o}	$UF_4^{o} \rightleftarrows U^{+4} + 4F^-$	5b, 43b
157 UF_5^{-}	$UF_5^{-} \rightleftarrows U^{+4} + 5F^-$	5b, 43b
158 UF_6^{--}	$UF_6^{--} \rightleftarrows U^{+4} + 6F^-$	5b, 43b
159 UCl^{+3}	$UCl^{+3} \rightleftarrows U^{+4} + Cl^-$	5b, 43b
160 $U(HPO_4)^{++}$	$U(HPO_4)^{++} \rightleftarrows U^{+4} + HPO_4^{--}$	2b, 43b
161 $U(HPO_4)_2^{o}$	$U(HPO_4)_2^{o} \rightleftarrows U^{+4} + 2HPO_4^{--}$	2b, 43b
162 $U(HPO_4)_3^{--}$	$U(HPO_4)_3^{--} + 3H^{+} \rightleftarrows U^{+4} + 3H_2PO_4^{-}$	2b, 43b
163 $U(HPO_4)_4^{-4}$	$U(HPO_4)_4^{-4} + 4H^{+} \rightleftarrows U^{+4} + 4H_2PO_4^{-}$	2b, 43b
164 $U(SO_4)^{++}$	$U(SO_4)^{++} \rightleftarrows U^{+4} + SO_4^{--}$	5b, 43b

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
165 $U(SO_4)_2^0$	$U(SO_4)_2^0 \rightleftarrows U^{+4} + 2SO_4^{--}$	5b, 43b
166 $U_6(OH)_{15}^{+9}$	$U_6(OH)_{15}^{+9} + 12H^+ \rightleftarrows 6U^{+4} + 30H^- + 12H_2O$	5b, 48b
167 $(UO_2)(OH)^+$	$(UO_2)(OH)^+ \rightleftarrows UO_2^{++} + OH^-$	5b, 43b
168 $(UO_2)(OH)_2^0$	$(UO_2)(OH)_2^0 \rightleftarrows UO_2^{++} + 2OH^-$	5b, 43b
169 $(UO_2)_2(OH)_2^{++}$	$(UO_2)_2(OH)_2^{++} \rightleftarrows 2UO_2^{++} + 2OH^-$	5b, 43b
170 $(UO_2)_3(OH)_5^+$	$(UO_2)_3(OH)_5^+ + 5H^+ \rightleftarrows 3UO_2^{++} + 5H_2O$	5b, 43b
171 $(UO_2)_3(OH)_7^-$	$(UO_2)_3(OH)_7^- + 7H^+ \rightleftarrows 3UO_2^{++} + 7H_2O$	5b, 43b
172 $UO_2(SO_4)^0$	$UO_2(SO_4)^0 \rightleftarrows UO_2^{++} + SO_4^{--}$	43b
173 $UO_2(SO_4)_2^{--}$	$UO_2(SO_4)_2^{--} \rightleftarrows UO_2^{++} + 2SO_4^{--}$	5c, 45c
174 UO_2F^+	$UO_2F^+ \rightleftarrows UO_2^{++} + F^-$	5b, 43b
175 $UO_2F_2^0$	$UO_2F_2^0 \rightleftarrows UO_2^{++} + 2F^-$	5b, 43b
176 $UO_2F_3^-$	$UO_2F_3^- \rightleftarrows UO_2^{++} + 3F^-$	5b, 43b
177 $UO_2F_4^{--}$	$UO_2F_4^{--} \rightleftarrows UO_2^{++} + 4F^-$	5b, 43b
178 UO_2Cl^+	$UO_2Cl^+ \rightleftarrows UO_2^{++} + Cl^-$	5b, 43b
179 $UO_2H_3SiO_4^+$	$UO_2H_3SiO_4^+ + H^+ \rightleftarrows UO_2^{++} + H_4SiO_4^0$	5c, 45c
180 $UO_2(HPO_4)^0$	$UO_2(HPO_4)^0 \rightleftarrows UO_2^{++} + HPO_4^{--}$	2b, 43b
181 $UO_2(HPO_4)_2^{--}$	$UO_2(HPO_4)_2^{--} \rightleftarrows UO_2^{++} + 2HPO_4^{--}$	2b, 43b
182 $UO_2(H_2PO_4)^+$	$UO_2(H_2PO_4)^+ \rightleftarrows UO_2^{++} + HPO_4^{--} + H^+$	2b, 43b
183 $UO_2(H_2PO_4)_2^0$	$UO_2(H_2PO_4)_2^0 \rightleftarrows UO_2^{++} + 2HPO_4^{--} + 2H^+$	2b, 43b
184 $UO_2(H_2PO_4)_3^-$	$UO_2(H_2PO_4)_3^- \rightleftarrows UO_2^{++} + 3HPO_4^{--} + 3H^+$	2b, 43b
185 $UO_2(CO_3)^0$	$UO_2(CO_3)^0 \rightleftarrows UO_2^{++} + CO_3^{--}$	5b, 43b
186 $UO_2(CO_3)_2^{--}$	$UO_2(CO_3)_2^{--} \rightleftarrows UO_2^{++} + 2CO_3^{--}$	5b, 43b
187 $UO_2(CO_3)_3^{-4}$	$UO_2(CO_3)_3^{-4} \rightleftarrows UO_2^{++} + 3CO_3^{--}$	5b, 43b
188 HVO_4^{-2}	$HVO_4^{--} \rightleftarrows VO_4^{-3} + H^+$	43c
189 $H_2VO_4^{-1}$	$H_2VO_4^- \rightleftarrows VO_4^{-3} + 2H^+$	43c
190 $H_3VO_4^0$	$H_3VO_4^0 \rightleftarrows VO_4^{-3} + 3H^+$	43c

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
191 $H_4VO_4^+$	$H_4VO_4^+ \rightleftarrows VO_4^{-3} + 4H^+$	43c
192 $NaHVO_4^-$	$NaHVO_4^- \rightleftarrows Na^+ + VO_4^{-3} + H^+$	2g
193 VO_2F^0	$VO_2F^0 \rightleftarrows VO_2^+ + F^-$	15g
194 $VO_2F_2^-$	$VO_2F_2^- \rightleftarrows VO_2^+ + 2F^-$	15g
195 $V(OH)^{++}$	$V(OH)^{++} \rightleftarrows V^{+3} + OH^-$	43g
196 $V(OH)_2^+$	$V(OH)_2^+ \rightleftarrows V^{+3} + 2OH^-$	43g
197 $V(OH)_3^0$	$V(OH)_3^0 \rightleftarrows V^{+3} + 3OH^-$	43g
198 $VOOH^+$	$VOOH^+ \rightleftarrows VO^{++} + OH^-$	43g
199 $VOSO_4^0$	$VOSO_4^0 \rightleftarrows VO^{++} + SO_4^{--}$	2g
200 $VOCl^+$	$VOCl^+ \rightleftarrows VO^{++} + Cl^-$	15g
201 VOF^+	$VOF^+ \rightleftarrows VO^{++} + F^-$	2g
202 VOF_2^0	$VOF_2^0 \rightleftarrows VO^{++} + 2F^-$	2g
203 $UO_2CH_3COO^+$	$UO_2CH_3COO^+ \rightleftarrows UO_2^{++} + CH_3COO^-$	15c
204 $UO_2(CH_3COO)_2^0$	$UO_2(CH_3COO)_2^0 \rightleftarrows UO_2^{++} + 2CH_3COO^-$	71c
205 UO_2^+	$UO_2^+ + Fe^{+3} \rightleftarrows UO_2^{++} + Fe^{++}$	43b, 44b
206 U^{+4}	$U^{+4} + Fe^{+3} + 2H_2O \rightleftarrows UO_2^+ + Fe^{++} + 4H^+$	43b, 44b
207 V^{+3}	$V^{+3} + Fe^{+3} + H_2O \rightleftarrows VO^{++} + Fe^{++} + 2H^+$	2b, 44b
208 VO^{++}	$VO^{++} + Fe^{+3} + 3H_2O \rightleftarrows VO_4^{-3} + Fe^{++} + 6H^+$	44c, 45c
209 $AlCH_3COO^{++}$	$AlCH_3COO^{++} \rightleftarrows Al^{+3} + CH_3COO^-$	49
210 $BaCH_3COO^+$	$BaCH_3COO^+ \rightleftarrows Ba^{++} + CH_3COO^-$	49c
211 $CaCH_3COO^+$	$CaCH_3COO^+ \rightleftarrows Ca^{++} + CH_3COO^-$	50c
212 $CuCH_3COO^0$	$CuCH_3COO^0 \rightleftarrows Cu^+ + CH_3COO^-$	49c
213 $FeCH_3COO^+$	$FeCH_3COO^+ \rightleftarrows Fe^{++} + CH_3COO^-$	51a
214 $Fe(CH_3COO)_2^0$	$Fe(CH_3COO)_2^0 \rightleftarrows Fe^{++} + 2CH_3COO^-$	51a
215 KCH_3COO^0	$KCH_3COO^0 \rightleftarrows K^+ + CH_3COO^-$	52c, 53c
216 $MgCH_3COO^+$	$MgCH_3COO^+ \rightleftarrows Mg^{++} + CH_3COO^-$	50c
217 $NaCH_3COO^0$	$NaCH_3COO^0 \rightleftarrows Na^+ + CH_3COO^-$	52c, 53c

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
218 $PbCH_3COO^+$	$PbCH_3COO^+ \rightleftarrows Pb^{++} + CH_3COO^-$	18c, 52c
219 $Pb(CH_3COO)_2^0$	$Pb(CH_3COO)_2^0 \rightleftarrows Pb^{++} + 2CH_3COO^-$	18c, 52c
220 $Pb(CH_3COO)_3^-$	$Pb(CH_3COO)_3^- \rightleftarrows Pb^{++} + 3CH_3COO^-$	18c, 52c
221 $SrCH_3COO^+$	$SrCH_3COO^+ \rightleftarrows Sr^{++} + CH_3COO^-$	50c
222 $ZnCH_3COO^+$	$ZnCH_3COO^+ \rightleftarrows Zn^{++} + CH_3COO^-$	18c, 38a
223 $HC_2O_4^-$	$HC_2O_4^- \rightleftarrows H^+ + C_2O_4^{--}$	49c, 52c
224 $H_2C_2O_4^0$	$H_2C_2O_4^0 \rightleftarrows 2H^+ + C_2O_4^{--}$	49c, 52c
225 $AlC_2O_4^+$	$AlC_2O_4^+ \rightleftarrows Al^{+3} + C_2O_4^{--}$	49c, 59c
226 $Al(C_2O_4)_2^-$	$Al(C_2O_4)_2^- \rightleftarrows Al^{+3} + 2C_2O_4^{--}$	49c, 59c
227 $BaC_2O_4^0$	$BaC_2O_4^0 \rightleftarrows Ba^{++} + C_2O_4^{--}$	25c. 49c
228 $CaC_2O_4^0$	$CaC_2O_4^0 \rightleftarrows Ca^{++} + C_2O_4^{--}$	25c, 49c
229 $FeC_2O_4^0$	$FeC_2O_4^0 \rightleftarrows Fe^{++} + C_2O_4^{--}$	25c, 49c
230 $FeC_2O_4^+$	$FeC_2O_4^+ \rightleftarrows Fe^{+3} + C_2O_4^{--}$	25c, 49c
231 $KC_2O_4^-$	$KC_2O_4^- \rightleftarrows K^+ + C_2O_4^{--}$	25c, 49c
232 $MgC_2O_4^0$	$MgC_2O_4^0 \rightleftarrows Mg^{++} + C_2O_4^{--}$	25c, 49c
233 $MnC_2O_4^0$	$MnC_2O_4^0 \rightleftarrows Mn^{++} + C_2O_4^{--}$	49c, 52c
234 $Mn(C_2O_4)_2^{--}$	$Mn(C_2O_4)_2^{--} \rightleftarrows Mn^{++} + 2C_2O_4^{--}$	49c, 52c
235 $Mn(C_2O_4)_3^{-4}$	$Mn(C_2O_4)_3^{-4} \rightleftarrows Mn^{++} + 3C_2O_4^{--}$	49c, 52c
236 $MnC_2O_4^+$	$MnC_2O_4^+ \rightleftarrows Mn^{+3} + C_2O_4^{--}$	49c, 52c
237 $NaC_2O_4^-$	$NaC_2O_4^- \rightleftarrows Na^+ + C_2O_4^{--}$	25c, 49c
238 $PbC_2O_4^0$	$PbC_2O_4^0 \rightleftarrows Pb^{++} + C_2O_4^{--}$	25f, 49f
239 $SrC_2O_4^0$	$SrC_2O_4^0 \rightleftarrows Sr^{++} + C_2O_4^{--}$	25c, 49c
240 $ZnC_2O_4^0$	$ZnC_2O_4^0 \rightleftarrows Zn^{++} + C_2O_4^{--}$	49c, 52c
241 $H(C_4H_4O_4)^-$	$H(C_4H_4O_4)^- \rightleftarrows H^+ + C_4H_4O_4^{--}$	49c
242 $H_2(C_4H_4O_4)^0$	$H_2(C_4H_4O_4)^0 \rightleftarrows 2H^+ + C_4H_4O_4^{--}$	49c
243 $AlC_4H_4O_4^+$	$AlC_4H_4O_4^+ \rightleftarrows Al^{+3} + C_4H_4O_4^{--}$	49f, 59f

Table 2. -- Dissociation reactions for aqueous complexes and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
244 $Al(C_4H_4O_4)_2^-$	$Al(C_4H_4O_4)_2^- \rightleftarrows Al^{+3} + 2C_4H_4O_4^{--}$	49f, 59f
245 $BaC_4H_4O_4^0$	$BaC_4H_4O_4^0 \rightleftarrows Ba^{++} + C_4H_4O_4^{--}$	25c, 49c
246 $CaC_4H_4O_4^0$	$CaC_4H_4O_4^0 \rightleftarrows Ca^{++} + C_4H_4O_4^{--}$	25c, 49c
247 $FeC_4H_4O_4^0$	$FeC_4H_4O_4^0 \rightleftarrows Fe^{++} + C_4H_4O_4^{--}$	25f, 49f
248 $FeC_4H_4O_4^+$	$FeC_4H_4O_4^+ \rightleftarrows Fe^{+3} + C_4H_4O_4^{--}$	25c, 49c
249 $KC_4H_4O_4^-$	$KC_4H_4O_4^- \rightleftarrows K^+ + C_4H_4O_4^{--}$	25c, 49c
250 $MgC_4H_4O_4^0$	$MgC_4H_4O_4^0 \rightleftarrows Mg^{++} + C_4H_4O_4^{--}$	25c, 49c
251 $MnC_4H_4O_4^0$	$MnC_4H_4O_4^0 \rightleftarrows Mn^{++} + C_4H_4O_4^{--}$	25c, 49c
252 $NaC_4H_4O_4^-$	$NaC_4H_4O_4^- \rightleftarrows Na^+ + C_4H_4O_4^{--}$	25c, 49c
253 $PbC_4H_4O_4^0$	$PbC_4H_4O_4^0 \rightleftarrows Pb^{++} + C_4H_4O_4^{--}$	25c, 49c
254 $SrC_4H_4O_4^0$	$SrC_4H_4O_4^0 \rightleftarrows Sr^{++} + C_4H_4O_4^{--}$	25c, 49c
255 $ZnC_4H_4O_4^0$	$ZnC_4H_4O_4^0 \rightleftarrows Zn^{++} + C_4H_4O_4^{--}$	25c, 49c
256 FeF^{++}	$FeF^{++} \rightleftarrows Fe^{+3} + F^-$	57c
257 SiF_6^{--}	$SiF_6^{--} + 4OH^- \rightleftarrows H_4SiO_4^0 + 6F^-$	58c
258 $Pb(HS)_2^0$	$Pb(HS)_2^0 \rightleftarrows Pb^{++} + 2HS^-$	2a, 55a, 56a
259 $Pb(HS)_3^-$	$Pb(HS)_3^- \rightleftarrows Pb^{++} + 3HS^-$	2a, 55a
260 $PbCO_3^0$	$PbCO_3^0 \rightleftarrows Pb^{++} + CO_3^{--}$	56a, 57a
261 $PbOH^+$	$PbOH^+ \rightleftarrows Pb^{++} + OH^-$	52a, 56a
262 $Zn(HS)_2^0$	$Zn(HS)_2^0 \rightleftarrows Zn^{++} + 2HS^-$	46a, 55a, 56a
263 $Zn(HS)_3^-$	$Zn(HS)_3^- \rightleftarrows Zn^{++} + 3HS^-$	46a, 55a
264 $ZnHCO_3^+$	$ZnHCO_3^+ \rightleftarrows Zn^{++} + HCO_3^-$	46a
265 $ZnOH^+$	$ZnOH^+ \rightleftarrows Zn^{++} + OH^-$	46a
266 $Zn(OH)_2^0$	$Zn(OH)_2^0 \rightleftarrows Zn^{++} + 2OH^-$	9a, 46a
267 $Zn(HS)(OH)^0$	$Zn(HS)(OH)^0 \rightleftarrows Zn^{++} + HS^- + OH^-$	46a

Oxidation-Reduction Reactions

Oxidation-reduction reactions are used in conjunction with mass-action reactions and mass-balance expressions to compute the distribution of the multivalent elements Fe, Cu, Hg, Mn, U, and V where the Eh of the solution is known. The reaction for iron is

$$Fe^{++} \rightleftarrows Fe^{+3} + e^{-} \quad , \tag{3}$$

where e^{-} represents an electron. The concentrations of Fe^{++} and Fe^{+3} are related by

$$Eh = E^{o} + \frac{RT}{nF} \ln \left[\frac{m_{Fe^{+3}} \cdot \gamma_{Fe^{+3}}}{m_{Fe^{++}} \cdot \gamma_{Fe^{++}}} \right] \quad , \tag{6}$$

where Eh is the oxidation potential referred to the hydrogen half cell, E^{o} is the standard state potential of the reaction, n is the number of electrons involved in the reaction, F is the Faraday constant and R is the gas constant. Values of E^{o}at temperatures from 0° to 350 °C, are calculated from equation

$$E^{o} = \frac{\Delta G_{r}^{o}}{nF} \quad , \tag{7}$$

where the Gibbs standard state free energies for the oxidation-reduction reactions (ΔG_{r}^{o}) are tabulated in the data files of the program (see below).

SOLMINEQ.88 will compute the Eh of a water sample at the desired temperature, if necessary, from the Emf of the Eh cell including the Calomel reference electrode (EHMC) or from the Emf of the Eh cell calibrated using Zobell's solution (EMFZSC). For a more detailed discussion of the theory of Eh, its field measurement and reduction, see Barnes and Back (1964), Barnes and Clarke (1969), Garrels and Christ (1965), and Thorstensen (1984).

Computations based on measured Eh have been kept to a minimum in SOLMINEQ.88 because of uncertainties in the measurement and interpretation of oxidation potentials (Barnes and Clarke, 1969; Wolery, 1983; Nordstrom and Munoz, 1985). However, the program can compute the distribution of species for elements with multiple redox states by assuming redox equilibrium between the species HS^{-} and SO_{4}^{--}. Kharaka and others (1980) have shown that oil field waters are strongly reducing (Eh < -200 mV) and that the sulfide-sulfate redox reaction

$$HS^- + 4H_2O \rightleftarrows SO_4^{--} + 9H^+ + 8e^- \quad , \qquad (4)$$

is probably the best of the possible redox couples for computing the Eh of these waters. However, in other natural systems alternative redox couples may be better indicators of the redox state of water (Freeze and Cherry, 1979; Kharaka and others, 1980; Nordstrom and Munoz, 1985).

The distribution of Fe species in SOLMINEQ.88 can be computed by combining HS^-/SO_4^{--}, and Fe^{+3}/Fe^{++} couples (Reactions 3 and 4) to give the reaction

$$8Fe^{+3} + 4H_2O + HS^- \rightleftarrows 8Fe^{++} + SO_4^{--} + 9H^+ \quad . \qquad (5)$$

The distribution of species for the other multivalent elements can be computed by combining them with the Fe^{+3}/Fe^{++} couple in reactions that eliminate the electron. In the case of Cu, for example, the reaction is

$$Fe^{+3} + Cu^+ \rightleftarrows Fe^{++} + Cu^{++} \quad . \qquad (6)$$

It must be emphasized in this section that the above computations assume a state of thermodynamic equilibrium that may not be applicable to many or all of the redox couples. For a detailed discussion of the real meaning of Eh, the related parameter pe and the numerous pitfalls and inconsistencies in their measurements and interpretations, the reader is referred to Barnes and Clarke (1969), Wolery (1983) and Thorstenson, (1984).

Speciation at Subsurface Conditions

The chemical compositions of subsurface water samples collected at the land surface may not correspond to their in-situ compositions. Volatile gases such as CO_2, H_2S, and NH_3 may exsolve due to a pressure decrease. Loss of these gases may drastically change (by up to 3 pH units) the pH of the remaining fluids. Changes in temperature and pressure alone will result in pH changes due to variations in the stabilities of hydrogen-bearing aqueous species. Changes in pH, temperature, and pressure may result in precipitation of solid phases such as calcium carbonate and amorphous silica, among others Increases in the Eh of waters containing Fe^{++} usually result in the precipitation of amorphous iron hydroxides and coprecipitation of trace metals.

The in situ water chemistry may be calculated for water-dominated geothermal and oil field systems where the amount and composition of gases

lost prior to water sampling are known. The main problem in these computations has been the estimation of an in situ pH which is critical to these computations. Two different approaches have been used (see Modeling Options) to compute the in-situ pH: (1) assuming equilibrium at subsurface conditions with a mineral (Merino, 1979) known to be present in the aquifer (calcite is generally selected), or (2) assuming mass balance for hydronium at surface and subsurface conditions (Truesdell and Singer, 1974; Kharaka and others, 1985).

SOLMINEQ.88 has options to compute the subsurface pH and resulting speciation and saturation states using either approach. The distribution of species in the mass-balance approach is carried out at surface conditions using the measured pH. The total hydrogen (m_{H,t,T_1}) and hydroxyl (m_{OH,t,T_1}) are then computed at the surface conditions from the equations

$$m_{H,t,T_1} = m_{H^+} + m_{HCO_3^-} + 2m_{H_2CO_3^o} + m_{HS^-} + 2m_{H_2S^o} + m_{CH_3COOH^o} + \ldots \quad , \quad (8)$$

$$m_{OH,t,T_1} = m_{OH^-} + m_{Ca(OH)^+} + m_{Mg(OH)^+} + m_{NH_4OH^o} + 2m_{Fe(OH)_2^o} + \ldots \quad . \quad (9)$$

For samples where known quantities of CO_2, H_2S, and NH_3 are lost prior to surface pH measurement, equations (8) and (9) are modified to include the lost gases. CO_2, H_2S, and NH_3 are included as $2m_{H_2CO_3}$, $2m_{H_2S}$, and m_{NH_4OH}, respectively, in the computed value of m_{H,t,T_2} and m_{OH,t,T_2} (see Modeling Options).

The distribution of species is then computed at the subsurface temperature assuming that the subsurface pH is equal to the measured surface pH. The total molalities of hydrogen (m_{H,t,T_2}) and hydroxyl (m_{OH,t,T_2}) at subsurface temperature (T_2) are then computed. The value of the tolerance factor (Y_H) for the hydronium given by:

$$Y_H = 1 - \frac{(m_{H,t,T_2} - m_{OH,t,T_2})}{(m_{H,t,T_1} - m_{OH,t,T_1})} \quad , \quad (10)$$

is then computed. The terms (m_{OH,t,T_1} and m_{OH,t,T_2}) are included in Equation (10) to account for the changes in the hydrogen mass-balance from hydrolysis

of water. Iterations are then carried out changing the pH by small increments (see below) until the value of Y is $\leq \pm 5x10^{-5}$ (or another user-defined value). The final computed pH is then used to compute the distribution of species and the states of saturation of the solution with respect to minerals.

Iteration Techniques

The distribution of cations in SOLMINEQ.88 is carried out using equations that, throughout all computations, meet the requirement of mass-balance (Equation 3). In the case of anions, however, the total (analytical) molality of each anion is initially assigned to the primary (generally the predominant) species of that anion to compute the molalities of the other species. This generally results in a sum of computed molalities that after the first iteration is higher than the analytical molality. In the case of sulfate, for example, $m_{SO_4}^{--}$ is initially made equal to $m_{SO_4,t}$ resulting in

$$m_{SO_4,t} < m_{SO_4}^{--} + m_{CaSO_4}^{o} + m_{NaSO_4}^{-} + \ldots \quad . \tag{11}$$

SOLMINEQ.88 uses a back - substitution iterative procedure (see code listing in Appendix IV.) for the distribution of anions. Iterations are continued until the tolerance factor for the anion (Y_A) defined by the ratio of the analytical molality of the anion to the computed sum of its species and given by

$$Y_A = 1 - \frac{m_{i,t}}{\Sigma\, n_{i,j}\, m_{j,i}} \quad , \tag{12}$$

is $\leq \pm 5x10^{-5}$. Almost all waters examined to date have met these requirements within 10 iteration cycles. Iteration problems, however, may be encountered especially in solutions with many ions or high pH values, incorrect or incomplete chemical analysis, and in high salinity brines when using the Pitzer equations to compute the activity coefficients.

The iterative algorithm for hydronium mass-balance in SOLMINEQ.88 has been modified to utilize a polynomial interpolating technique. Initially, the pH is adjusted (the initial adjustment is 1.0 pH unit) until either convergence is achieved, (as defined by equation (10)), or the sign of Y_H is reversed. Once the sign of Y_H has reversed, values of pH and Y_H are fit to a

polynomial, the order of which is one less than the number of pH and Y_H values (up to a maximum of 6 points). The polynomial is then used to interpolate the value of pH where Y_H "should be" zero. This value is checked to insure that it is between the bracketing values. If it is not, a polynomial of decreased order is re-fit to the values and a new value of pH is obtained. This is continued until the pH is between the bracketing values. The aqueous species are then redistributed by iteration until Y_A is satisfied and a new value of Y_H obtained. This procedure continues until Y_H passes the convergence test. This technique results in a much faster solution than the back-substitution approach used in the original program, and allows imposition of a smaller tolerance factor. The smaller tolerance factor avoids an erroneous calculation of pH when one H^+- or OH^-- bearing species is predominant in the solution (see Morel, 1983, p. 96-97).

All of the options which modify the solution composition and can be treated as a function of a single variable (addition/removal of a volatile, precipitation/dissolution of a mineral, etc.; see Modeling Options) use a similar procedure to obtain pH convergence; the only difference is the function for Y and the independent variable. For example, for mineral saturation, Y is a function of the saturation index (SI) of the minerals and it is varied as a function of the amount of material added to or removed from the solution.

Before the polynomial interpolation is used, the sign of Y must change. This is done by increasing or decreasing the independent variable. The choice of step size is critical. With the exception of the pH modification (discussed earlier), the step size is based on the difference between the current parameters (SI's, amount in solution, etc.), and the anticipated values of the parameter when convergence has been reached. If the first step does not cause Y to change sign, either the step size is increased or its direction reversed, depending on the current derivative. This process is continued until either Y changes sign, an impossible solution is reached (for example, negative mass of an element) or it can be demonstrated that no answer exists.

Saturation States of Minerals

The saturation state of a mineral in a given solution determines its interactions with that solution. In SOLMINEQ.88, two saturation indices are used to test for possible dissolution or precipitation of minerals. The program computes the Gibbs free energy difference (ΔG_{diff}) between the actual and equilibrium states of a mineral in a given subsurface water (equal to the chemical affinity **A**) as well as the saturation index SI given by:

$$SI = \ln(Q/K) \quad . \tag{13}$$

ΔG_{diff} is given by:

$$\Delta G_{diff} = -RT\ln K - (-RT\ln Q) = RT\ln(Q/K) \quad , \tag{14}$$

where R is the gas constant, T is temperature in degrees Kelvin, Q is the reaction quotient (equal to the ion activity product (AP)), and K is the equilibrium constant at the specified temperature and pressure.

Mineral reactions used in SOLMINEQ.88 are for complete hydrolysis (Table 3); no incongruent reactions which require additional assumptions (e.g., conserving Al) are used. For anorthite, the reaction is

$$CaAl_2Si_2O_{8(s)} + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + 2H_4SiO_4^o \quad . \tag{7}$$

The reaction quotient (Q) for reaction (7) is given by:

$$Q_{anorthite} = \frac{a_{Ca^{++}} \cdot a^2_{Al^{+3}} \cdot a^2_{H_4SiO_4^o}}{a^8_{H^+} \cdot a_{anorthite}} \quad , \tag{15}$$

where (a) is the activity of the subscripted species at the specified temperature and pressure; $a_{anorthite}$ is the activity of anorthite. With the exception of minerals entered using the unknown mineral option, the activity of all minerals is assumed to be equal to 1.0 at any temperature and pressure.

At equilibrium, $Q = K$ and $\Delta G_{diff} = 0$. In this case, the subsurface water is in equilibrium with the mineral and no dissolution or precipitation should take place. Where $\Delta G_{diff} < 0$, anorthite cannot precipitate from that subsurface water because of undersaturation, but anorthite probably will dissolve if the mineral is present in the reservoir rocks. Where $\Delta G_{diff} > 0$, anorthite will not dissolve because of supersaturation, but rather will likely precipitate if kinetic factors allow.

Table 3. -- Reactions for the congruent dissolution of minerals and sources of thermochemical data

ID # and Name	Reaction	References
1 Adularia	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$	7a
2 Akermanite	$Ca_2MgSi_2O_7 + 6H^+ + H_2O \rightleftarrows 2Ca^{++} + Mg^{++} + 2H_4SiO_4^0$	5b, 61b
3 Albite	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$	5b, 61b
4 Albite, Low	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$	5b, 61b
5 Albite, High	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$	5b, 61b
6 Alunite	$KAl_3(SO_4)_2(OH)_6 + 6H^+ \rightleftarrows K^+ + 3Al^{+3} + 2SO_4^{--} + 6H_2O$	5b, 6b, 62b
7 Amesite, 14A	$Mg_2Al_2SiO_5(OH)_4 + 10H^+ \rightleftarrows 2Mg^{++} + 2Al^{+3} + H_4SiO_4^0 + 5H_2O$	66a
8 Analcime	$NaAlSi_2O_6 \cdot H_2O + 4H^+ + H_2O \rightleftarrows Na^+ + Al^{+3} + 2H_4SiO_4^0$	6b, 72b
9 Andalusite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^0 + H_2O$	5b, 6b
10 Andesine	$Ca_{.4}Na_{.6}Al_{1.4}Si_{2.6}O_8 \rightleftarrows .4CaAl_2Si_2O_8 + .6NaAlSi_3O_8$	2a
11 Anhydrite	$CaSO_4 \rightleftarrows Ca^{++} + SO_4^{--}$	39b, 63b
12 Annite	$KFe_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Fe^{++} + Al^{+3} + 3H_4SiO_4^0$	6b, 72b
13 Anorthite	$CaAl_2Si_2O_8 + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + 2H_4SiO_4^0$	6b, 72b
14 Apatite, Cl	$Ca_5(PO_4)_3Cl \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + Cl^-$	7a
15 Apatite, F	$Ca_5(PO_4)_3F \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + F^-$	2b, 6b
16 Apatite, OH	$Ca_5(PO_4)_3OH \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + OH^-$	6b, 61b
17 Aragonite	$CaCO_3 \rightleftarrows Ca^{++} + CO_3^{--}$	35a
18 Augite	$CaAl_2SiO_6 + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + H_4SiO_4^0 + 2H_2O$	6b, 72b
19 Azurite	$Cu_3(CO_3)_2(OH)_2 \rightleftarrows 3Cu^{++} + 2CO_3^{--} + 2OH^-$	6b, 72b

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
20 Barite	$BaSO_4 \rightleftarrows Ba^{++} + SO_4^{--}$	6b, 63b
21 Boehmite	$AlO(OH) + 3H^+ \rightleftarrows Al^{+3} + 2H_2O$	6b, 62b
22 Brucite	$Mg(OH)_2 \rightleftarrows Mg^{++} + 2OH^-$	6b, 61b
23 Bytownite	$Ca_{.8}Na_{.2}Al_{1.8}Si_{2.2}O_8 \rightleftarrows .8CaAl_2Si_2O_8 + .2NaAlSi_3O_8$	2a
24 Calcite	$CaCO_3 \rightleftarrows Ca^{++} + CO_3^{--}$	35a
25 Celestite	$SrSO_4 \rightleftarrows Sr^{++} + SO_4^{--}$	6b, 61b
26 Chalcedony	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	5b, 6b
27 Chamosite, 7A	$Fe_2Al_2SiO_5(OH)_4 + 10H^+ \rightleftarrows 2Fe^{++} + 2Al^{+3} + H_4SiO_4^0 + 5H_2O$	66a
28 Chlorite, 7A	$Mg_5Al_2Si_3O_{10}(OH)_8 + 16H^+ \rightleftarrows 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4^0 + 6H_2O$	5b, 6b
29 Chlorite, 14A	$Mg_5Al_2Si_3O_{10}(OH)_8 + 16H^+ \rightleftarrows 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4^0 + 6H_2O$	5b, 6b
30 Chrysotile	$Mg_3Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 3Mg^{++} + 2H_4SiO_4^0 + H_2O$	6b, 61b
31 Clinoenstatite	$MgSiO_3 + 2H^+ + H_2O \rightleftarrows Mg^{++} + H_4SiO_4^0$	6b, 61b
32 Clinoptilolite Sodium	$Na_2Al_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows 2Na^+ + 2Al^{+3} + 10H_4SiO_4^0$	76a
33 Clinoptilolite, Potassium	$K_2Al_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows 2K^+ + 2Al^{+3} + 10H_4SiO_4^0$	76a
34 Clinoptilolite, Calcium	$CaAl_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 10H_4SiO_4^0$	76a
35 Clinoptilolite, Magnesium	$MgAl_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows Mg^{++} + 2Al^{+3} + 10H_4SiO_4^0$	76a
36 Corundum	$Al_2O_3 + 6H^+ \rightleftarrows 2Al^{+3} + 3H_2O$	5b, 6b
37 Cristobalite,α	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	67a

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
38 Cristobalite,β	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	67a
39 Dickite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^0 + H_2O$	6b, 61b
40 Diopside	$CaMgSi_2O_6 + 4H^+ + 2H_2O \rightleftarrows Ca^{++} + Mg^{++} + 2H_4SiO_4^0$	6b, 61b
41 Dolomite	$CaMg(CO_3)_2 \rightleftarrows Ca^{++} + Mg^{++} + 2CO_3^{--}$	5b, 6b
42 Dolomite (DSORD)	$CaMg(CO_3)_2 \rightleftarrows Ca^{++} + Mg^{++} + 2CO_3^{--}$	5b, 6b
43 Enstatite	$MgSiO_3 + 2H^+ + H_2O \rightleftarrows Mg^{++} + H_4SiO_4^0$	5b, 6b
44 Epidote	$Ca_2FeAl_2Si_3O_{12}(OH) + 13H^+ \rightleftarrows 2Ca^{++} + Fe^{+3} + 2Al^{+3} + 3H_4SiO_4^0 + H_2O$	6b, 72b
45 Fayalite	$Fe_2SiO_4 + 4H^+ \rightleftarrows 2Fe^{++} + H_4SiO_4^0$	6b, 61b
46 Fluorite	$CaF_2 \rightleftarrows Ca^{++} + 2F^-$	68a
47 Forsterite	$Mg_2SiO_4 + 4H^+ \rightleftarrows 2Mg^{++} + H_4SiO_4^0$	6b, 61b
48 Gibbsite, Am	$Al(OH)_3 \rightleftarrows Al^{+3} + 3OH^-$	7a
49 Gibbsite	$Al(OH)_3 \rightleftarrows Al^{+3} + 3OH^-$	6b, 62b
50 Greenalite	$Fe_3Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 3Fe^{++} + 2H_4SiO_4^0 + H_2O$	66a
51 Gypsum	$CaSO_4 \cdot 2H_2O \rightleftarrows Ca^{+2} + SO_4^{-2} + 2H_2O$	6b, 63b
52 Halite	$NaCl \rightleftarrows Na^+ + Cl^-$	6b, 61b
53 Halloysite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^0 + H_2O$	6b, 61b
54 Heulandite	$CaAl_2Si_7O_{18} \cdot 6H_2O + 8H^+ + 4H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 7H_4SiO_4^0$	6b, 78b
55 Huntite	$CaMg_3(CO_3)_4 \rightleftarrows Ca^{++} + 3Mg^{++} + 4CO_3^{--}$	5b, 6b
56 Hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 3H_2O \rightleftarrows 5Mg^{++} + 4CO_3^{--} + 2OH^- + 3H_2O$	6b, 69b
57 Hydrophilite	$CaCl_2 \rightleftarrows Ca^{++} + 2Cl^-$	5b, 61b
58 Illite	$K_{.6}Mg_{.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 8H^+ + 2H_2O \rightleftarrows .6K^+ + .25Mg^{++} + 2.3Al^{+3} + 3.5H_4SiO_4^0$	7a

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
59 Kaolinite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^0 + H_2O$	6b, 72b
60 Kenyaite	$NaSi_{11}O_{20.5}(OH)_4 \cdot 3H_2O + H^+ + 16.5H_2O \rightleftarrows Na^+ + 11H_4SiO_4^0$	7e
61 K-Feldspar	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$	6b, 72b
62 Kyanite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^0 + H_2O$	6b, 61b
63 Labradorite	$Ca_{.6}Na_{.4}Al_{1.6}Si_{2.4}O_8 \rightleftarrows .6CaAl_2Si_2O_8 + .4NaAlSi_3O_8$	2a
64 Larnite	$Ca_2SiO_4 + 4H^+ \rightleftarrows 2Ca^{++} + H_4SiO_4^0$	5b, 61b
65 Laumontite	$CaAl_2Si_4O_{12} \cdot 4H_2O + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + 4H_4SiO_4^0$	5b, 61b
66 Leucite	$KAlSi_2O_6 + 4H^+ + 2H_2O \rightleftarrows K^+ + Al^{+3} + 2H_4SiO_4^0$	5b, 61b
67 Lime	$CaO + 2H^+ \rightleftarrows Ca^{++} + H_2O$	5b, 61b
68 Magadite	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O \rightleftarrows Na^+ + 7H_4SiO_4^0$	7e
69 Magnesio-ferrite	$MgFe_2O_4 + 8H^+ \rightleftarrows Mg^{++} + 2Fe^{+3} + 4H_2O$	7a
70 Magnesite	$MgCO_3 \rightleftarrows Mg^{++} + CO_3^{--}$	6b, 69b
71 Chloro-magnesite	$MgCl_2 \rightleftarrows Mg^{++} + 2Cl^-$	7a
72 Marialite	$(NaAlSi_3O_8)_3 \cdot NaCl + 12H^+ + 12H_2O \rightleftarrows 4Na^+ + 3Al^{+3} + Cl^- + 9H_4SiO_4^0$	7a, 74a
73 Merwinite	$Ca_3MgSi_2O_8 + 8H^+ \rightleftarrows 3Ca^{++} + Mg^{++} + 2H_4SiO_4^0$	5b, 61b
74 Microcline	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$	6b, 72b
75 Meionite	$(CaAl_2Si_2O_8)_3 \cdot CaCO_3 + 24H^+ \rightleftarrows 4Ca^{++} + 6Al^{+3} + CO_3^{--} + 6H_4SiO_4^0$	6b, 75b

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
76 Mirabilite	$Na_2SO_4 \cdot 10H_2O \rightleftarrows 2Na^+ + SO_4^{--} + 10H_2O$	2b, 5b
77 Monticellite	$CaMgSiO_4 + 4H^+ \rightleftarrows Ca^{++} + Mg^{++} + H_4SiO_4^0$	5b, 6b
78 Mordenite, Na	$NaAlSi_5O_{12} \cdot 3H_2O + 4H^+ + 5H_2O \rightleftarrows Na^+ + Al^{+3} + 5H_4SiO_4^0$	76a
79 Mordenite, K	$KAlSi_5O_{12} \cdot 3H_2O + 4H^+ + 5H_2O \rightleftarrows K^+ + Al^{+3} + 5H_4SiO_4^0$	76a
80 Muscovite	$KAl_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Al^{+3} + 3H_4SiO_4^0$	6b, 61b
81 Nahcolite	$NaHCO_3 \rightleftarrows Na^+ + HCO_3^-$	5b, 71b
82 Nathermite	$Na_2CO_3 \cdot H_2O \rightleftarrows 2Na^+ + CO_3^{--} + H_2O$	2b
83 Natron	$Na_2CO_3 \cdot 10H_2O \rightleftarrows 2Na^+ + CO_3^{--} + 10H_2O$	5b, 71b
84 Nepheline	$NaAlSiO_4 + 4H^+ \rightleftarrows Na^+ + Al^{+3} + H_4SiO_4^0$	6b, 72b
85 Nesquehonite	$MgCO_3 \cdot 3H_2O \rightleftarrows Mg^{++} + CO_3^{--} + 3H_2O$	6b, 72b
86 Nontronite, Na	$Na_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33Na^+ + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
87 Nontronite, K	$K_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33K^+ + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
88 Nontronite, H	$H_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 6.99H^+ + 2.68H_2O \rightleftarrows 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
89 Nontronite, Ca	$Ca_{.165}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Ca^{++} + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
90 Nontronite, Mg	$Mg_{.165}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Mg^{++} + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
91 Oldhamite	$CaS + H^+ \rightleftarrows Ca^{++} + HS^-$	7b
92 Oligoclase	$Ca_{.2}Na_{.8}Al_{1.2}Si_{2.8}O_8 \rightleftarrows .2CaAl_2Si_2O_8 + .8NaAlSi_3O_8$	2a

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
93 Paragonite	$NaAl_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows Na^+ + 3Al^{+3} + 3H_4SiO_4$	6a, 75a
94 Pargasite	$NaCa_2Mg_4Al_3Si_6O_{22}(OH)_2 + 22H^+ \rightleftarrows Na^+ + 2Ca^{++} + 4Mg^{++} + 3Al^{+3} + 6H_4SiO_4^0$	6b, 72b
95 Periclase	$MgO + 2H^+ \rightleftarrows Mg^{++} + H_2O$	5b, 61b
96 Phillipsite	$Na_{.5}K_{.5}AlSi_3O_8 \cdot H_2O + 4H^+ + 3H_2O \rightleftarrows .5Na^+ + .5K^+ + Al^{+3} + 3H_4SiO_4^0$	7a
97 Phlogopite, OH	$KMg_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Mg^{++} + Al^{+3} + 3H_4SiO_4^0$	6b, 72b
98 Fluor-phlogopite	$KMg_3AlSi_3O_{10}F_2 + 8H^+ + 2H_2O \rightleftarrows K^+ + 3Mg^{++} + Al^{+3} + 2F^- + 3H_4SiO_4^0$	5b, 61b
99 Portlandite	$Ca(OH)_2 \rightleftarrows Ca^{++} + 2OH^-$	5b, 61b
100 Potassium Oxide	$K_2O + 2H^+ \rightleftarrows 2K^+ + H_2O$	5b, 61b
101 Prehnite	$Ca_2Al_2Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows 2Ca^{++} + 2Al^{+3} + 3H_4SiO_4^0$	6b, 72b
102 Pyrophyllite	$Al_2Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftarrows 2Al^{+3} + 4H_4SiO_4^0$	6b, 72b
103 Quartz	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	70a
104 Sanidine, High	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$	5b, 61b
105 Saponite, Na	$Na_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33Na^+ + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
106 Saponite, K	$K_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33K^+ + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
107 Saponite, H	$H_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 6.99H^+ + 2.68H_2O \rightleftarrows 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
108 Saponite, Ca	$Ca_{.165}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Ca^{++} + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
109 Saponite, Mg	$Mg_{3.165}Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Mg^{++} + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^0$	66a
110 Sepiolite	$Mg_4Si_6O_{15}(OH)_2 \cdot 6H_2O + 8H^+ + H_2O \rightleftarrows 4Mg^{++} + 6H_4SiO_4^0$	72a, 77a
111 Silica, Amorphous	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	70a
112 Silica Gel	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$	7a
113 Sillimanite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^0 + H_2O$	6b, 72b
114 Smectite, Ca	$Ca_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .167Ca^{++} + 2.33Al^{+3} + 3.67H_4SiO_4^0$	7a
115 Smectite, K	$K_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .33K^+ + 2.33Al^{+3} + 3.67H_4SiO_4^0$	7a
116 Smectite, Mg	$Mg_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .167Mg^{++} + 2.33Al^{+3} + 3.67H_4SiO_4^0$	7a
117 Smectite, Na	$Na_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .33Na^+ + 2.33Al^{+3} + 3.67H_4SiO_4^0$	7a
118 Sodium Monoxide	$Na_2O + 2H^+ \rightleftarrows 2Na^+ + H_2O$	5b, 61b
119 Spinel	$MgAl_2O_4 + 8H^+ \rightleftarrows Mg^{++} + 2Al^{+3} + 4H_2O$	5b, 61b
120 Stilbite	$CaAl_2Si_7O_{18} \cdot 7H_2O + 8H^+ + 3H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 7H_4SiO_4^0$	6b, 78b
121 Strengite	$FePO_4 \cdot 2H_2O \rightleftarrows Fe^{+3} + PO_4^{-3} + 2H_2O$	7a
122 Strontianite	$SrCO_3 \rightleftarrows Sr^{++} + CO_3^{--}$	40a
123 Sylvite	$KCl \rightleftarrows K^+ + Cl^-$	6a, 61a
124 Talc	$Mg_3Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftarrows 3Mg^{++} + 4H_4SiO_4^0$	6a, 72b, 75b

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
125 Thenardite	$Na_2SO_4 \rightleftarrows 2Na^+ + SO_4^{--}$	5b, 61b
126 Tremolite	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 14H^+ + 8H_2O \rightleftarrows 2Ca^{++} + 5Mg^{++} + 8H_4SiO_4^o$	6b, 72b
127 Trona	$Na_2CO_3NaHCO_3 \cdot 2H_2O \rightleftarrows 3Na^+ + CO_3^{--} + HCO_3^- + 2H_2O$	6b, 71b
128 Vivianite	$Fe_3(PO_4)_2 \cdot 8H_2O \rightleftarrows 3Fe^{++} + 2PO_4^{-3} + 8H_2O$	7a
129 Wairakite	$CaAl_2Si_4O_{12} \cdot 2H_2O + 8H^+ + 2H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 4H_4SiO_4^o$	6b, 72b
130 Witherite	$BaCO_3 \rightleftarrows Ba^{++} + CO_3^{--}$	6b, 61b
131 Wollastonite	$CaSiO_3 + 2H^+ + H_2O \rightleftarrows Ca^{++} + H_4SiO_4^o$	6b, 72b
132 Zoisite	$Ca_2Al_3Si_3O_{12}(OH) + 13H^+ \rightleftarrows 2Ca^{++} + 3Al^{+3} + 3H_4SiO_4^o + H_2O$	6b, 72b
133 Silver	$Ag + Fe^{+3} \rightleftarrows Ag^+ + Fe^{++}$	5b, 61b
134 Cerargyrite	$AgCl \rightleftarrows Ag^+ + Cl^-$	11a
135 Acanthite	$Ag_2S + H^+ \rightleftarrows 2Ag^+ + HS^-$	5b, 61b
136 Copper, Native	$Cu + Fe^{+3} \rightleftarrows Cu^+ + Fe^{++}$	5b, 6b
137 Malachite	$Cu_2CO_3(OH)_2 \rightleftarrows 2Cu^{++} + CO_3^{--} + 2OH^-$	6b, 61b
138 Tenorite	$CuO + 2H^+ \rightleftarrows Cu^{++} + H_2O$	6b, 61b
139 Cuprite	$Cu_2O + 2H^+ \rightleftarrows 2Cu^+ + H_2O$	5b, 6b
140 Covellite	$CuS + H^+ \rightleftarrows Cu^{++} + HS^-$	6b, 61b
141 Chalcocite	$Cu_2S + H^+ \rightleftarrows 2Cu^+ + HS^-$	6b, 61b
142 Chalcopyrite	$CuFeS_2 + 2H^+ \rightleftarrows Cu^{++} + Fe^{++} + 2HS^-$	65a
143 Bornite	$Cu_5FeS_4 + 4H^+ \rightleftarrows 4Cu^+ + Cu^{++} + Fe^{++} + 4HS^-$	5b, 6b
144 Lawrencite	$FeCl_2 \rightleftarrows Fe^{++} + 2Cl^-$	7b
145 Molysite	$FeCl_3 \rightleftarrows Fe^{+3} + 3Cl^-$	7b
146 Siderite	$FeCO_3 \rightleftarrows Fe^{++} + CO_3^{--}$	5b, 6b
147 Ferrous Oxide	$FeO + 2H^+ \rightleftarrows Fe^{++} + H_2O$	5b, 6b
148 Hematite	$Fe_2O_3 + 6H^+ \rightleftarrows 2Fe^{+3} + 3H_2O$	5b, 6b

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
149 Maghemite	$Fe_2O_3 + 6H^+ \rightleftarrows 2Fe^{+3} + 3H_2O$	7a
150 Magnetite	$Fe_3O_4 + 8H^+ \rightleftarrows 2Fe^{+3} + Fe^{++} + 4H_2O$	5b, 6b
151 $Fe(OH)_3$	$Fe(OH)_3 \rightleftarrows Fe^{+3} + 3OH^-$	7a
152 Goethite	$FeOOH + 3H^+ \rightleftarrows Fe^{+3} + 2H_2O$	5b, 6b
153 Pyrrotite	$FeS + H^+ \rightleftarrows Fe^{++} + HS^-$	6b, 72b
154 Troilite	$FeS + H^+ \rightleftarrows Fe^{++} + HS^-$	5b, 6b
155 Pyrite	$FeS_2 + H_2O \rightleftarrows Fe^{++} + 1.75HS^- + 0.25SO_4^{--} + 0.25H^+$	5b, 6b
156 Greigite	$Fe_3S_4 + 4H^+ \rightleftarrows 2Fe^{+3} + Fe^{++} + 4HS^-$	7a
157 Mercury (L)	$Hg + 2Fe^{+3} \rightleftarrows Hg^{++} + 2Fe^{++}$	2b, 5b
158 Mercurous Chloride	$HgCl_2 \rightleftarrows Hg^{++} + 2Cl^-$	7a
159 Calomel	$Hg_2Cl_2 \rightleftarrows Hg_2^{++} + 2Cl^-$	7a
160 Montroydite	$HgO + 2H^+ \rightleftarrows Hg^{++} + H_2O$	6b, 61b
161 Cinnabar	$HgS + H^+ \rightleftarrows Hg^{++} + HS^-$	6b, 61b
162 Cinnabar, Meta-	$HgS + H^+ \rightleftarrows Hg^{++} + HS^-$	6b, 61b
163 Scacchite	$MnCl_2 \rightleftarrows Mn^{++} + 2Cl^-$	5b, 61b
164 Rhodochrosite	$MnCO_3 \rightleftarrows Mn^{++} + CO_3^{--}$	5b, 61b
165 Manganosite	$MnO + 2H^+ \rightleftarrows Mn^{++} + H_2O$	5b, 6b
166 Pyrolusite	$MnO_2 + Mn^{++} + 4H^+ \rightleftarrows 2Mn^{+3} + 2H_2O$	5b, 6b
167 Alabandite	$MnS + H^+ \rightleftarrows Mn^{++} + HS^-$	5b, 61b
168 Cotunnite	$PbCl_2 \rightleftarrows Pb^{++} + 2Cl^-$	5b, 61b
169 Cerussite	$PbCO_3 \rightleftarrows Pb^{++} + CO_3^{--}$	5b, 6b
170 Litharge	$PbO + 2H^+ \rightleftarrows Pb^{++} + H_2O$	72a
171 Massicot	$PbO + 2H^+ \rightleftarrows Pb^{++} + H_2O$	5b, 61b
172 Galena	$PbS + H^+ \rightleftarrows Pb^{++} + HS^-$	46a
173 Anglesite	$PbSO_4 \rightleftarrows Pb^{++} + SO_4^{--}$	6b, 63a
174 Smithsonite	$ZnCO_3 \rightleftarrows Zn^{++} + CO_3^{--}$	46a

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
175 Zincite	$ZnO + 2H^{+} \rightleftarrows Zn^{++} + H_2O$	46a
176 Sphalerite	$ZnS + H^{+} \rightleftarrows Zn^{++} + HS^{-}$	46a
177 Zincosite	$ZnSO_4 \rightleftarrows Zn^{++} + SO_4^{--}$	5b, 61b
178 Rutherfordine	$UO_2CO_3 \rightleftarrows UO_2^{++} + CO_3^{--}$	6b, 44b, 61b
179 Uramphite	$(NH_4)_2(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows 2NH_4^{+} + 2UO_2^{++} + 2HPO_4^{--}$	2b, 45b, 61b
180 Przhevalskite	$Pb(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Pb^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 7b, 44b
181 Torbernite	$Cu(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Cu^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 45b, 61b
182 Saleeite	$Mg(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Mg^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 45b, 74b
183 Autunite, Sr	$Sr(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Sr^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 61b, 74b
184 Uranocircite	$Ba(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Ba^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 45b, 61b
185 Bassetite	$Fe(UO_2)_2(PO_4)_2 + 2H^{+} \rightleftarrows Fe^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 44b, 45b
186 Clarkeite	$UO_3 + 2H^{+} \rightleftarrows UO_2^{++} + H_2O$	43b
187 Gummite	$UO_3 + 2H^{+} \rightleftarrows UO_2^{++} + H_2O$	43b, 45b
188 $UO_2(OH)_2$	$UO_2(OH)_2 \rightleftarrows UO_2^{++} + 2OH^{-}$	5b, 45b
189 $UF_4 \cdot 2.5H_2O$	$UF_4 \cdot 2.5H_2O \rightleftarrows U^{+4} + 4F^{-} + 2.5H_2O$	5b, 43b, 61b
190 $U(HPO_4)_2 \cdot 4H_2O$	$U(HPO_4)_2 \cdot 4H_2O \rightleftarrows U^{+4} + 2HPO_4^{--} + 4H_2O$	5b, 43b, 61b
191 Ningyoite	$CaU(HPO_4)_2 \cdot 2H_2O + 2H^{+} \rightleftarrows Ca^{++} + U^{+4} + 2HPO_4^{--} + 2H_2O$	5b, 45b, 61b
192 U_3O_8	$U_3O_8 + 4H^{+} \rightleftarrows UO_2^{++} + 2UO_2^{+} + 2H_2O$	43b, 61b

Table 3. -- Congruent dissolution of minerals and sources of thermochemical data -- (Continued)

ID # and Name	Reaction	References
193 Uraninite, Amorphous	$UO_2 + 4H^+ \rightleftarrows U^{+4} + 2H_2O$	43b
194 Uraninite	$UO_2 + 4H^+ \rightleftarrows U^{+4} + 2H_2O$	43b
195 U_4O_9	$U_4O_9 + 10H^+ \rightleftarrows 2U^{+4} + 2UO_2^+ + 5H_2O$	43b, 61b
196 Coffinite	$USiO_4 + 4H^+ \rightleftarrows U^{+4} + H_4SiO_4^o$	44b
197 Autunite, H	$H_2(UO_2)_2(PO_4)_2 \rightleftarrows 2UO_2^{++} + 2HPO_4^{--}$	44b
198 Autunite, Na	$Na_2(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows 2Na^+ + 2UO_2^{++} + 2HPO_4^{--}$	2b, 61b
199 Autunite, K	$K_2(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows 2K^+ + 2UO_2^{++} + 2HPO_4^{--}$	5b, 45b, 61b
200 Autunite	$Ca(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Ca^{++} + 2UO_2^{++} + 2HPO_4^{--}$	5b, 45b, 61b
201 Carnotite	$K_2(UO_2)_2(VO_4)_2 \rightleftarrows 2K^+ + 2UO_2^{++} + 2VO_4^{-3}$	5b, 45b, 61b
202 Tyuyamunite	$Ca(UO_2)_2(VO_4)_2 \rightleftarrows Ca^{++} + 2UO_2^{++} + 2VO_4^{-3}$	5b, 45b, 61b
203 Uranophane	$Ca(UO_2)_2(HSiO_4)_2 + 6H^+ \rightleftarrows Ca^{++} + 2UO_2^{++} + 2H_4SiO_4^o$	5b, 45b, 61b
204 Schoepite	$UO_2(OH)_2 \cdot H_2O \rightleftarrows UO_2^{++} + 2OH^- + H_2O$	43b, 61b
205 $MgUO_4$	$MgUO_4 + 4H^+ \rightleftarrows Mg^{++} + UO_2^{++} + 2H_2O$	5b, 44b, 61b
206 $CaUO_4$	$CaUO_4 + 4H^+ \rightleftarrows Ca^{++} + UO_2^{++} + 2H_2O$	5b, 44b, 61b
207 $BaUO_4$	$BaUO_4 + 4H^+ \rightleftarrows Ba^{++} + UO_2^{++} + 2H_2O$	5b, 44b, 61b
208 UO_2F_2	$UO_2F_2 \rightleftarrows UO_2^{++} + 2F^-$	5b, 44b, 61b
209 US_3	$US_3 + 2H_2O \rightleftarrows UO_2^{++} + 3HS^- + H^+$	5b, 44b, 61b
210 Karelianite	$V_2O_3 + 6H^+ \rightleftarrows 2V^{+3} + 3H_2O$	2b, 45b
211 Vanadium Tetro-	$V_2O_4 + 4H^+ \rightleftarrows 2VO^{++} + 2H_2O$	2b, 45b
212 Vanadium Pento-	$V_2O_5 + 3H_2O \rightleftarrows 2VO_4^{-3} + 6H^+$	2b, 45b
213 $VOSO_4 \cdot 6H_2O$	$VOSO_4 \cdot 6H_2O \rightleftarrows VO^{++} + SO_4^{--} + 6H_2O$	2b, 61b
214 $Pb_3(VO_4)_2$	$Pb_3(VO_4)_2 \rightleftarrows 3Pb^{++} + 2VO_4^{-3}$	2b, 5b, 61b

Sources of Thermochemical Data for Reactions in Tables 2 and 3

1) Plummer and Busenberg (1982)
2) Naumov and others (1974)
3) Marshall and Frank (1981)
4) Busey and Mesmer (1977)
5) Helgeson and others (1981)
6) Helgeson (1985 Version of SUPCRT)
7) Kharaka and Barnes (1973)
8) Arnorsson and others (1982)
9) Baes and Mesmer (1981)
10) May and others (1979)
11) Seward (1976)
12) Lown and others (1970)
13) Jacobson and Langmuir (1974)
14) Kalyanaraman and others (1973)
15) Smith and Martell (1976)
16) Crerar and Barnes (1976)
17) Crerar and others (1978)
18) Wagman and others (1968; 1969)
19) Helgeson and others (1978)
20) Mesmer and others (1972)
21) Helgeson (1969)
22) Bryzgalin and Rafelski (1982)
23) Barnes and others (1967)
24) Smith and others (1986)
25) Sillen and Martell (1964)
26) Siebert and Hostetler (1977)
27) Wolley and Hepler (1977)
28) Kublanovskii (1977)
29) Harned and Owen (1958)
30) Seward (1981)
31) Drummond (1981)
32) Lafon (1969)
33) Reardon (1975)
34) Lafon and Truesdell (1971)
35) Plummer and others (1984)
36) Seward (1984)
37) Patterson and others (1982)
38) Giordano and Drummond (1987)
39) Møller (1988)
40) Busenberg and others (1984)
41) Ruaya and Seward (1986)
42) Katayama (1976)
43) Lemire and Tremaine (1980)
44) Hemingway (1982)
45) Langmuir (1978)
46) Bourcier and Barnes (1987)
47) Tremaine and others (1981)
48) Phillips (1982)
49) Martell and Smith (1977)
50) Nancollas (1956)
51) Palmer and Drummond (1988)
52) Wagman and others (1982)
53) Wagman and others (1976)
54) Shanks and Bischoff (1977)
55) Giordano and Barnes (1981)
56) Wood and others (1987)
57) Hogfeldt (1982)
58) Roberson and Barnes (1978)
59) Bilinski and others (1986)
60) Daniele and others (1981)
61) Robie and others (1978)
62) Tremaine (1987)
63) DeKock (1986)
64) Cobble and others (1982)
65) Conard and others (1980)
66) Wolery (1986)
67) Richet and others (1982)
68) Nordstrom and Jenne (1977)
69) Tanger and Helgeson (1988)
70) Fournier and Potter (1982)
71) Vanderzee (1982)
72) Tugarinov and others (1975)
73) Hovey and others (1988)
74) Zen (1972)
75) Berman and others (1985)
76) Kerrisk (1983)
77) Stoessell (1988)
78) Cho and others (1987)
79) Williams-Jones and Seward (1988)

Letters following numerical references in Tables 2 and 3 refer to the method of computation used to calculate the equilibrium constants as described in the section, Equilibrium Constants.

ACTIVITY and ACTIVITY COEFFICIENTS

The activity of all minerals is assumed to be equal to unity, with the possible exception of the minerals entered using the unknown mineral option (see the description of the input file). The activity of water used in many equations is computed in SOLMINEQ.88 from the semiempirical expression given by Garrels and Christ (1965) as

$$a_{H_2O} = 1 - 0.017 \sum_i m_i \quad . \tag{16}$$

The summation covers the molalities (m_i) of all the species in solution. Alternatively, a more accurate value for the activity of water can be obtained from the Pitzer expressions (Pitzer, 1973; 1981) where

$$\log (a_{H_2O}) = 0.007823 \ (\Sigma \ m_i)\phi \quad , \tag{17}$$

where ϕ is the osmotic coefficient of the solution. Values of ϕ are calculated by equations and parameters given by Pitzer (1973) and Pitzer (1981). Equations (16) and (17) give approximately the same value for the activity of water in NaCl solutions (0 - 6 molal) at temperatures of 25 °C to 200 °C; the activity of water is somewhat lower in $CaCl_2$ than in NaCl solutions (see Table 6.2 in Kharaka and Mariner, 1989). The activity of water can be approximated for most natural waters using equation (16). Equation (17), however, should be used for waters where the concentrations of divalent cations comprise more than about 20 percent of the total cations.

The program uses equation (16), but the user can specify equation (17) by selecting the appropriate input switch. Values for the osmotic coefficients of NaCl, $CaCl_2$ and other electrolytes as a function of temperature and molality were obtained from Staples and Nuttall (1977), Holmes and others (1978, 1981) and Pitzer (1981).

The activities of aqueous species are computed from

$$a_i = m_i \gamma_i \quad , \tag{18}$$

where γ_i is the activity coefficient of species i. The standard state adopted for the aqueous species is that where the activity is equal to molality in a hypothetical infinitely dilute solution at any pressure and temperature.

Activity Coefficients for Neutral Species

Several methods are used by geochemists to calculate the activity coefficients of neutral species, each give different results. The activity coefficients of all neutral species are generally assumed equal to that of dissolved CO_2 in NaCl solutions (Helgeson, 1969). The activity coefficients for CO_2 (γ_{CO_2}) maybe calculated using:

$$\gamma_{CO_2}(T) = \frac{k_m}{k} \quad , \tag{19}$$

where k and k_m are the Henry's law coefficients (atm/mole) in pure water and sodium chloride solutions of molality m at temperature T (°K). Values for k_m and k are available as a function of temperature (0°-350 °C) and molality of NaCl (0 - 6 molal) from Ellis and Golding (1963) and Drummond (1981). SOLMINEQ.88 has the option to compute γ_{CO_2} and all the other neutral species (except H_2S and H_4SiO_4) using a modified expression from Drummond (1981):

$$\ln k_{CO_2} = 21.2752 - 0.0176036T - 1.0312m - \frac{3885.6}{T} + \frac{0.4445}{(m-1)} + 0.0012806\ mT + \frac{255.9m}{T} - \frac{0.001606\ T}{(m-1)} \quad . \tag{20}$$

The activity coefficient for H_2S can be calculated from a similar expression, also modified from Drummond (1981) which is:

$$\ln k_{H_2S} = 11.1255 - 0.0071704T + 0.2905T - \frac{2021.5}{T} + \frac{0.5705}{(m-1)} - 0.0001574mT - \frac{46.2m}{T} - \frac{0.001777T}{(m-1)} \quad . \tag{21}$$

In both equations (20) and (21), m is the molality of NaCl.

The expressions of Marshall (1980) and Chen and Marshall (1982) are preferred for calculating the activity coefficient of $H_4SiO_4^o$. Their activity coefficients for $H_4SiO_4^o$ were derived from data on the solubility of amorphous silica as a function of temperature (0° - 350 °C), and NaCl salinity (0 - 6 molal). The expression is:

$$\log (\gamma_{H_4SiO_4^o}) = (0.00978 \times 10^{(280/T)}) \times m \quad . \tag{22}$$

Sodium and chloride are by far the dominant aqueous species in most formation waters from sedimentary basins (Kharaka and others, 1985), and equation (22) can be applied directly to these waters. However, the concentrations of other species, especially calcium, can be high, requiring modification of equation (22). Data in Marshall (1980) and Chen and Marshall (1982) show that equation (22) can be generalized to:

$$\log (\gamma_{H_4SiO_4^o}) = (0.00489 \times 10^{(280/T)}) \cdot \Sigma_i \, z_i^2 \, m_i \quad , \tag{23}$$

where z_i and m_i are the charge and molality of species (i). The summation includes all of the species in the formation water.

Activity Coefficients for Charged Species

In SOLMINEQ.88, the activity coefficients (γ) for the charged aqueous species are computed using $B^{\cdot}$ method (Lewis and Randall, 1961; Helgeson, 1969).

$$\log \gamma_i = \frac{-A_\gamma z_i^2 \, I^{1/2}}{1 + a_i^o \, B_\gamma I^{1/2}} + B^{\cdot} I \quad , \tag{24}$$

where a_i^o is the ion size parameter, A_γ and B_γ are the molal Debye-Hückel coefficients (described below) at temperature T, z_i is the charge of the ith ion, I is the true ionic strength, and $B^{\cdot}$ is a deviation function. The ionic strength (I) of a given solution is given by:

$$I = 1/2 \sum_i n_i \, z_i^2 \quad . \tag{25}$$

The Debye-Hückel coefficients, A_γ and B_γ, are given by:

$$A_\gamma(T) = \frac{1.8248 \times 10^6 \, \rho^{1/2}}{(\epsilon T)^{3/2}} \quad , \tag{26}$$

and

$$B_\gamma(T) = \frac{50.29 \times 10^8 \, \rho^{1/2}}{(\epsilon T)^{1/2}} \quad , \tag{27}$$

where ρ and ϵ are the density and the dielectric constant of water at temperature T. The values of A_γ and B_γ in the above equations are given in Table 4 and are from Helgeson and others (1981). The density and dielectric constants are corrected for pressure using functions based on data in Helgeson and Kirkham (1974).

The a_i^o values used (Appendix IA) are mainly from Kielland (1937), with unpublished data for U and V species from Goodwin (1982). Arbitrary a^o values of 4.0, 5.0 and 6.0 were assigned, respectively, to those monovalent, divalent and trivalent species not reported in the literature; for U and V species, values of 4.5, 3.5, 2.5, 5.0 and 9.0 were assigned respectively to -2, -1, +1, +2, and +3 charged species as suggested by Goodwin (1982).

The values for the deviation function, $B^\bullet$, used in equation (24) vary as a function of temperature (Appendix ID) and are from Helgeson (1969). The $B^\bullet$ values used are for NaCl solutions, a close approximation for most subsurface waters. The presence of appreciable amounts of divalent and trivalent cations and anions in solution with their higher degree of hydration will make the γ_i obtained lower than the true values. The $B^\bullet$ option should not be used for waters with ionic strengths higher than about one molal. In these cases the Pitzer equations, as discussed in the following section, should be selected in the input file.

Table 4. Values of the Debye-Hückel coefficients A_γ and B_γ along the vapor pressure curve of water (Helgeson and others, 1981).

t (°C)	A_γ ($kg^{1/2}mole^{-1/2}$)	B_γ ($kg^{1/2}mole^{-1}cm^{-1} \times 10^8$)
0	0.4913	0.3247
10	0.4976	0.3261
20	0.5050	0.3276
30	0.5135	0.3291
40	0.5231	0.3307
50	0.5336	0.3325
60	0.5450	0.3343
70	0.5573	0.3362
80	0.5706	0.3381
90	0.5848	0.3401
100	0.5998	0.3422
125	0.6417	0.3476
150	0.6898	0.3533
200	0.8099	0.3655
250	0.9785	0.3792
300	1.2555	0.3965
350	1.9252	0.4256

Pitzer Equations

SOLMINEQ.88 has an option to compute the activity coefficients of the aqueous species using Pitzer equations (Pitzer, 1981; Harvie and others, 1984). This modification was necessary because the $B^{\bullet}$ method used for calculating the activity coefficients (Helgeson, 1969) gives results that are much lower than the true values for solutions with salinities higher than about one molal (Figure 1). Pitzer equations are based on an ion-interaction or virial-coefficient model where the effects of ion association are implicitly incorporated in stoichiometric activity coefficients calculated by virial expansion of the Debye-Hückel theory (Pitzer, 1973, 1981; Silvester and Pitzer, 1978). A number of investigations (Whitfield, 1975; Harvie and Weare, 1980; Harvie and others, 1984; Gueddari and others, 1983) have shown that the use of the Pitzer equations has resulted in accurate predictions of mineral sequences in very concentrated brines at low temperatures.

The basic equations for the activity coefficients of positively (M) and negatively (X) charged species in terms of second and third virial coefficients (Pitzer, 1973; Harvie and others, 1984) are given below.

$$\ln \gamma_M = z_M^2 F + \sum_{a=1}^{N_a} m_a(2B_{Ma} + ZC_{Ma}) + \sum_{c=1}^{N_c} m_c(2\Phi_{Mc} + \sum_{a=1}^{N_a} m_a \psi_{Mca})$$

$$+ \sum_{a=1}^{N_{a-1}} \sum_{a'=a+1}^{N_a} m_a m_{a'} \psi_{aa'M} + |z_M| \sum_{c=1}^{N_c} \sum_{a=1}^{N_a} m_c m_a C_{ca} \quad , \qquad (28)$$

$$\ln \gamma_X = z_X^2 F + \sum_{c=1}^{N_c} m_c(2B_{cX} + ZC_{cX}) + \sum_{a=1}^{N_a} m_a(2\Phi_{Xa} + \sum_{c=1}^{N_c} m_c \psi_{Xac})$$

$$+ \sum_{c=1}^{N_{c-1}} \sum_{c'=c+1}^{N_c} m_c m_{c'} \psi_{cc'X} + |z_X| \sum_{c=1}^{N_c} \sum_{a=1}^{N_a} m_c m_a C_{ca} \quad , \qquad (29)$$

where m_c and z_c are the molality and charge of cation c and N_c is the total number of cations. Similar definitions apply for anions (subscript a). The following terms are defined for use in the above equations:

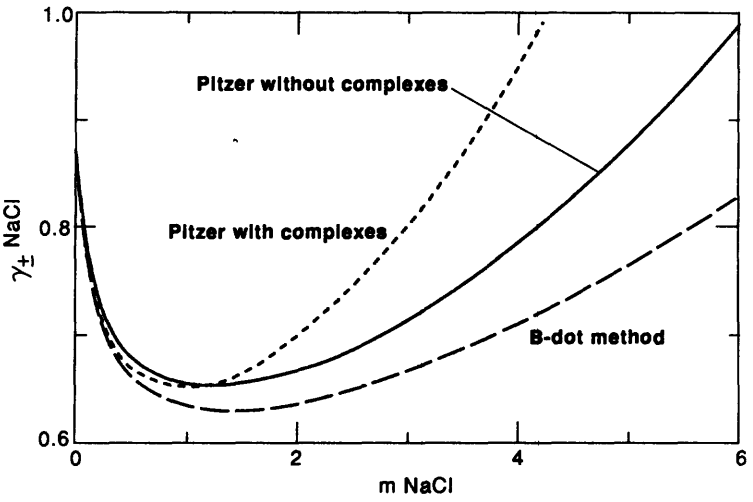

Figure 1. -- Pitzer and Ion Pair Activity Coefficients for NaCl solutions as a function of Ionic Strength.

$$F = -A^{\phi}\left[\frac{I^{1/2}}{1+1.2I^{1/2}} + \frac{2}{1.2}\ln(1+1.2I^{1/2})\right] + \sum_{c=1}^{N_c}\sum_{a=1}^{N_a} m_c m_a B'_{ca}$$

$$+ \sum_{c=1}^{N_{c-1}}\sum_{c'=c+1}^{N_c} m_c m_{c'} \Phi'_{cc'} + \sum_{a=1}^{N_{a-1}}\sum_{a'=a+1}^{N_a} m_a m_{a'} \Phi'_{aa'} \quad , \tag{30}$$

$$C_{MX} = C^{\phi}_{MX} / 2|z_M z_X|^{1/2} \quad , \tag{31}$$

$$Z = \Sigma\, m_i |z_i| \quad , \tag{32}$$

and

$$A^{\phi} = \frac{2.303}{3.0} A_{\gamma} \quad , \tag{33}$$

where A_{γ} is the Debye-Huckel constant and I is the stoichiometric ionic strength. The second virial coefficients (B) and (Φ) are given the following ionic strength dependence:

$$B_{MX} = \beta^{(0)}_{MX} + \beta^{(1)}_{MX} g(\alpha_{MX}\sqrt{I}) + \beta^{(2)}_{MX} g(12\sqrt{I}) \quad , \tag{34}$$

$$B'_{MX} = \beta^{(1)}_{MX} g'(\alpha_{MX}\sqrt{I})/I + \beta^{(2)}_{MX} g'(12\sqrt{I})/I \quad , \tag{35}$$

$$\Phi_{ij} = \theta_{ij} + {}^{E}\theta_{ij}(I) \quad , \tag{36}$$

$$\Phi'_{ij} = {}^{E}\theta'_{ij}(I) \quad . \tag{37}$$

The functions, g and g', are defined by the equations

$$g(x) = 2(1 - (1+x)e^{-x})/x^2 \quad , \tag{38}$$

$$g'(x) = -2(1 - (1 + x + \frac{x^2}{2})e^{-x})/x^2 \quad , \tag{39}$$

where $x = \alpha_{MX}\sqrt{I}$ or $12\sqrt{I}$. When either cation M or anion X is univalent, $\alpha_{MX} = 2.0$. For 2 - 2, or higher valence pairs, $\alpha_{MX} = 1.4$. In most cases $\beta^{(2)}$ equals zero. The functions of ${}^{E}\theta_{ij}(I)$ and ${}^{E}\theta'_{ij}(I)$ account for the

electrostatic effects of unsymmetrical unmixing (Pitzer, 1981). They are only significant in complex 1-2 and 1-3 electrolytes at high ionic strength.

A relatively large and expanding database is now available to calculate the activities of alkali and alkaline earth metals in concentrated chloride and sulfate solutions at temperatures of up to at least 200 °C (Pitzer, 1981; Holmes and Mesmer, 1983; Pabalan and Pitzer, 1987; Møller, 1988; and many others).

The complete set of parameters required to calculate the activities of these species are: $\beta^{(0)}_{MX}$, $\beta^{(1)}_{MX}$, $\beta^{(2)}_{MX}$, and C^{ϕ}_{MX} for each cation-anion pair, θ_{ij} for each cation-cation and anion-anion pair; ψ_{ijk} for each cation-cation-anion and anion-anion-cation triplet. The interaction parameters for seven cations and four anions were calculated from various published data and are tabulated in the database of SOLMINEQ.88 (Appendix IG) at 25 °C intervals from 0° to 150 °C and at 50 °C intervals from 150 ° to 350 °C. The parameters are interpolated to the specified temperature (from 0° to 350 °C) by the Lagrange subroutine (TLUV) used to interpolate the K values (see below).

SOLMINEQ.88 has an option to compute the activity coefficients of the seven cations and four anions using Pitzer equations. It must be emphasized here that these equations are based on an ion interaction model that assumes no ion associations or complexing. The distribution of species in SOLMINEQ.88, on the other hand, is based on an ion association model. This inconsistency is resolved by incrementing the ion activity coefficients obtained from the Pitzer equations for these species so the final activity for the species is equal to that computed from Pitzer equations. In the case of Na, for example, the final value for γ_{Na^+}, is given by

$$\gamma_{Na^+} = \frac{m_{Na,t} \cdot \gamma_{Na,P}}{m_{Na^+}} \quad , \tag{40}$$

where $\gamma_{Na,P}$ is the activity coefficient for Na obtained from the Pitzer equations. The activity coefficients for a large number of species and complexes in SOLMINEQ.88 can not be computed using Pitzer's equations because there are no published virial coefficients for them, especially at high temperatures. The activity coefficients for these species (γ_i) are calculated using a modified ($B^{\bullet}$) equation given by:

$$\log \gamma_i = \frac{- z_i^2 \; A_\gamma I^{1/2}}{1 + a_i^o \; B_\gamma I^{1/2}} + B^* I \quad , \tag{41}$$

where B^* is a deviation function. The value of B^* used to calculate the activity coefficients for univalent cations, anions, and complexes (B_u^*) is obtained from:

$$B_u^* = \frac{1}{I} \left(\log \gamma_{Na^+} + \frac{A_\gamma I^{1/2}}{1 + 4.0 \times 10^{-8} \; B_\gamma I^{1/2}} \right) \quad , \tag{42}$$

where γ_{Na^+} is obtained for a hypothetical minor concentration of Na^+ equal to 0.01 m using Pitzer equations. The value of B_m^* used to calculate the activity coefficients for multivalent cations, anions and complexes with no virial coefficients data to calculate their activities by Pitzer equations is obtained from:

$$B_m^* = \frac{1}{I} \left(\log \gamma_{Ca^{++}} + \frac{4.0 \; A_\gamma I^{1/2}}{1 + 6.0 \times 10^{-8} \; B_\gamma I^{1/2}} \right) \quad , \tag{43}$$

where $\gamma_{Ca^{++}}$ is again obtained using Pitzer equations for a hypothetical 0.01 m concentrations of Ca^{++}. Hypothetical 0.01 concentrations of Na^+ and Ca^{++} are used because at concentrations higher than about 0.1 m, γ_i is a function of concentration (Pitzer, 1981; Tanger and Helgeson, 1988).

Using Na^+ and Ca^{++} as the "typical minor or trace" species to calculate the activity coefficients for the majority of the dissolved species is clearly not thermodynamically rigorous, but is an operational approach. However, comparison of values of activity coefficients obtained by this approach and by Pitzer equations for a number of dissolved species shows that this approach allows the operational $B^\bullet$ method (Helgeson, 1969) to be extended to about 3 to 6m solutions. Research to obtain virial coefficients for carbonate, aluminum and other important species is clearly needed.

EQUILIBRIUM CONSTANTS

The equilibrium constants (K) for the dissociation of aqueous complexes (Table 2) and congruent dissolution of minerals (Table 3) are the most important part of the database in geochemical codes such as SOLMINEQ.88. Examples of dissociation reactions (Reactions 1 and 2) and the corresponding equations (1 and 2) are given in an earlier section; the corresponding equation for the dissolution of anorthite reaction (7) is:

$$K_{an} = \frac{\bar{a}_{Ca^{++}} \cdot \bar{a}^{2}_{Al^{+3}} \cdot \bar{a}^{2}_{H_4SiO_4^{o}}}{\bar{a}_{an} \cdot \bar{a}^{8}_{H^{+}}} \quad , \tag{44}$$

where $\bar{a}_i$ is the activity of the ith species at equilibrium. The equilibrium constants for the reactions shown in Tables 2 and 3 are in a data file labeled DATA.TBL. The K(T) values reported (Appendix IB and IC) at intervals of 25 °C from 0-150 °C and at intervals of 50 °C from 150°-350 °C were computed assuming a total pressure equal to the vapor pressure of water. (The correction for pressure is described in a following section.)

The equilibrium constants were obtained from references listed in Table 2 and by the methods described below, which are listed in decreasing order of reliability. The uncertainties in the computed equilibrium constants are generally higher for the aqueous species especially at temperatures higher than about 150 °C because their heat capacities can not be accurately estimated. In the case of minerals, if heat capacity functions are not available, they can be estimated from those of their oxides (Helgeson, 1969; Berman and others, 1985).

(a) Reported experimental data (solubility, free energy, and other data) or reported K values as a function of temperature over the temperature range of 25° to at least 200 °C. The values were extrapolated and interpolated to the temperature values used in this code.

(b) Computed using KELYCOB (Helgeson, 1971a) and SUPCRT (Helgeson, 1985), which computes the equilibrium constants of a given reaction (log K_r) as a function of temperature and pressure. Generally the input to these programs for solids are the coefficients A, B, and C for the Maier-Kelley heat capacity power function (Kelly, 1960) given below

$$C_p = A + BT + \frac{C}{T^2} \quad , \tag{45}$$

the standard state enthalpies of formation (H_f^o), and the standard state entropies (S_i^o) of all the components involved in the reaction. KELYCOB computes the K(T) values from an integrated form of Van't Hoff's equation (Helgeson, 1969),

$$\log K(T) = \log K_{298.15} - \frac{H_r^o}{2.303R}\left(\frac{1}{T} - \frac{1}{298.15}\right) - \frac{1}{2.303RT}\int_{298.15}^{T} \Delta C_{p,r}^o (T)dT + \frac{1}{2.303R}\int_{298.15}^{T} \Delta C_{p,r}^o (T)d\ln T \quad . \tag{46}$$

The heat capacity of the aqueous species Na^+, K^+, Li^+, Ag^+, NH_4^+, Cu^+, Mg^{+2}, Ca^{+2}, Sr^{+2}, Ba^{+2}, Pb^{+2}, Zn^{+2}, Cu^{+2}, Hg^{+2}, Fe^{+2}, Mn^{+2}, Fe^{+3}, Al^{+3}, F^-, Cl^-, OH^-, HS^-, HCO_3^-, SO_4^{-2}, $NaCl^o$, and SiO_2^o can be described by this equation (Helgeson and others, 1981; Helgeson, 1985):

$$C_p = C_{1i} + \frac{C_{2i}T}{T - \theta_i} - w_i Tx \quad , \tag{47}$$

where C_{1i}, C_{2i}, θ_i and w_i are empirical constants derived separately for each aqueous species, i, and x is the derivative of the variation of the dielectric constant of water, ϵ, with temperature (Helgeson and others, 1981).

A program called IONK was created which performs the function of KELYCOB, but uses the coefficients in equation (45) or those in equation (47) as input. IONK was used when the coefficients C_{1i}, C_{2i}, θ_i, and w_i were available.

KELYCOB and IONK were used to generate log K values at 25 °C intervals from 0° to 350 °C for most of the solubility reactions reported on Appendix IC. A number of log K values for the dissociation reactions of aqueous complexes were also obtained by this method.

The heat capacity power function for many minerals reported in this program are not known. They were approximated by summing up the heat capacity power functions for the oxides. The expression

$$(7.11 + .0082\ T)\text{cal mole}^{-1}\ \text{deg}^{-1} \quad ,$$

(structural water) was used to represent H_2O in these approximations (Helgeson and others, 1978). For several ions (i.e., those containing U, V, or P) heat capacity was represented by a constant. The solubility constants of minerals containing these elements are only reliable below 200 °C (Langmuir, 1978).

(c) Computed using DQUANT (Helgeson, 1971b). This program requires only that $\Delta H^o_r\ (T_r)$ and $\Delta S^o_r\ (T_r)$ be known; it was used where no heat capacity data of any kind are available for one or more of the species involved in the reaction. This last condition covers many of the aqueous reactions reported in Table 2. DQUANT computes K(T) values by evaluating (Helgeson, 1967)

$$\log K(T) = \frac{\Delta S^o_r\ (T_r)}{2.303RT}\ [T_r - \frac{\theta}{W}\ (1 - \exp(\exp(b + aT) - c + \frac{(T - T_r)}{\theta}))] - \frac{\Delta H^o_r(T_r)}{2.303RT}\ , \qquad (48)$$

where θ, W, a, b, and c are temperature-independent constants characteristic of the solvent, and R is the gas constant.

DQUANT assumes that $\Delta C^o_{p,r}$ changes monotonically but nonlinearly with temperature. Dissociation constants computed from this program are often much closer approximations of actual dissociation constants at higher temperatures than those computed assuming $\Delta C^o_{p,r}(T) = 0$ or $\Delta C^o_{p,r}(T) =$ a constant (Helgeson, 1969). K(T) values obtained with DQUANT are reasonable approximations only to about 150 °C.

A correction factor was applied to some of the K(T) values generated with DQUANT at temperatures higher than 150 °C. These factors were generated either graphically by comparison with the K(T) values of similar complexes or by generating $\Delta C^o_{p,r}$ using K(T) values from 0° to 150 °C, then using them in equation (46). Even with the application of these correction factors, the errors involved in the values of K(T) at temperatures higher than 200 °C are large; this introduces large uncertainties in computations carried out with SOLMINEQ.88 at these high temperatures.

(d) Values for K are available at two or more generally low temperatures. Values for ΔH^o_r and ΔS^o_r are derived from this data using two equations of the form:

$$\frac{\log K(T)}{2.303RT} = \Delta H_r^o - T\Delta S_r^o \quad , \tag{49}$$

and solving for ΔH_r^o and ΔS_r^o algebraically. This method was used only when ΔC_p^o could not be derived from available data. Values for K at higher temperatures were calculated using Equation (48).

(e) Entropy was estimated by Arnorsson and others (1982) using correlation plots of the known entropies of ions as a function of molecular weight. Enthalpy was then calculated from the stability constant using Equation (49).

(f) A value for K is available only at 25 °C; it was extrapolated using the assumption that the curve of log K as a function of temperature is parallel to that of a similar species.

(g) A value for K is available only at 25 °C; it was extrapolated using Bryzgalin's method (Bryzgalin and Rafal'skiy, 1982):

$$-\log K(T) = \frac{298}{T} (-\log K(298)) + \frac{72600\ Z}{aT} \left(\frac{1}{\epsilon} - 0.0128 \right) \quad , \tag{50}$$

where

$$Z = Lz_C z_A - Qz_A^2 + \frac{pz_C^2 L}{2a^3} - \left[\frac{pz_C}{a^3} \right]^2 \frac{Q}{2} \quad , \tag{51}$$

and

$$Q = \frac{3L^2 - 5L + 2}{8} \quad , \tag{52}$$

ϵ is the dielectric constant of water, a is the sum of the Goldschmidt radii of the simple ions from which the ion complex is formed, z_A, and z_C are the charge of the anion and cation, respectively, L is the number of ligands ($PbCl_3$ has three ligands), and p is polarizability. Where p was not known it was assumed to be zero.

Equilibrium Constants at Desired Temperature

Values of log K for aqueous complexes and minerals at the desired temperature are interpolated from data in Appendix 1 by the subroutine TLUV. The interpolation of the log K values uses the cubic function:

$$Y = a + bX + cX^2 + dX^3 \quad , \tag{53}$$

where X is the independent variable (temperature at which K values are listed), Y is the dependent variable (log K values at the listed and specified sample temperature), and a, b, c, and d are constants. This subroutine calculates interpolated log K values between the reported intervals (25 °C from 0-150 °C and 50 °C from 150-350 °C) that are in good agreement with the original values.

Equilibrium Constants at Desired Pressure

The equilibrium constants (K) tabulated in SOLMINEQ.88 are computed at the vapor pressure of water. SOLMINEQ.88 has an option to compute the solubility of minerals at a specified pressure using data tabulated in Appendix 1E. The pressure dependence of the equilibrium constant is given by

$$\left(\frac{\partial \ln K}{\partial P}\right)_T = \frac{-\Delta V_r^o}{RT} \quad , \tag{54}$$

where ΔV_r^o is the volume change of the reaction in the standard state. Values of ΔV_r^o at higher temperatures and pressures for the dissolution reactions of minerals can be obtained from the data of Helgeson and others (1978, 1981) and Robie and others (1978). However, ΔV_r^o values at higher T and P for the dissociation reactions of most of the aqueous complexes are not available and, therefore, Equation (54) cannot be used to calculate K values at higher pressures for these complexes.

Correction of the solubility constants for pressure

Changes in the partial molal volume of aqueous species ($\bar{V}$) and water with pressure are the main contributors to the volume change in dissolution reactions (ΔV_r^o); minerals are assumed to be incompressible (Helgeson and others, 1981). Data on the molal volume of water were obtained from Helgeson and Kirkham (1974). Values for the partial molal volumes of aqueous species $\bar{V}_i$ are sparse. They are calculated for the primary species using the data and equations reported in Helgeson and others (1981) and given by:

$$\bar{V}_i = a_{1i} + a_{2i}P + a_{3i}T + \frac{a_{4i}PT}{T - \theta_i} - w_iQ \quad , \tag{55}$$

where a_{1i} is the intrinsic volume of species i which is independent of pressure and temperature; $w_i Q$ is the volume of solvation, the component of partial molal volume related to the orientation of water dipoles around the aqueous species. The remaining portion of Equation (55) is the volume of collapse, that is, the component of the partial molal volume related to the collapse of the water structure in the vicinity of the aqueous species. The constants a_{1i}, a_{2i}, a_{3i}, and a_{4i} are empirically derived; θ_i is a constant; P is in bars and T is in degrees K.

The pressure effect on the K values for minerals was estimated at 500 and 1,000 bars and temperatures of 100°, 150°, 200°, 300°, and 350 °C. The data were fit to a curve with the general formula

$$\log \left[\frac{K_p}{K} \right] = A + Bt + Ct^6 \quad , \tag{56}$$

where t is in °C, and the constants A, B and C were calculated for each solid phase at 500 and 1,000 bars. The term Ct^6 reflects the extreme changes in the partial molal volume (and therefore in K values) which occur above 300 °C. Values for the constants A, B and C for each mineral are listed in Appendix 1E.

The subroutine PCLOGK calculates solubility constants at selected pressure (P) below 500 bars using the following interpolation:

$$\log K_P = \log K + \frac{\Delta \log K_{500} P}{500} \quad , \tag{57}$$

and for pressures above 500 bars using:

$$\log K_P = \log K + \Delta \log K_{500} + \frac{(\Delta \log K_{1,000} - \Delta \log K_{500})\ (P - 500)}{500} \quad . \tag{58}$$

The pressure correction is significant when the pressure is several hundred bars or more, especially at temperatures above about 150 °C. For example, in Figure 2 it can be seen that at 1,000 bars the solubility product of anorthite is increased relative to saturation pressure of water by factors of about 30, 300 and 100,000,000, at 100°, 250° and 350 °C, respectively.

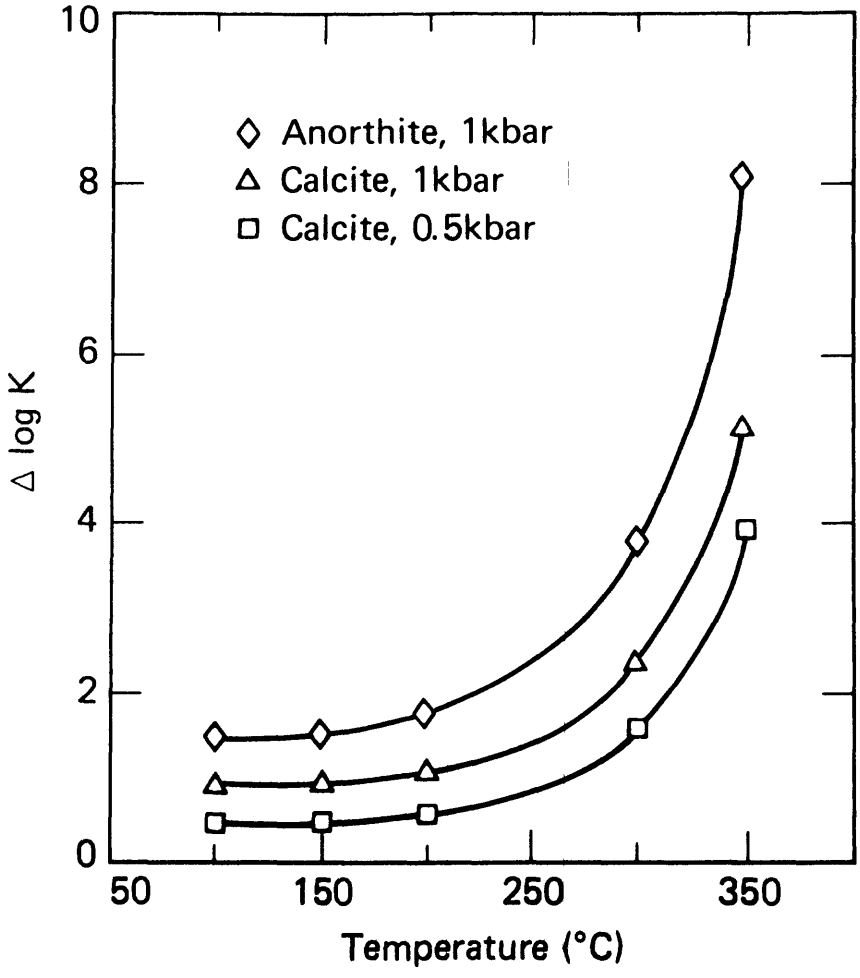

Figure 2. -- Effects of pressure on the solubilities of calcite and anorthite. Note that the difference between the solubilities of minerals at higher pressure and at vapor pressure of water (Δ log K) becomes very large at temperatures higher than about 200°C (Kharaka and others, 1985).

Correction of Dissociation Constants for Pressure

Values for the partial molal volume of most aqueous complexes are not available at high temperatures and pressures and, therefore, equation (54) can not be used to calculate K values at higher pressures. The pressure dependence of K for aqueous complexes in SOLMINEQ.88 is obtained by the method of Marshall and Mesmer (1981), in which K at pressure P is given by:

$$\ln K(P) = \ln K(S) - \frac{\Delta V(T)}{RT\,\beta} \ln \left(\frac{\rho(P)}{\rho(S)}\right) \quad , \tag{59}$$

where K(S) is the value of K at saturation water pressure and ρ is either the density of water at pressure (P) or at saturation vapor pressure of water (S); β is the coefficient of isothermal compressibility of water at temperature T; and $\Delta V(T)$ is the volume change of the dissociation reaction at temperature T and pressure S. It has been observed that the heat capacity and, by analogy, ΔV of "isocoulombic" reactions (reactions which are symmetrical with respect to the number of ions of each charge type) is nearly independent of temperature (Lindsay, 1980; Murray and Cobble, 1980). Thus, Equation (59) can be used with the 25 °C value of ΔV if the reaction is "isocoulombic", or is made so by the addition or subtraction of the dissociation reaction for water. For example, the dissociation reaction of the aqueous complex $H_2CO_3^o$:

$$H_2CO_3^o = HCO_3^- + H^+ \tag{8}$$

can be written in the isocoulombic form as:

$$H_2CO_3^o + OH^- = HCO_3^- + H_2O \tag{9}$$

by combining reaction (8) with the ionization reaction of water

$$H_2O = H^+ + OH^- \quad . \tag{10}$$

The equilibrium constant at higher pressures for (8) can be obtained from

$$\ln K_8(P) = \ln K_9(P) + \ln K_{10}(P) \quad , \tag{60}$$

and

$$\ln K_9(P)_T = \ln K_9(S)_T - \frac{n}{RT\beta} \ln \left(\frac{\rho(P)}{\rho(S)}\right) \quad , \tag{61}$$

where $n = \Delta V_8(S) - \Delta V_{10}(S)$ at 25 °C.

Values of $\Delta V_{10}(S)$ and of K_{10} at higher temperatures and pressures are well known and are incorporated in SOLMINEQ.88. Values of ΔV for dissociation

reactions even at 25 °C and saturation pressure are poorly known; however, they can be estimated from methods based on the electrostatic theory (Hemmes, 1972; Hemmes' method is based on the Fuoss (1958) equation), or empirical correlations (Millero, 1972; Swaddle and Mak, 1983). The ΔV values of dissociation reactions for 48 complexes used in SOLMINEQ.88 have been obtained either from available experimental data, or by estimation based on one of the above methods. They are tabulated in Appendix IF together with the number of water ionization reactions that must be added to convert the dissociation reaction or the complex to an "isocoulombic" form. The specific equations used to generate the data in Appendix IF and the original sources are detailed by Aggarwal and others (1989).

The dissociation constants generally increase with increasing pressures leading to an increase in the activity of the dissociated species and a decrease in the activity of the complexes. The increases are relatively high for the complexes of carbonate, bisulfide, ammonium and acetate species. The increase in the activity of dissociated species when the pressure effects are taken into account generally leads to reduced solubility products for minerals. In the case of calcite, for example, the increase in solubility shown in Figure 2 are reduced by more than a factor of 2 when the pressure effects on the dissociation of carbonate and calcium complexes are taken into account (see Aggarwal and others, 1989, for more details).

MODELING OPTIONS

SOLMINEQ.88 uses the chemical analysis of an aqueous fluid to calculate speciation-solubility relations at a given temperature and the vapor pressure of water or at a higher temperature and pressure with (1) a constant mass or with (2) a transfer of mass (Figure 3). The mass transfer options include:

(a) addition of the gases, CO_2, H_2S, NH_3, CH_4, which may have been lost prior to pH measurement,

(b) partitioning of the gases CO_2, H_2S, and CH_4 between water, oil and/or gas phases,

(c) mixing with a second solution,

(d) dissolution/precipitation of a given amount of a mineral; this may be continued to saturation with this or another mineral,

(e) addition or subtraction of a given amount of one or more components of solution; this may be continued to saturation with a selected mineral,

(f) boiling (formation of steam coupled with loss of volatiles into the steam), and

(e) ion exchange and adsorption.

Calculations with a Constant Mass

The calculations with a constant mass can be carried out at a given temperature as well as at the subsurface (or experimental) temperature. These calculations can be performed with six options: (i) carbon; (ii) high-temperature carbon; (iii) pH; (iv) one or two additional (user defined) anions; (v) one additional cation; and (vi) one to five additional minerals.

Carbon Option

At a given pH, the distribution of carbonate species requires a value for any one of the following: (i) total inorganic carbon (TIC); (ii) bicarbonate and/or carbonate alkalinity (ALK); or (iii) total alkalinity (ALKTOT).

TIC, the sum of the concentrations of all aqueous species of inorganic carbon, is given as:

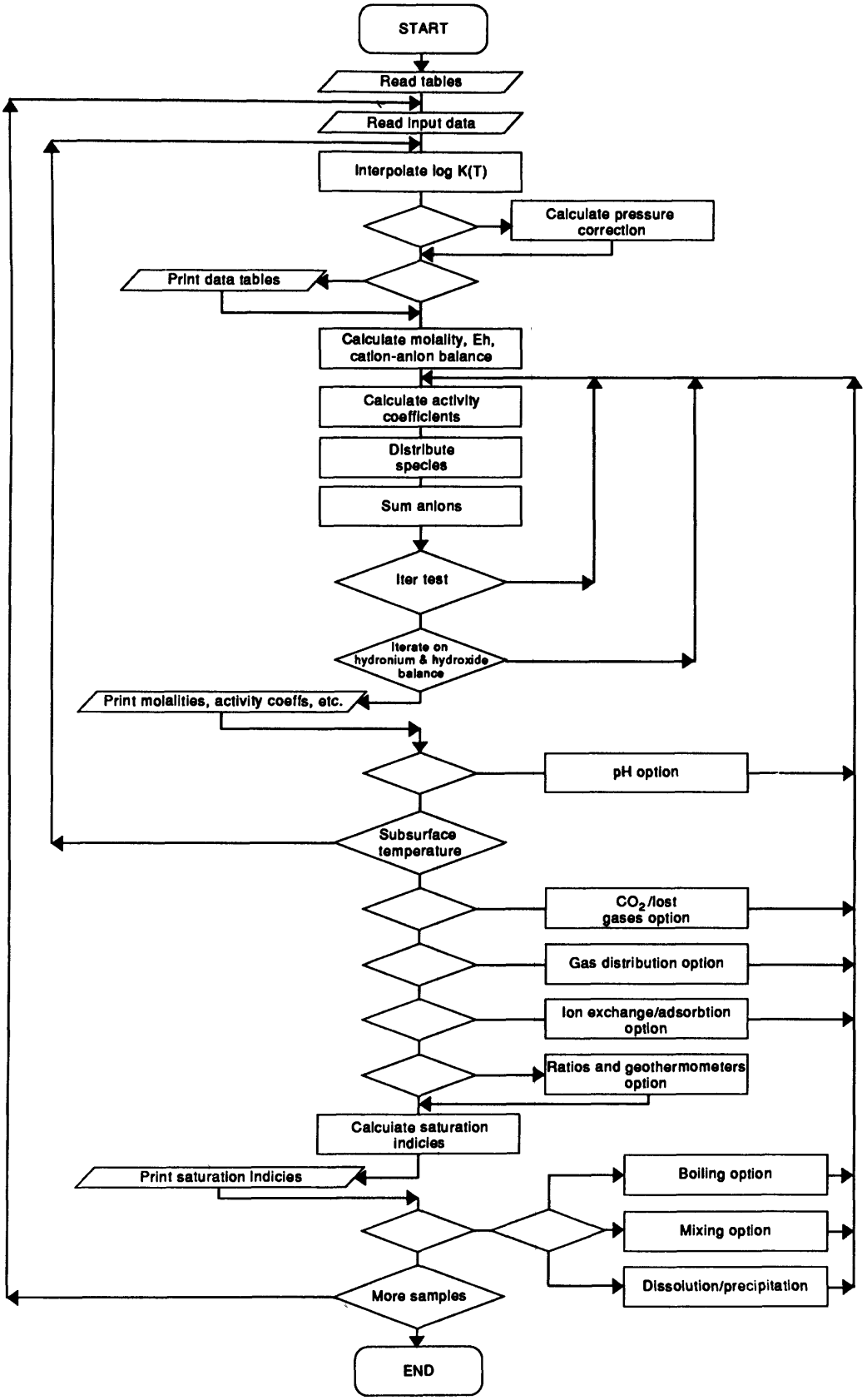

Figure 3. -- Flow Chart for SOLMINEQ.88

$$m_{TIC} = m_{H_2CO_3^o} + \Sigma\, m_{HCO_3^-} + \Sigma\, m_{CO_3^{--}} \quad , \tag{62}$$

where the summation covers the species and complexes of the summed species. ALK, the sum of the equivalents contributed to the alkalinity titration analysis by all the bicarbonate and carbonate species, is given as:

$$ALK = \Sigma\, m_{HCO_3^-} + \Sigma\, 2m_{CO_3^{--}} \quad . \tag{63}$$

ALKTOT specifies that in addition to HCO_3^- and CO_3^{--} species, other inorganic and organic species (e.g., $Al(OH)_4^-$, $Ba(OH)^+$, CH_3COO^-) were also titrated during the alkalinity determination, and is given as:

$$ALKTOT = \Sigma\, m_{HCO_3^-} + \Sigma\, 2m_{CO_3^{--}} + \Sigma\, m_{CH_3COO^-} + m_{BaOH^+} + \ldots \quad . \tag{64}$$

The carbon option in SOLMINEQ.88 is used to specify the criterion (TIC, ALK, or ALKTOT) for the distribution of carbonate species. The choice of any one of these criteria depends on the nature of the chemical analysis available. The other two are calculated and all three are printed in the output.

High-Temperature Carbon Option

When a value for TIC is available, the distribution of carbonate species at a higher temperature is performed with a constant TIC. However, if a value for only ALK or ALKTOT is available, two alternatives exist for the distribution of carbonate species at high temperature: (a) constant alkalinity (ALK or ALKTOT) or (b) constant TIC. The value of TIC used at high temperature is calculated at the end of the low-temperature species distribution. If the high temperature calculations are carried out with a constant alkalinity, the resulting value of TIC in the solution may be significantly different from that at the low temperature because of the shift in carbonate equilibria with temperature. Similarly, a constant TIC at high temperature may result in a change in the value of calculated alkalinity.

pH Option

This option is most useful when the pH of the solution was not determined or may be in error, and the water is known to have been in equilibrium with a carbonate mineral. Formation water in reservoir rocks are often in equilibrium with calcite at depth; thus, this option can be used to calculate

the pH of this water. If it is known that the solution was in equilibrium with calcite, dolomite or siderite, then SOLMINEQ.88 will adjust the pH of the solution until log(AP/K) of the specified mineral is less than or equal to 0.05 (or to a value defined by the user = FSAT).

The equilibrium pH is guessed by SOLMINEQ.88, the distribution species is calculated, and the saturation index (SI) of the desired mineral is calculated. The SI is calculated in terms of the most abundant species of CO_2, that is, the SI will be calculated according to one of the following reactions:

$$MCO_{3(s)} + 2H^+ \rightleftarrows M^{++} + H_2CO_3^o \quad , \tag{11}$$

$$MCO_{3(s)} + H^+ \rightleftarrows M^{++} + HCO_3^- \quad , \tag{12}$$

$$MCO_{3(s)} \rightleftarrows M^{++} + CO_3^{--} \quad , \tag{13}$$

where MCO_3 (s) is either of the carbonate minerals, calcite or siderite, and M is Ca^{++} or Fe^{++}, respectively. If saturation with dolomite is specified; reaction (11), for example, is written as

$$CaMg(CO_3)_2 + 4H^+ \rightleftarrows Ca^{++} + Mg^{++} + 2H_2CO_3^o \quad . \tag{14}$$

If the SI is not within the tolerance limit (0.05 log units or a value defined by the user), the pH is adjusted. The initial adjustment is determined through the use of reaction (11), (12), or (13). Subsequent adjustments increase either the size or direction of the pH step until the SI sign changes. Once this occurs, an interpolating polynomial in SI and pH is repeatedly used to obtain new values until the FSAT criterion is satisfied. Mineral saturation using the pH option is attempted within the pH limits of 0.0 and 14.0. The pH option is calculated after the initial distribution of species, and before the "HITEMP" calculation.

Additional Anions Option

SOLMINEQ.88 is particularly useful for modeling water-rock interactions in sedimentary basins where aqueous organic species may be present at high concentrations (up to 10,000 mg/L) (Figure 4) and can play an important role in these interactions. The total number of possible aqueous organic species is extremely large and it is not possible or even useful to incorporate all of them in this code. However, recent work (Carothers and Kharaka, 1978; Kharaka and others, 1986; Lundegard and Land, 1986; MacGowan and Surdam, 1988) has

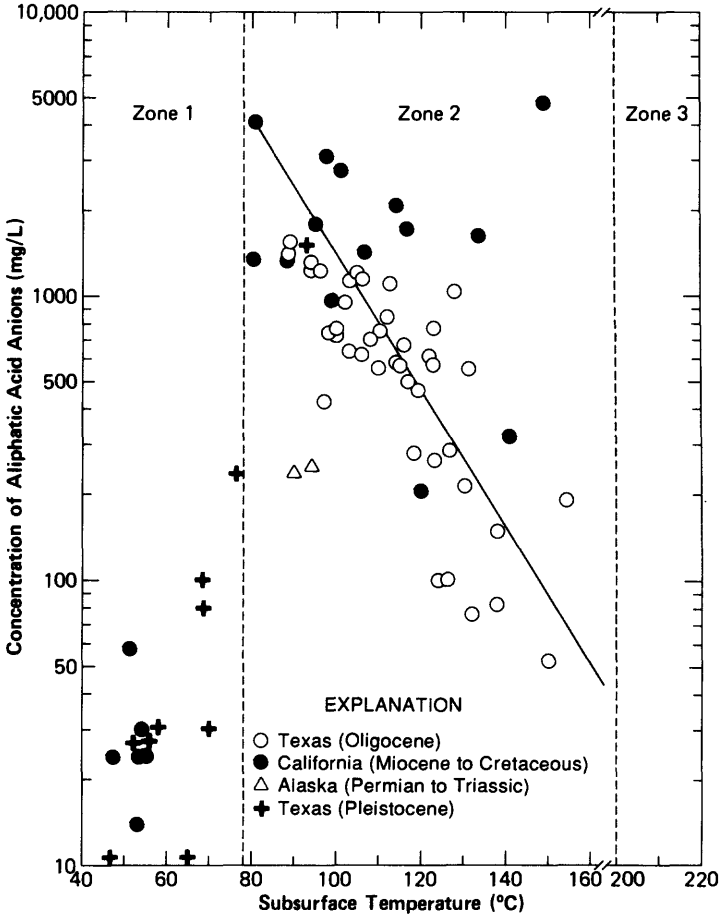

Figure 4. -- Distribution of organic species in oil field waters from United States of America. Note that the highest concentrations are in waters from reservoirs at temperatures of 80°C to 100°C.

shown that acetate, oxalate and succinate are the dominant organic species in oil field waters. These ligands and their complexes are incorporated in the code.

SOLMINEQ.88 has an option to add two user-defined organic ligands to the above three. This option is included because a total of five organic ligands is probably adequate to examine the role of organics on inorganic interactions in any natural-water system. The number of organic ligands examined can be increased as desired by making several runs of the program with the same input except for changing the list of the user-defined organic ligands in each run. This option has also been included because it is anticipated that potentially important new aqueous organics will be discovered in natural waters as better methods of sample preservation and analysis are used (Kharaka and others, 1986) and as more systems are studied.

The equations necessary for distribution of these user-defined ligands and their complexes with 14 inorganic cations are incorporated in SOLMINEQ.88. These ligands and their complexes are already included in the equations that compute titrated alkalinity and total hydronium. The ligands can have a charge of -1 to -4. Table 5 gives the identification number and the list of possible cations that may form complexes with these ligands. The dissociation constant for each complex must be supplied by the user. Otherwise, the complexes are treated as being unstable. In the case of Na-Anion #1, for example, the dissociation reaction, assuming Z charge for the ligand, is

$$\text{Na-Anion \#1}^{(1-Z)} \rightleftarrows \text{Na}^{+} + \text{Anion \#1}^{Z} \qquad (15)$$

The input subroutine to this code (see INPUT) prompts the user to provide the dissociation constants and other data necessary to implement this option.

Additional Cation Option

This option allows the user to study speciation-saturation states of one (during any one simulation) user-defined cation that is not in SOLMINEQ.88. As in the case of additional anions, all the equations necessary for the distribution of this cation and its complexes with all the anions (including the user defined anions) in the code are incorporated in SOLMINEQ.88. Again, the input subroutine to this code prompts the user to provide the dissociations constants and other data necessary to implement this option.

Table 5 Index numbers of user-defined anions and cations and their complexes

1)	Anion#1	Anion#2	Cation
2)	H^+ - Anion#1	H^+ - Anion#2	Cation - Cl^-
3)	$2H^+$ - Anion#1	$2H^+$ - Anion#2	Cation - SO_4^{--}
4)	Al^{+3} - Anion#1	Al^{+3} - Anion#2	Cation - HCO_3^-
5)	Ba^{++} - Anion#1	Ba^{++} - Anion#2	Cation - OH^-
6)	Ca^{++} - Anion#1	Ca^{++} - Anion#2	Cation - PO_4^{-3}
7)	Cu^+ - Anion#1	Cu^+ - Anion#2	Cation - F^-
8)	Fe^{++} - Anion#1	Fe^{++} - Anion#2	Cation - CH_3COO^-
9)	K^+ - Anion#1	K^+ - Anion#2	Cation - CO_3^{--}
10)	Mg^{++} - Anion#1	Mg^{++} - Anion#2	Cation - HS^-
11)	Mn^{++} - Anion#1	Mn^{++} - Anion#2	Cation - $C_2O_4^{--}$
12)	Na^+ - Anion#1	Na^+ - Anion#2	Cation - $C_4H_4O_4^{--}$
13)	Pb^{++} - Anion#1	Pb^{++} - Anion#2	Cation - Anion#1
14)	Sr^{++} - Anion#1	Sr^{++} - Anion#2	Cation - Anion#2
15)	Zn^{++} - Anion#1	Zn^{++} - Anion#2	

Additional Minerals Option

SOLMINEQ.88 has 220 minerals in its data base. This number can be increased as this option allows the user to include up to five new minerals during any simulation. This option also can be used to input data for minerals present in the code in order to investigate the geochemical implications of using solubility constants that are different from those in the existing data base. This option should prove particularly useful in the study of the interactions of minerals with variable chemical composition (solid solutions). If the solubility constants for the end members are available in Appendix IC, the user can calculate the solubility of the impure phase assuming ideal mixing, then use the calculated values in the input for this option. The solubility constant for an ideal binary solid solution (K_i) is given by:

$$\log K_i = X\log K_1 + (1-X)\log K_2 + X\log X + (1-X)\log(1-X) \qquad (65)$$

where K_1 and K_2 are the solubility constants for the end-member minerals and X and (1-X) are the mole fractions of these end members in the phase. Most solid solutions, it should be noted, require a more rigorous treatment and additional parameters to calculate their solubility constants (Navrotsky, 1987).

The reactions for the congruent dissolution of optional minerals are completely general and may involve up to eight of the aqueous species in Table 6 together with a numerical constant. The numerical constant is included in the solubility reaction to simulate the effects of one or more aqueous species not present in Table 6 or in the user defined anions or cation. The input subroutine to SOLMINEQ.88 prompts the user to provide the solubility constants and the aqueous species and their stoichiometry to implement this option.

Calculations Involving Mass Transfer

Addition of Lost Gases

During sampling of subsurface fluids, volatiles (including CO_2, H_2S, NH_3, and CH_4) may be lost before the solution pH is measured. These gases can have a significant impact on the calculated, in-situ pH of the solution and must be included in the analyzed composition of the fluid. Three options are available in SOLMINEQ.88 which can be used for titrating the lost gases back into the solution (Figure 5): (a) gas-water option, (b) gas-water-oil option, and (c) CO_2 option.

(a) Gas-Water Option: this option is used when the amount of lost gases is known. The amount of a gas lost is added to the total concentration of its constituent component in the water and an equivalent amount is added to the summation of hydronium ions in the water as:

$$TIC = TIC + m_{CO_2\ (lost)} \tag{66}$$

$$m_{H_2S,t} = m_{H_2S,t} + m_{H_2S\ (lost)} \tag{67}$$

$$m_{NH_3,t} = m_{NH_3,t} + m_{NH_3\ (lost)} \tag{68}$$

and

$$(\Sigma m_{H_f^+} - \Sigma m_{OH_f^-}) = (\Sigma m_{H_i^+} - \Sigma m_{OH_i^-}) + 2m_{CO_2} + 2m_{H_2S} - m_{NH_3} \tag{69}$$

where the final (f) and initial (i) summations cover all the species with H^+ and OH^-. Methane, of course, does not affect the hydronium balance.

(b) Gas-Water-Oil Distribution Option: samples of oil-field waters for chemical analysis are generally collected after they have been separated from the oil phase. During the separation process, a gas phase (commonly containing CO_2 and CH_4, but sometimes with H_2S) is also produced which may consist of gases derived from one or more of the three subsurface phases: oil, water, and natural gas. Because dissolved CO_2 gas has a significant impact on the in situ pH of the water, it is important to know the distribution of gas between the three phases in the in situ environment. The Gas-Water-Oil distribution option in SOLMINEQ.88 has been designed to perform such calculations. The necessary equations for equilibrium distribution of gases between oil (o),

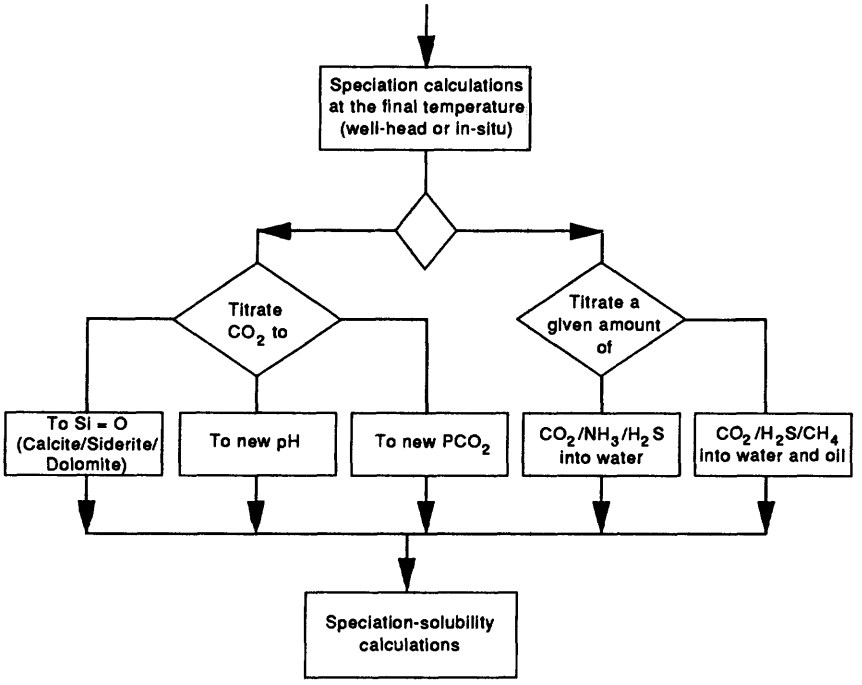

Figure 5. -- Flow chart for calculations with addition of gases to water and oil.

water (w), and natural gas (g) are as follows:

$$k_{CO_2,w} = \frac{P_{CO_2}}{m_{CO_2,w}} \; ; \; k_{CH_4,w} = \frac{P_{CH_4}}{m_{CH_4,w}} \; ; \; k_{H_2S,w} = \frac{P_{H_2S}}{m_{H_2S,w}} \quad , \tag{70}$$

$$k_{CO_2,o} = \frac{P_{CO_2}}{m_{CO_2,o}}; \; k_{CH_4,o} = \frac{P_{CH_4}}{m_{CH_4,o}}; \; k_{H_2S,o} = \frac{P_{H_2S}}{m_{H_2S,o}} \quad , \tag{71}$$

$$M_{CO_2,t} = Cm_{CO_2,o} + m_{CO_2,w} + M_{CO_2,g} \quad , \tag{72}$$

$$M_{CH_4,t} = Cm_{CH_4,o} + m_{CH_4,w} + M_{CH_4,g} \quad , \tag{73}$$

$$M_{H_2S,t} = Cm_{H_2S,o} + m_{H_2S,w} + M_{H_2S,g} \quad , \tag{74}$$

$$C = \frac{W_o}{W_w} \quad , \tag{75}$$

$$\frac{M_{CO_2,g}}{P_{CO_2}} = \frac{M_{CH_4,g}}{P_{CH_4}} = \frac{M_{H_2S,g}}{P_{H_2S}} = \frac{M_{H_2O,g}}{P_{H_2O}} \quad , \tag{76}$$

$$P_t = P_{CH_4} + P_{CO_2} + P_{H_2S} + P_{H_2O} \quad , \tag{77}$$

where k is the Henry's law coefficient for the solubility of the subscripted gas in water or oil, m is the molality, M is total moles of a gas, C is the weight ratio of oil (W_o) to water (W_w), and P_t is the reservoir pressure. Note that the Henry's law coefficients are expressed in the molality convention (moles of gas/Kg of water or oil) and not in the mole fraction convention (moles of gas/mole of fluid) because the term mole cannot be applied to oil which is a heterogeneous mixture of many compounds. The above equations are derived with the assumption that all gases (CO_2, CH_4, H_2S, H_2O), and their mixtures, behave as ideal gases (i.e., fugacity coefficients = 1).

The Henry's law constants for the water phase are calculated from Drummond's (1981) equations described in the section on the activity coefficients of neutral species. For the oil phase, the constants must be obtained and entered by the user. The user can calculate the Henry's law constants for oil (density range of 0.63 to 0.90 g/cm^3) using the data (Figure 6) and equations summarized by ASTM (1985) and reported in Beerbower (1980). The density of oil at 15 °C (≈60 °F) in kg/L or its API gravity at 15 °C must be known by the user.

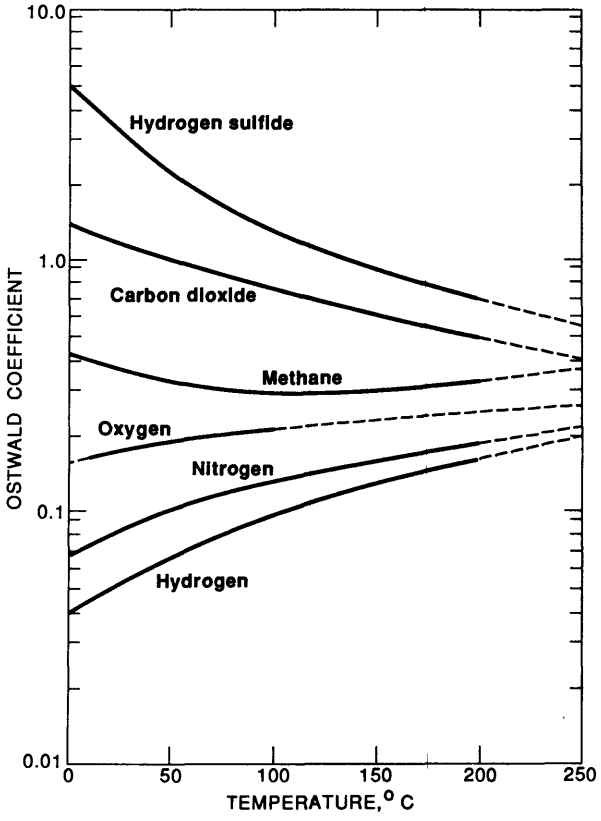

Figure 6. -- Solubility constants of selected gases in oil (density = 0.85 g/ml at 15°C) modified from ASTM (1985)

Water samples are commonly collected from the test separator. If the separator pressure is greater than 1 atmosphere some dissolved gas will be lost during water sampling. To compensate for this, an additional SOLMINEQ.88 run must be made to equilibrate the water with the separator gas phase at the separator pressure by titrating CO_2, H_2S and CH_4 back in. The concentrations of CO_2, H_2S and CH_4 in the water must be calculated from equations (70-77). The CO_2 and H_2S options are then used to equilibrate the separator water at the separator pressure for the separator P_{CO_2} and P_{H_2S}. The user must then enter the modified $m_{H_2S,w}$, $m_{CH_4,w}$, TIC and pH into SOLMINEQ.88, and activates the water-oil-gas distribution option which calculates the distribution of gases at reservoir pressure and temperature assuming that the gas phase in the separator was derived from only two phases, water and oil. If this assumption leads to the condition

$$P_{CH_4} + P_{CO_2} + P_{H_2S} + P_{H_2O} > P_t \quad , \tag{78}$$

then the third phase, vapor, is included in the distribution calculations. Once the pH and the distribution of the aqueous species are determined, SOLMINEQ.88 calculates the concentration of the volatiles in the water, oil, and vapor phases by simultaneously solving equations (70) to (77). At this point a check is made on the mass balance of the volatiles (including all their aqueous complexes). If not satisfied, the TIC, total H_2S and/or total CH_4 in the water are adjusted in the correct direction. A new pH and distribution of species is calculated. This cycle is repeated until mass balance is achieved.

(c) CO_2 Saturation Option: this option can be used for a variety of field and experimental conditions. In many cases, the amount of CO_2 lost from a subsurface fluid is not correctly known. However, it may be known that the fluid was in equilibrium with calcite, dolomite, or siderite. The CO_2 option can be used to determine the amount of CO_2 required to achieve saturation with the specified mineral and thus the subsurface pH of the solution. Another use of the CO_2 option is in the case of certain experiments where the amount of CO_2 exsolved between two pH measurements is not known; the CO_2 option can be used to determine the amount of CO_2 lost. A third use of the CO_2 option is in

calculating the pH and distribution of species in experimental solutions where the experiments were carried out at a constant P_{CO_2}. In some such cases, the pH of the solutions cannot be measured at the imposed pressure of CO_2. However, it can be calculated using the CO_2-option to achieve a specified P_{CO_2} or $m_{H_2CO_3}$ in solution.

The algorithm used for the CO_2 option is similar to that used in the pH option. The equilibrium test (FSAT) is formulated as one of the following relationships:

$$FSAT = pH_{(desired)} - pH_{(calculated)} \quad (79)$$

or

$$FSAT = m_{H_2CO_3\,(desired)} - m_{H_2CO_3(calculated)} \quad (80)$$

or

$$FSAT = P_{CO_2(desired)} - P_{CO_2(calculated)} \quad (81)$$

or

$$FSAT = \text{Saturation Index (SI) (calcite/siderite/dolomite)} \quad . \quad (82)$$

The saturation index of one of the carbonate minerals is calculated using the most abundant species of CO_2, as discussed earlier in the pH option.

CO_2 is incremented, species distribution is recalculated and convergence is achieved in the aqueous model and on hydronium mass-balance. If the absolute value of FSAT is increasing, the step size or direction is modified such that the absolute value of FSAT decreases. Once the absolute value of FSAT is decreasing, step size is increased until FSAT changes sign. The value of FSAT and total CO_2 are then fit with a polynomial in order to interpolate to a new value of FSAT. This process is continued until FSAT is less than the user defined limit (default value = 0.05 log units).

Boiling Option

SOLMINEQ.88 may be used to predict the changes in solution composition and the saturation states of minerals as a consequence of boiling. There are two major effects of boiling:

1. Loss of steam.
2. Loss of gases such as CO_2, H_2S, and NH_3.

The loss of steam can be simulated by subtracting pure water of neutral pH from the solution. This is accomplished by multiplying the molality of each of the species and ($\Sigma m_{H^+} - \Sigma m_{OH^-}$) by the factor 1/(1 - X) where X is the fraction of water removed by boiling; and is given by

$$X = \frac{W_{H_2O,v}}{W_{H_2O,t}} = \frac{n_{H_2O,v}}{n_{H_2O,\ell} + n_{H_2O,v}} \quad , \tag{83}$$

where n = is the number of moles and W = the weight of water in the vapor (v), liquid (ℓ), and total (t) system, respectively.

If the P-V-T relationships of all the gases are known, the amount of each gas lost due to boiling can be calculated. The partitioning of volatiles CO_2, CH_4, NH_3, and H_2S is calculated following Drummond (1981) by making use of the volatility ratio, VR. For example, VR for CO_2 is calculated from:

$$VR_{CO_2} = \frac{55.51\ k_H\ \bar{V}^v_{H_2O}}{\chi_{CO_2} Z_{CO_2}\ R\ T} \quad , \tag{84}$$

where k_H is the Henry's Law constant given by $\frac{f_{CO_2}}{m_{CO_2}}$,

and $\bar{V}^v_{H_2O}$ is the specific volume of water vapor, and χ and Z are the fugacity coefficient and compressibility factor of CO_2, respectively. In the calculation, the product χZ is set equal to 1.0 which is a reasonable assumption at relatively low pressures. The VR is defined by:

$$VR_{CO_2} = \frac{n^v_{CO_2}}{n^\ell_{CO_2}} \cdot \frac{n^\ell_{H_2O}}{n^v_{H_2O}} = \frac{n^v_{CO_2}}{n^\ell_{CO_2}} \cdot \frac{(1-X)}{X} \quad , \tag{85}$$

where n = number of moles of CO_2 or H_2O. Normalizing to 1000 grams of H_2O (i.e., assuming that 1,000 grams of H_2O are present in each of the liquid and vapor phases), equation (85) becomes:

$$VR = \frac{m^v_{CO_2}}{m^\ell_{CO_2}} \quad , \tag{86}$$

where m is molality.

The boiling calculation is based on a system containing 1000 grams of water. Therefore the mass balance equation for CO_2 becomes

$$m^{\ell,i}_{CO_2} = n^{\ell,i}_{CO_2} = n^\ell_{CO_2} + n^v_{CO_2} \quad , \tag{87}$$

where the superscript i refers to the molality or number of moles before any boiling occurs. For a given fraction of water, X, removed by boiling, equation (85) may be combined with equation (87) to give:

$$n^v_{CO_2} = \frac{m^{\ell,i}_{CO_2} VR_{CO_2}}{VR_{CO_2} + \frac{(1-X)}{X}} \quad . \tag{88}$$

SOLMINEQ.88 solves for the partitioning of volatiles by estimating from equation (88) the amount lost to vapor. Because the effect of a change in pH is to increase or decrease the amount of $n^\ell_{CO_2}$ or $n^\ell_{NH_3}$ by reactions such as:

$$HCO_3^- + H^+ = CO_2 + H_2O \quad , \tag{16}$$

and

$$NH_4^+ + OH^- = NH_3 + H_2O \quad , \tag{17}$$

SOLMINEQ.88 then utilizes an iterative scheme by increasing or decreasing the total concentration of the volatile components in water (i.e. TIC); calculating the new pH and aqueous species distribution; and repartitioning the volatiles between vapor and liquid until the mass balance for volatiles in both phases (including all aqueous species) is achieved.

Mixing of Two Solutions Option

SOLMINEQ.88 has an option to mix two solutions in specified proportions (by weight) at constant or varying temperature. Mixing is performed based on analytical molalities. The mass-balance criteria for the mixture are formulated as follows:

$$\Sigma m_i \text{ (mixture)} = X_1 \Sigma m_{i,1} + X_2 \Sigma m_{i,2} \quad , \tag{89}$$

$$(\Sigma m_{H^+} - \Sigma m_{OH^-})\text{mixture} = X_1(\Sigma m_{H^+} - \Sigma m_{OH^-})_1 + X_2(\Sigma m_{H^+} - \Sigma m_{OH^-})_2 \quad , \tag{90}$$

where m_i is the analytical molality of the species of the ith element and X_1 and X_2 are the proportion of water (by weight) in which solutions 1 and 2 are to be mixed. The carbon mass-balance in the mixture is carried out using the TIC option.

Dissolution/Precipitation Option

The dissolution/precipitation option in SOLMINEQ.88 can be used to carry out the reactions listed below.

1-Dissolve/precipitate a given amount of mineral;

2-dissolve/precipitate a mineral to saturation;

3-dissolve/precipitate a mineral to saturation with an other mineral;

4-add/subtract aqueous components to saturation with a mineral; and

5-add/subtract components from a congruent, incongruent, or net reaction. Reaction may follow a kinetic rate law.

This option allows the user to titrate in (or out) a specified amount of aqueous components (see Table 6) (or of a titrant mineral) to (or from) the aqueous solution. The amount to be titrated may be specified by the user in moles of component per kilogram of solution. Alternatively, the amount may be determined by adding or subtracting the aqueous components (see Table 6) (or titrant mineral) until saturation is reached with any of the 214 minerals in the database of SOLMINEQ.88.

If a mineral is specified to be dissolved/precipitated, equilibration is achieved by dissolving (if the titrant mineral is undersaturated) or precipitating (if the titrant mineral is supersaturated) the titrant mineral. A series of reaction steps (i.e., moles of components or titrant mineral), initially based on the concentration of the least abundant component of the

Table 6 List of aqueous species components

No.	Species	No.	Species	No.	Species
1	Ca^{++}	2	Mg^{++}	3	Na^{+}
4	K^{+}	5	Cl^{-}	6	SO_4^{--}
7	HCO_3^{-}	8	H^{+}	9	OH^{-}
10	H_2O	12	$SiO_2(aq)$	13	Ag^{+}
14	Al^{+3}	15	Ba^{++}	16	Cu^{+}
18	Fe^{++}	21	Hg^{++}	22	Li^{+}
23	Mn^{++}	25	Pb^{++}	26	Sr^{++}
27	Zn^{++}	28	$H_2AsO_3^{-}$	29	PO_4^{-3}
30	F^{-}	31	$H_3BO_3(aq)$	32	$NH_3(aq)$
33	$H_2S(aq)$	48	CH_3COO^{-}	98	CO_3^{--}
136	NO_3^{-}	169	UO_2^{++}	210	VO_4^{-3}
246	$C_2O_4^{--}$	265	$C_4H_4O_4^{--}$	285	$CH_4(aq)$

The species numbers in the input refer to the index number of selected species in the data file which are organized above. The species (with the exception of H^{+} and OH^{-}) are those normally entered in the input data file for SOLMINEQ.88, and are the only species allowed to be used in the dissolution/precipitation options and ion exchange/adsorption options. For the ion exchange/adsorption options, vacant surface site is assigned the number zero. Presently moles of H_2O is fixed in the program at 1 kilogram.

mineral to be saturated and its degree of departure from equilibrium (eg. saturation index, SI), are executed in order to find an interval where the SI changes its sign. An interpolating polynomial technique is then used to find the amount of mineral to be dissolved/precipitated for which SI is sufficiently close to zero.

It is not always possible to achieve saturation with a mineral. Suppose the user wished to dissolve/precipitate gibbsite to reach saturation with kaolinite. If the SI of gibbsite is negative, it can only be dissolved. Dissolving gibbsite will increase the SI of kaolinite. If the SI of kaolinite is already positive, it will steadily increase as more gibbsite is dissolved into the aqueous phase. Clearly the SI of the kaolinite must be negative in order to reach a possible solution.

A mixture or solid which is not in the database can be titrated in and out by specifying its components (listed in Table 6). In this way a congruent or incongruent reaction can be followed. The reaction may be a simple one involving one or two minerals and aqueous components; or it may be the sum of several reactions (a net reaction) involving several minerals and aqueous components. The simple or net reaction may follow a rate law (user defined) which allows the knowledgeable user to compute changes in composition through time and/or space. The mass-balance criteria are formulated as:

$$\Sigma m_{i,t} = \Sigma(m_{i,soln} + Am_{i,j}) \quad , \tag{91}$$

$$(\Sigma m_{H^+} - \Sigma m_{OH^-})_t = (\Sigma m_{H^+} - \Sigma m_{OH^-})_{soln} + (\Sigma m_{H^+} - \Sigma m_{OH^-})_{added} \quad , \tag{92}$$

where m_i is the analytical molality of the species of the i^{th} element. $Am_{i,j}$ is the molality of the jth species of i^{th} element to be added to the solution. To illustrate the use of this option for a congruent reaction of a mineral not in the database, let us consider the dissolution of one mole of clinochlore ($Mg_5Al_2Si_3O_{10}(OH)_{8(s)}$) according to the reaction:

$$Mg_5Al_2Si_3O_{10}(OH)_{8(s)} + 16H^+ = 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4^o + 6H_2O \quad . \tag{18}$$

For every mole of clinochlore dissolved, 5 moles of Mg, 2 moles of Al, and 3 moles of silica will be released and 16 moles of hydronium will be

consumed. The net hydronium balance of the solution will be decreased by only 4 moles of hydronium because $H_4SiO_4^o$ is included in the hydronium summation. Thus, the mixture would have the following constraints on the mass-balance that will be different from the original solution:

$$m_{Al,t} = m_{Al,soln} + 2 \quad , \tag{93}$$

$$m_{Mg,t} = m_{Mg,soln} + 5 \quad , \tag{94}$$

$$m_{Si,t} = m_{Si,soln} + 3 \quad , \tag{95}$$

$$(\Sigma m_{H^+} - \Sigma m_{OH^-})_t = (\Sigma m_{H^+} - \Sigma m_{OH^-})_{soln} - 4 \quad . \tag{96}$$

Note that the hydronium balance is decreased only by 4 because 12 of the 16 moles of hydronium lost will be added back by $H_4SiO_4^o$.

If a mineral in the database is specified, SOLMINEQ.88 automatically determines the component stoichiometry to be added to the solution, saving time for the user.

Ion Exchange and Adsorption Option

Surface chemical processes can be simulated in SOLMINEQ.88 using two models: ion exchange and a preliminary adsorption option. The ion exchange model treats the exchange of cations or anions on a constant charge surface; the adsorption model simulates the exchange process on a surface where the surface charge is developed due to the ionization of surface sites at the solution-surface interface. The major distinction between the two models is in the treatment of the activity of aqueous species on the surface. In the ion-exchange model, the surface activity of aqueous species is considered to be the same as in the bulk solution. For the adsorption model, an electrical potential term is used to calculate the surface activity from the activity of the species in the bulk solution. Excellent discussions of the ion exchange and adsorption processes are given in several references (Hohl and others, 1980; Westall, 1980; Westall and Hohl, 1980; Bolt, 1982; James and Parks, 1982; Sposito, 1982) and the user should read these articles to understand the limitations inherent in modeling surface chemical processes and to obtain values for the selectivity constants to be used for modeling.

The ion exchange and adsorption models in SOLMINEQ.88 are completely general and can be used to simulate the interaction of any of the aqueous

species in the data file (Appendix IA) through the use of the appropriate components (Table 6). A maximum of 10 aqueous species (components) may be selected for each run to interact with a single surface of constant or varying charge. It is assumed that the activity coefficients of surface functional groups (X or SO^-) and surface species (e.g. NaX or SONa) are equal to one. The ion exchange process, for example for a surface with no vacant sites and of constant charge exchanging with Na, Ca, and K, is given by the following reactions:

$$Na^+ + KX = K^+ + NaX \quad , \tag{19}$$

$$2Na^+ + CaX_2 = Ca^{++} + 2NaX \quad , \tag{20}$$

where X represents a surface site. These would be specified to SOLMINEQ.88 using the following three association reactions:

$$X^- + Na^+ = NaX \quad , \tag{21}$$

$$X^- + K^+ = KX \quad , \tag{22}$$

$$2X^- + Ca^{++} = CaX_2 \quad . \tag{23}$$

The cation exchange capacity (CEC) is the sum given by:

$$CEC = NaX + KX + 2CaX_2 \quad , \tag{97}$$

and is expressed in meq/kg of the solvent. The CEC is given by:

$$CEC\ (meq/kg) = \frac{A_T \cdot N_S \cdot 1000}{N_A} \quad , \tag{98}$$

where A_T is total area of the exchanging surface per kg of water, N_S is the number of sites per unit area of the surface, and N_A is Avogadro's number. The equilibrium constants for reactions (21), (22), and (23) must sum to the equilibrium constants for reactions (19) and (20). They can be combined with equation (98) to solve for the concentration of surface and aqueous species by using an iterative technique similar to that used for the distribution of species.

The adsorption model in SOLMINEQ.88 is based on the Gouy-Chapman theory following Healy and White (1978) for the distribution of charge and potential at the solution-surface interface, which states that:

$$\sigma_o + \sigma_d = 0 \quad , \tag{99}$$

where σ is the charge density at the surface (o) or in the diffuse layer made up of coions and counterions (d). To illustrate the implementation of the Gouy-Chapman model, let us consider an amphoteric surface with ionizable

surface sites, SOH, in an NaCl solution. The intrinsic ionization of these sites is given as:

$$SOH_2^+ = SOH + H_s^+ \quad , \tag{24}$$

$$SOH = SO^- + H_s^+ \quad , \tag{25}$$

and the specific adsorption of ions as:

$$SOH + Na_s^+ = SONa^o + H_s^+ \quad , \tag{26}$$

$$SOH + H_s^+ + Cl_s^- = SOH_2Cl^o \quad , \tag{27}$$

where the subscript "s" refers to the surface ions. The relation between the activities of ions in bulk solution and surface is given by

$$a_s = a_{aq} \exp(-z \cdot Y_o); \; Y_o = \frac{e \cdot \psi}{\kappa T} \quad , \tag{100}$$

where a_{aq} is the activity of an ion in the bulk solution, z is its charge, e is the electron charge, ψ is the surface potential, κ is Boltzman's constant and T is the temperature in Kelvin. The mass-action equations for (24) to (27), with the surface concentration described by equation (100), are:

$$K_{24} = \frac{E_{SOH} \cdot a_{H_s^+}}{E_{SOH_2^+}} \quad , \tag{101}$$

$$K_{25} = \frac{E_{SO^-} \cdot a_{H_s^+}}{E_{SOH}} \quad , \tag{102}$$

$$K_{26} = \frac{E_{SONa^o} \cdot a_{H_s^+}}{E_{SOH} \cdot a_{Na_s^+}} \quad , \tag{103}$$

$$K_{27} = \frac{E_{SOH_2Cl^o}}{a_{H_s^+} \cdot E_{SOH} \cdot a_{Cl_s^-}} \quad . \tag{104}$$

Now,

$$\sigma_o = eN_sA_T\alpha \quad , \tag{105}$$

LIMITATIONS OF GEOCHEMICAL MODELING

Geochemical models are extremely powerful and useful tools for understanding the processes of water-rock interactions and predicting their consequences. However, uncertainties involved in computations carried out using SOLMINEQ.88 and similar computer codes should be recognized by all users. Major uncertainties may be imposed by the amount and quality of thermochemical and other data used to calculate the equilibrium constants (K) for the dissociation of complexes and dissolution of minerals. Uncertainties in the computed activity coefficients of aqueous species are probably less severe except for those species (including aluminum and carbonate) that have no published Pitzer coefficients in concentrated brines at high temperatures. Usefulness of the results obtained is limited also by the completeness and reliability of the reported physical and chemical parameters used as input to the codes. It is also important to take the necessary precautions to insure that the sample is "representative" of the water in a specified part of the aquifer (Hull and others, 1985).

Physical Parameters

Accurate temperature and pressure values are needed to model water-rock interactions, especially in deep sedimentary basins where these values may be high. In these basins, oil and gas wells are the primary sources of temperature data. Unfortunately, the accuracy of temperatures obtained from oil wells varies widely (Meyer and McGee, 1985). Many operators do not recognize the importance of temperatures in exploration and production of petroleum and make no attempt to gather accurate data. Also, most temperatures are obtained from wells during drilling when the temperature distribution in the hole is under maximum thermal disturbance. The most reliable temperatures are those obtained from static bottom-hole pressure and temperature surveys generally conducted in production wells. Temperatures obtained from drill-stem tests are of intermediate accuracy. However, the majority of temperatures are obtained from electric log headings; these give the least reliable data, and are generally lower than the true subsurface values. Meyer and McGee (1985) showed that the discrepancy between log-header and static bottom-hole test temperatures from the Wattenberg field, Colorado, is large, ranging from 11 °C to 61 °C.

$$\alpha = \frac{E_{SOH_2^+} - E_{SO^-}}{E_{SOH_2^+} + E_{SO^-} + E_{SONa^o} + E_{SOH_2\,Cl^o} + E_{SOH}} \quad , \tag{106}$$

where E refers to the equivalent fraction of surface sites occupied by the species. The dominator of equation (106) thus is unity and α is the fractional surface charge. Following Hunter (1981),

$$\sigma_d = \{2\epsilon_o \epsilon \kappa T \sum_i n_i (\exp(-Z_i \cdot Y_o) - 1)\}^{1/2} \quad , \tag{107}$$

where n_i is the number of ions of i per gram of the solution ($n_i = 1{,}000 N_A m_i$; m_i being the molality of each charged species in solution), ϵ_o is the permittivity of the vacuum, and ϵ is the dielectric constant of water.

Equations (99) and (101) to (107) are sufficient to uniquely solve for the concentrations of the surface species in equilibrium with the solution at a given pH, temperature and surface potential, ψ. The calculation routine in SOLMINEQ.88 satisfies equation (99) by iteratively changing the value of Y_o until its sign changes. An interpolation polynomial is then used to solve for the final value of Y_o.

Chemical geothermometers, based on the concentration of silica and proportions of sodium, potassium, lithium, calcium and magnesium in water from hot springs and geothermal wells, have been used successfully to estimate the subsurface temperatures of the reservoir rocks (Fournier and Truesdell, 1973; Fournier, 1981). Modified versions of these geothermometers and a new chemical geothermometer, based on the concentrations of magnesium and lithium (Table 7), were developed (Kharaka and others, 1985; Kharaka and Mariner, 1988) to estimate the subsurface temperatures (30 °C to 200 °C) in sedimentary basins where water salinities and hydraulic pressures are generally much higher than those in geothermal systems. SOLMINEQ.88 computes all the chemical geothermometer listed in Table 7.

Quartz, Mg-Li, Mg-corrected Na-K-Ca, and Na-Li geothermometers generally give concordant subsurface temperatures that are within 10 °C of the measured values for reservoir temperatures higher than about 70 °C. Mg-Li, Na-Li, and chalcedony geothermometers give the best results for reservoir temperatures from 30 °C to 70 °C. Subsurface temperatures calculated by chemical geothermometers are at least as reliable as those obtained by conventional methods. Chemical and conventional methods should be used together where reliable temperature data are required. The user then makes the selection of the temperature to be used for the high temperature option in SOLMINEQ.88. For more details see Kharaka and Mariner (1988).

Hydraulic pressure, as discussed earlier, is also an important parameter that affects the equilibrium constants for the aqueous species and minerals, especially at temperatures higher than about 150 °C. Assuming a hydrostatic pressure gradient of 0.45 psi/ft (10.2 kPa/m) is generally reasonable for petroleum wells immediately after drilling. However, in geopressured geothermal systems, initial hydraulic pressure gradients may reach lithostatic pressure gradient of 1.0 psi/ft (22.6 kPa/m). Production wells may have hydraulic pressures that are much lower than the original (virgin) shut-in pressure of the well. Accurate pressure readings at regular time intervals are generally available from the operator and should be extrapolated or interpolated to the time of sampling.

Table 7 Chemical Geothermometers in SOLMINEQ.88

(from Kharaka and Mariner, 1988)

Geothermometer	Equation (Concentrations are in mg/L; t in °C)
1. Quartz	$t = \frac{1309}{0.41 - \log (k \cdot pf)} - 273.15$; $k = \frac{\alpha H_4SiO_4}{\alpha H_2O^2}$; $pf = (1-7.862\times10^{5}\ e^{(3.61\times10^{3}\cdot t)}{}_{p(bar)})$
2. Chalcedony	$t = \frac{1032}{-0.09 - \log (k \cdot pf)} - 273.15$
3. Mg-Li	$t = \frac{2200}{\log (\sqrt{Mg/Li}) + 5.47} - 273.15$
4. Na-K	$t = \frac{1180}{\log (Na/K) + 1.31} - 273.15$
5. Na-K-Ca	$t = \frac{699}{\log (Na/K) + \beta\ [\log(\sqrt{Ca/Na}) + 2.06] + 0.489} - 273.15$ $\beta = 4/3$ for $t<100$; $= 1/3$ for $t>100$
6. Mg-Corrected, Na-K-Ca	$t = t_5 - \Delta t_{Mg}$. For R values of 0.5 to 5. $\Delta t_{Mg} = 1.03 + 59.971 \log R + 145.05(\log R)^2 - 36711\ (\log R)^2/T(K) - 1.67\times10^{7} \log (R/T^2)$; For R values of 5 to 50 $\Delta t_{Mg} = 10.66 - 47415\ R + 325.87(\log R)^2 - 1.032\times10^{5}(\log R)^2/T - 1.968\times10^{7}(\log R)^2/T^2 + 1.605\times10^{7}(\log R)^3/T^2$; No correction should be attempted if R > 50. $R = \frac{Mg}{Mg + 0.61\ Ca + 0.31\ K} \cdot 100$
7. Na/Li	$t = \frac{1590}{\log (Na/Li) + 0.779} - 273.15$

Chemical Analysis

Chemical data may be a major source of uncertainty in the computation of water-rock interactions. Uncertainty may result from:

1. Incomplete analyses. Chemical data collected by oil companies from wells drilled in search of, or for production of oil and gas are plentiful but almost always inadequate for these computations because data are available only for a limited number of major cations and anions. There are very few analyses of trace constituents from oil-field or geothermal waters. A major problem of almost all chemical data is the paucity of Al determinations that are essential for computing the states of reaction of water and aluminosilicates. Barnes (1975) showed that Al concentrations in natural waters at near-neutral pH values are generally less than 57 micrograms per liter (μg/l). Analyses of Al in oil-field and geothermal waters give values that are generally less than 20 μg/l (Kharaka and others, 1985). Concentrations of this magnitude are difficult to determine reliably and some possibility exists that a portion of Al may have precipitated from water prior to sampling (MacGowan and Surdam, 1988).

Another major limitation of many chemical analyses is lack of data on the concentrations of dissolved organic species (Thurman, 1985). It is now generally accepted that mono- and dicarboxylic acid anions may be present at high concentrations (up to 10,000 mg/L) in waters from sedimentary basins (Carothers and Kharaka, 1978; Kharaka and others, 1986; MacGowan and Surdam, 1988). Detailed studies of organic species in oil field waters were initiated (Willey and others, 1975), to a large degree, because computations using SOLMNEQ (Kharaka and Barnes, 1973) had shown that oil field waters at Kettleman North Dome, California, were supersaturated by up to 3 kcal/mole with respect to calcite (Willey and others, 1975; Merino, 1975). Willey and others (1975) showed that the high supersaturation resulted because the alkalinities of the waters were attributed only to inorganic species (mainly HCO_3^-, CO_3^-, and HS^-). They further showed that organic acid anions (C_2 - C_5) contributed up to 99 percent of the measured alkalinities. Carothers and Kharaka (1978) and Lundegard and Land (1986) showed that up to 100 percent of field determined alkalinities in oil field waters are contributed by organic species (Figure 7).

2. Unreliable chemical analyses. The reliability of many chemical analyses is uncertain because of the method of sample collection, treatment,

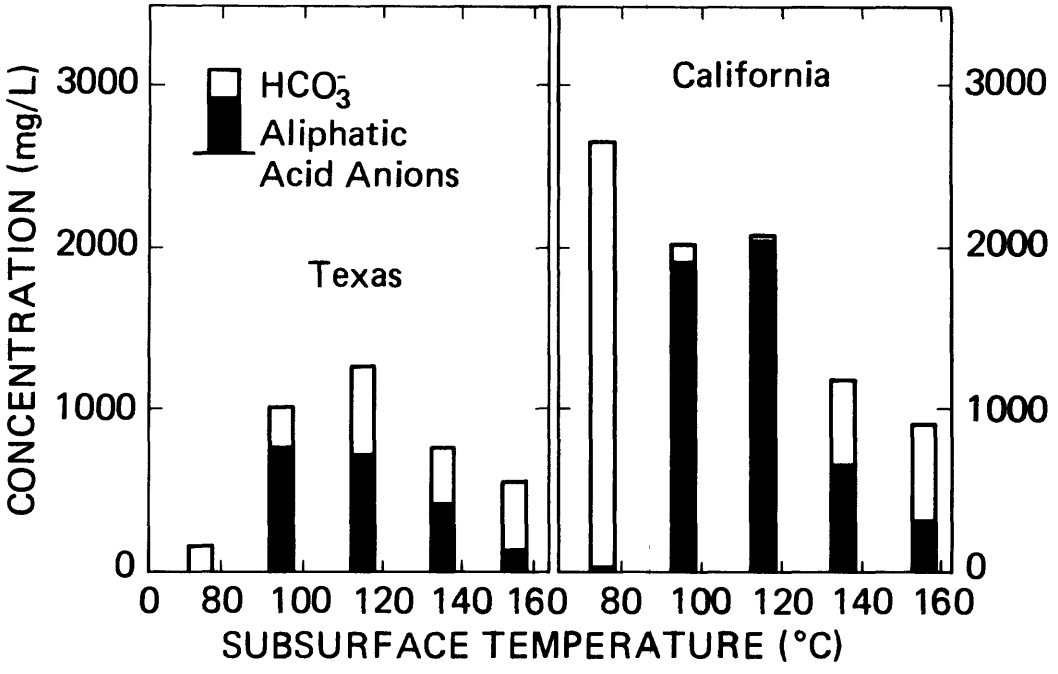

Figure 7. -- Average concentrations of aliphatic acid anions and bicarbonate in oil-field waters from Texas and California (from Carothers and Kharaka, 1978)

and analysis (Hem, 1985). Values of pH, alkalinity, H_2S, and NH_3 not determined in the field are always suspect (Presser and Barnes, 1974; Lico and others, 1982). Field treatment of the samples should include filtration through a 0.1 or 0.45 μm pore-size membrane filter for the major cations, anions, and organics and, in the case of cations, acidification with concentrated HCl to pH of about 2. An aliquot of the filtrate is diluted with distilled deionized water to decrease the silica concentration to less than 100 mg/L to prevent polymerization. Aluminum should be extracted in the field after filtration through a 0.1 μm filter (Barnes, 1975). Filtration through a 0.1 μm filter and acidification to pH 1.5 with high-purity nitric acid is also required for reliable determination of other trace metals (Kennedy and others, 1974). Mercuric chloride or sodium azide, and potassium permanganate should be added to preserve dissolved organics and mercury, respectively, (Hull and others, 1985).

Laboratory analyses require methodologies and instruments that give the best results for the samples selected. Analysis of cations is generally performed by atomic absorption (AA), flame emission spectrophotometry and inductively-coupled plasma atomic emission spectrometry (ICP-AES). Graphite-furnace AA with Zeeman background correction is used for the determination of most trace metals. An increasing number of anionic species, including sulfate, bromide, and iodide, are being determined by ion chromatographic techniques. Dissolved organics are determined by gas and ion chromatography and other instrumentation, such as mass spectrometry. The reader is referred to recent reviews by Parsons and others (1983) and Hull and others (1985).

A high level of analytical skill is required to obtain reliable data from the highly sophisticated instruments described above. Ellis (1976), in an international laboratory-comparison program, showed that the analytical precision for many chemical constituents was poor. The reported silica concentration of a geothermal sample, for example, ranged from 70 to 920 ppm. Lowest precisions were reported for geothermal and alkaline spring waters of unusual composition. Friedman and Erdmann (1982) provide some guidance for setting up a quality assurance program.

3. Incorrect interpretation of chemical determinations. We have already discussed the problems associated with assuming that alkalinities are contributed only by inorganic species. Similar problems may arise if the iodometric titration method, which measures the concentrations of bisulfides, sulfites, polysulfides and other oxidizable species, is assumed to titrate only the bisulfide species. In oil field waters, H_2S values obtained by

specific sulfide electrode are more accurate and are much lower (by a factor of up to 10) than those obtained by titration (Lico and others, 1982).

Equilibrium Constants

Reliability of equilibrium constants for the dissociation of complexes and dissolution of minerals is highly variable, depending on the quality and the nature of the thermochemical data used in these computations (Arnorsson and others, 1982; Nordstrom and Munoz, 1985; Apps and others, 1987). The range of available thermochemical data is large. The Gibbs free energy values reported for the same mineral may vary by more than 10 kcal/mole (Tardy and Garrels, 1974; Berman and others, 1985). For instance reported values of the equilibrium constant at 25 °C for fluorite range from 10^{-8} to 10^{-13} (Nordstrom and Jenne, 1977); those for the second dissociation constant of H_2S range from 10^{-12} to 10^{-19} (Schoonen and Barnes, 1988). Equilibrium constants computed from solubility or free energy determinations over the temperature range of interest are probably the most reliable. As discussed earlier, equilibrium constants for most minerals and a few aqueous complexes used in SOLMINEQ.88 are computed from an integrated form of the Van't Hoff equation (Equation 37). These equilibrium constants are the most reliable for the pure mineral samples used to generate thermochemical data in laboratory experiments. However, minerals in natural systems often show large variations in chemical composition, surface characteristics, degree of crystallinity, order-disorder, and lattice imperfections. Clays and zeolites are two major groups of minerals for which large uncertainties in equilibrium constants may result from these imperfections (Tardy and Garrels, 1974; Bassett and others, 1979; May and others, 1986).

Heat-capacity data are not available for most aqueous complexes. Equilibrium constants for these complexes are computed from empirical relation using a large number of assumptions and extrapolations (see previous section). Equilibrium constants calculated from these empirical equations, nonetheless, more closely approximate the actual values at higher temperatures than those computed assuming a constant or zero-heat capacity of reaction. However, very large errors may be present in log K values calculated from these equations, especially at temperatures above 200 °C (Apps and others, 1988). Equilibrium constants for many minerals and aqueous complexes (especially with organic ligands) are either not available or are available only at 25 °C.

Equilibrium constants are unquestionably the most important parameters used in geochemical codes like SOLMINEQ.88. However, these constants are subject to continuous refinements, modifications or major changes (Hovey and Tremaine, 1986; Apps and and others, 1988), and the user should carry out literature searches to select the most reliable constants for the critical minerals and aqueous species in their study. SOLMINEQ.88 allows computations to be carried out using a set of up to six (at low and high temperatures) user selected equilibrium constants for minerals and aqueous complexes. The INPUT routine prompts the user to enter the desired equilibrium constants which will be used for any computations during that run. Permanent changes in the equilibrium constants, of course, can be made by changing the values for the desired complex or mineral in the permanent data file listed in Appendix IB and IC.

Limitations of Modeling Options

All of the modeling options in SOLMINEQ.88 have been designed to allow modification of the analyzed chemistry of a water sample to the in situ chemistry of the water and its mineral saturations. The options, also, can be used to study the consequences of the various hypothetical or planned water-rock interactions including sensitivity calculations.

The carbon option may be used to validate a chemical analysis if independent determinations of alkalinity and TIC exist. Given a value for one, SOLMINEQ.88 will calculate a value for the other. This can be compared to the analytical value (see Merino 1979 for examples). For high temperature calculations the assumption of constant TIC or constant alkalinity will affect the predictions differently. Constant alkalinity can only be enforced by allowing CO_2 to enter or leave the water, whereas constant TIC is a closed system. If CO_2 is known to have been lost from the system, it can be titrated back in with the gas-option. However, it is difficult to measure the ratio of gas/water in a flowing well. If the aim is to combine the masses of gas and water as they are in situ, large uncertainties exist because once gas separates from liquid water the two can travel at different velocities to the wellhead. If oil is present in the system, the gas lost from the oil must also be titrated back using the gas-water-oil option to reconstruct the in situ conditions. However, data on gas solubilities in oil have large uncertainties because of differences in the physical and chemical properties of oil. The gas-water-oil option will not run if the total pressure of the

gas phase (at high or low temperature) is less than the vapor pressure of water at that temperature and pressure. These calculations are carried out assuming that Henry's law does not vary with pressure and ideal mixing of gases. Although these assumption are good along the vapor pressure curve for water, significant errors will be introduced when pressures exceed several hundred bars at low temperatures; such conditions exist in deep wells in sedimentary basins. In addition, at high pressures, a significant mass of water vapor may exist in the natural gas phase which may condense in the well leading to erroneously low concentrations of dissolved species (Kharaka and others, 1985). Presently, all the water is assigned to the liquid phase in SOLMINEQ.88 except for the boiling option. The boiling and mixing options can handle loss or addition of water to in situ water, however, the fraction of boiling or the composition and amount of water mixing with the in situ water must be accurately known.

Minerals can also be used to compute the water chemistry at subsurface conditions. If the amount of gas which is lost is unknown, for example, an estimate can be made by assuming equilibrium with an in situ carbonate mineral using the CO_2 option; commonly equilibrium is assumed with calcite. If other minerals are controlling the water chemistry, a user specified set of components can be dissolved into or precipitated out of the water to reach saturation with a specified mineral. Even if the in situ mineralogy is known in detail, the extent to which a mineral controls the water chemistry depends on its surface area and reactivity, which are usually unknown. In addition, most minerals are solid solutions which are not presently included in the database of SOLMINEQ.88.

The mineral saturation option may be used to calculate the concentrations of unknown or suspect components. This option, for example, may be used to calculate the concentrations of SiO_2 (assuming quartz saturation) and Al (assuming equilibrium with kaolinite). This use of saturation options should only be used as a last resort because of the large uncertainties involved. If the pH is unknown or suspect, equilibrium with calcite is commonly assumed and the pH changed to attain equilibrium using the pH option. This case is only correct as long as significant amounts of the other ions in solution have not been added or subtracted at the same time the pH changed. Presently, SOLMINEQ.88 allows only equilibration with one mineral phase even when the reaction is incongruent, involving several minerals.

The water chemistry can also be changed by ion exchange or adsorption. Large uncertainties exist in the values for the ion exchange constants.

Consequently, in the ion exchange option, these constants must be specified by the user. Surface complexes are assumed to behave ideally. Smectites, the clays which control most of the ion exchange, are poorly characterized chemically. The double layer, one-site model chosen for adsorption calculations is probably too simple, but even this simple a model is difficult to use because of paucity of data. Consequently, mineral surface-water equilibrium calculations lag far behind mineral-water equilibrium predictions in accuracy.

The above discussion is included in this report because the uncertainties in the predictions made by these options can be large. The user should be cautioned to understand fully the assumptions and simplifications made in both the data and the calculations in order to use the model successfully.

INPUT FOR SOLMINEQ.88

The input to SOLMINEQ.88 consists of two sets of data: fixed and variable. The fixed set contains the chemical composition of an aqueous fluid and options for processing these data. The variable set consists of input data required for using the modeling options. Multiple samples may be processed during each run. The arrangement of input data is shown in Table 8. A list of input variable names and their description is given below. An interactive FORTRAN-77 program, SOLINPUT, is also available which can be used to generate or modify an input file. This program prompts the user for input data with a brief description of the required data. The user is prompted to press the "RETURN" key in cases where data are not available and where the default values are preferred. An abbreviated terminal session for building a data file using SOLINPUT is given in Appendix II. An interactive input-output management program (shell) that can be used with personal computers (PCs) is also available (Wiwchar and others, 1988) for SOLMINEQ.88

A. Input Data for the Fixed Set

TITLE	Sample identification and description.
TEMP	Temperature at which the pH of the solution was measured.
HITEMP	In-situ temperature, different from TEMP, at which a new pH is to be calculated.
DENS	Measured or desired density. If density is not entered, it is calculated based on the following empirical relationship (Kharaka, unpublished data): Density = $1.0 + 6.88 \times 10^{-7}$ * Total Dissolved Solids (mg/L)
PRESS	Total in-situ pressure (in bars). K values of the aqueous and mineral reactions will be adjusted for the pressure difference of (PRESS-P_{H_2O}). The K values are adjusted at only one temperature, TEMP or HITEMP. If PRESS is greater than P_{H_2O} at TEMP and a value for HITEMP is entered, the K values are adjusted only at HITEMP.
PH	Measured pH of the solution.
EHM	Measured or calculated Eh relative to the hydrogen electrode potential in volts, otherwise a default value of 9.0 is entered by the program.

EHMC — Measured Eh relative to the Calomel electrode potential in volts, otherwise a default value of 9.0 is entered by the program.

EMFZSC — Measured Eh using Zobell's solution in volts, otherwise a default value of 9.0 is entered in the program.

UNITS — Concentration units in which the chemical composition of the solution will be entered.

MG/L = milligrams/liter
PPM = parts per million
MOL/L = moles/liter (molar units)
MOL/K = moles/kg of solvent (molal units)
MEQ/L = milli-equivalents/liter

Total or analytical concentration of the specified component. The concentrations must be entered for the specified formula of the component (for example, sodium is entered as Na, silica as SiO_2, phosphorous as PO_4). The components are listed in Table 6.

TIC — Concentration of total inorganic carbon in solution, if measured, in the same units used for the rest of the components. If UNITS is "MEQ/L", carbon concentration should not be entered as TIC; instead it should be entered as alkalinity (ALK).

ALK — Criterion for the distribution of carbonate species.

"0" indicates that the entered concentration of HCO_3^- and for CO_3^{--} represent "TOTAL ALKALINITY" that includes inorganic and organic species.

"1" indicates that the entered concentrations of HCO_3^- and for CO_3^{--} represent "CARBONATE ALKALINITY" only.

"2" indicates that the entered concentrations of HCO_3^- and CO_3^{--} represent "TIC".

It should be noted if ALK = 2 and TIC = 0.0, the entered concentration of HCO_3^- and CO_3^{--} will be treated as TIC after conversion to the molality of carbon; if TIC is greater than 0.0, ALK will be set equal to 2 and the concentrations of HCO_3^- and CO_3^{--}, if entered, will be disregarded.

ITIC — Criterion for the distribution of carbonate species at HITEMP "1" if this distribution is to be done with the value of TIC calculated at the end of low-temperature species distribution. Note that if a value for TIC is entered, ITIC will be automatically set equal to "1".

NUFLAG — Sets the activity coefficients of neutral species;

"1" for setting them equal to unity;

"0" for setting them equal to the activity coefficient of aqueous CO_2.

IPIT — Enter "1" if activity coefficients are to be calculated using the Pitzer equations.

FLAGS(I) — Flags for the calculation of redox equilibria. If these flags are set equal to "1" the distribution of redox species will be calculated using the measured or calculated Eh and equations of the type:

$$Fe^{++} = Fe^{3+} + e^-$$

else, if equal to "0", the H_2S^o/SO_4^{--} and Fe^{++}/Fe^{+3}, will be used to determine redox species distribution.

FLAG(1) for Fe
FLAG(2) for Cu
FLAG(3) for Hg
FLAG(4) for Mn
FLAG(5) for U
FLAG(6) for V

INFORM — Flag for printing all the log K values in Tables 2 and 3. Set INFORM equal to "1" if you want the tables printed.

RATIO — Flag for printing the analytical and calculated activity ratios of major elements. Set RATIO equal to "1" if you want the ratios printed.

GEOTH — Flag for printing the temperature estimates from the chemical geothermometers. Set GEOTH equal to "1" if you want the geothermometers printed.

IPRIN1 — Flag for printing the data on iteration of anions, set equal to "1" for output.

IPRIN2 — Flag for printing the data on $(m_{H,t,T} - m_{OH,t,T})$ whenever a new pH is calculated. Set IPRIN2 equal to "1" to print data.

CONV1 Tolerance factor for convergence on distribution of anions. Enter the desired factor if different from a default value of 0.5E-4. Use of a lower value may result in greater accuracy but more computer time.

CONV2 Tolerance factor for pH calculation using hydronium mass-balance equation. Enter a desired factor if different from a default value of 0.5E-4. Use of a higher value may result in faster execution, but a larger pH difference between calculated and in situ.

OUTIN A restart file will be generated with the file name located in OUTIN. The restart file will contain data from the current SOLMINEQ.88 run. Leave blank if a restart file is not to be created.

B. Input for Gas, PH, and CO_2 options

DCO2 Concentration of CO_2 gas (moles/kg of water) that was lost before pH measurement.

DH2S Concentration of H_2S gas (moles/kg of water) that was lost before pH measurement.

DNH3 Concentration of NH_3 gas (moles/kg of water) that was lost before pH measurement.

DCH4 Concentration of CH_4 gas (moles/kg of water) that was lost before pH measurement.

ICCSAT Switch for the pH option (calculation of pH in equilibrium with carbonate mineral). "1" for calcite; "2" for dolomite; "3" for siderite. Default is "0"

IMCO3 Switch for the application of the CO_2 option.

"0" = do not use option (default).
"1" Enter for saturation with calcite.
"2" Enter for saturation with dolomite.
"3" Enter for saturation with siderite.
"4" for fixing a molality of H_2CO_3 specified by FIXIT.
"5" for fixing a pH specified by FIXIT.
"6" for fixing a P_{CO_2} specified by FIXIT.

FIXIT — Specify the value to be fixed using the CO_2 option above if IMCO3 = 4, 5, or 6.

FCCSAT — Tolerance factor for satisfying the equilibrium criterion in the PH and CO_2 options (default = 0.05). The equilibrium is tested in log units.

C. Input for the Gas Distribution option

TCO2M — Total moles of CO_2 (per kg of water) to be distributed between Oil, Water, and Vapor.

TCH4M — Total moles of CH_4 (per kg of water) to be distributed between Oil, Water, and Vapor.

TH2SM — Total moles of H_2S (per kg of water) to be distributed between Oil, Water and Vapor.

WROIL — Oil to water weight ratio.

KCO2OL — Henry's law coefficient for the solubility of CO_2 in oil. If value entered is "0", which is the default value, then the value is calculated in the program.

KCH4OL — Henry's law coefficient for the solubility of CH_4 in oil. If value entered is "0", which is the default value, then the value is calculated in the program.

KH2SOL — Henry's law coefficient for the solubility of H_2S in oil. If value entered is "0", which is the default value, then the value is calculated in the program.

DSEP — Density of oil at 15 °C needed to calculate Henry's law coefficients for the solubility of gas in oil.

D. Input for the Ion Exchange or Adsorption Option

ADEX — Flag for surface chemistry option:
"A" for adsorption, "E" for ion exchange.

CEC — Cation exchange capacity in milliequivalents/kg of water. Either a value for CEC or values for TAREA and SAREA must be specified.

TAREA — Site density per unit area (N_s) in sites/cm^2.

SAREA — Total surface area per kilogram of solvent in cm^2.

INSP — Total number of surface species (10 maximum)

ISCHG(I) — Charge of each surface site (e.g. ISCHG = 0 for NaX; -1 for X^-), where X represents vacant surface site.

MBASE(I) — Equivalent fraction of surface sites occupied by each surface species. If vacant surface sites occupy an appreciable fraction of total, then a dummy reaction $X \rightleftarrows X$ must be specified.

SPN(I) — Name of each of the surface species.

KRXN(I) — K_D for the association reaction of the surface species.

ISCOMP(I) — Total number of components in the association reaction of SPN(I).

COEF(I,J) — Stoichiometric coefficient of each of the reacting species (only those in Table 6) in the association reaction of SPN(I).

IDN(I,J) — ID#s of the ISCOMP(I) components in the association reaction of SPN(I). It is important that the K_D and coefficients for the species be specified as for an association reaction; and that all association reactions use only the vacant surface site X as the reactant surface site.

E. Input for the Dissolution/Precipitation, Mixing, and Boiling Option

IBMIX — Switch for the mixing and mass transfer option.
"1" for dissolution/precipitation.
"2" for mixing two solutions.
"3" for boiling-off or adding steam.

ITMIX — Total number of species to be added when IBMIX=1. If ITMIX is zero, it is used as the switch for the mineral saturation option. That is, if IBMIX = 1 and ITMIX = 0, then the program would look for the ID# of the mineral to be saturated. If ITMIX is not equal to zero, then a specified amount of mineral will be added if ITMIX = -1. If ITMIX = n, where n is greater than zero, then specified amounts of n aqueous components will be added.

IDSAT — ID# (from 1 to 214) of the mineral to be equilibrated (i.e. SI=0). (See Table 3.)

IDDP — ID # (from 1 to 214) of the mineral to be dissolved or precipitated. If IDDP equals "0", then a number of aqueous species are added or subtracted from the water.

ITT — Total number of aqueous species to be added to or subtracted from the water.

DP — Dissolution/precipitation switch. If DP is positive it will dissolve minerals or add aqueous components into solution; if negative, it will precipitate or subtract them out. The absolute value of DP is also used to scale the amount of material being added or subtracted. If the default value of zero is used then the program will determine the path to acheive equilibrium.

IRXDP(I) — ID# of the aqueous species to be added (only the species listed in Table 6 can be used).

RXDP(I) — Stoichiometric coefficient of the aqueous species to be added.

IDMIX(I) — ID number of the aqueous species to be added (only the species listed in Table 6 can be used).

AMOL(I) — Molality (Moles/kg of H_2O) of the aqueous or mineral species to be added.

INMIX — Total number of mixtures of the two solutions to be mixed.

DFRAC1 — Smallest fraction of solution 1 to be mixed with solution 2.

DINC — Increment of solution 1 to be added (INMIX-1) times. For example, if INMIX = 3, DINC = 0.25 and DFRAC1 = 0.10, a total of THREE mixtures will be prepared with the following fractions of the two solutions:

(1) solution 1 = 0.10; solution 2 = 0.90
(2) solution 1 = 0.35; solution 2 = 0.65
(3) solution 1 = 0.60; solution 2 = 0.40

MIXFLE — Name of second data file to form the mixture. No other mass transfer options can be executed as part of mixing.

FBOIL — Fraction of the solution to be boiled-off as steam.

F. Input for variable K values at TEMP and then again at HIGHTEMP

ODUM(I) — Switch for data base. If KT is for an aqueous complex dissociation reaction, enter "A"; if for a mineral dissociation reaction enter "M".

NDUM(I) — ID# of the mineral (Table 3) or aqueous complex (Table 2) whose (KT) is to be changed.

XDUM(I) — Log (KT) for the dissociation reaction specified in Tables 2 or 3.

G. Input for additional anions.

ANS1, ANS2	Switches for additional anion option. If ANS1 or ANS2 are not zero, the value of ANS1 or ANS2 is the number of lines (one line per complex with anion) to follow. If ANS1 = 0 (default option) and ANS2 = 0, skip option. If ANS1 > 0 and ANS2 = 0, or vice versa then add one additional anion. If ANS1 > 0 and ANS2 > 0, then add both additional anions.
PAGE1	Name of additional anions.
CUNITS	Total concentration (same UNITS as other components) of additional anions.
GFW	Gram formula weight of additional anion.
Z	Charge of additional anion (-1 to -4).
DHA	Debye Hückel radius of additional anion (default values are available).
NAME(I)	Name of each complex formed by association with the additional anion.
INDEX(I)	ID# of the dissociation reaction (Table 5) for the anion complex, NAME(I).
LOWKT(I)	Low temperature log (KT) for the INDEX(I) dissociation reaction.
HIGHKT(I)	High temperature log (KT) for the INDEX(I) dissociation reaction.

H. Input for additional cation.

NUMCOM	Number of complexes entered for the additional cation.
Z	Charge of additional cation (+1 to +4).
DHA	Debye Hückel radius of additional cation (default values are available).
GFW	Gram formula weight of additional cation.
CUNITS	Total concentration (same UNITS as other components) of additional cation.
NAME(I)	Name of each complex formed by association with the additional cation.
INDEX(I)	ID# of the dissociation reaction (Table 5) for the cation complex, NAME(I).
LOWKT(I)	Low temperature log K(T) for the INDEX(I) dissociation reaction.
HIGHKT(I)	High temperature log K(T) for the INDEX(I) dissociation reaction.

J. Input for additional minerals.

NUMINS	Number of minerals to be added (up to 5 allowed)
LOWKT	Low temperature log K(T) for the congruent dissolution of the mineral
HIGHKT	High temperature log K(T) for the congruent dissolution of the mineral
ADDACT	An additional activity parameter which can be added to the dissolution reaction of mineral
NAME	Name of the mineral
COEFF(I)	Coefficient of aqueous species (I) in the dissolution reaction of the mineral.
INDEX(I)	Index number of aqueous species (I) in the dissolution reaction of the mineral

Table 8 Arrangement of data for input to SOLMINEQ.88.

Line	Variable	Format
1	TITLE	A80
2	TEMP, HITEMP, DENS, PRESS	4E10.4
3	PH, EHM, EHMC, EMFZSC, UNITS	4E10.4, A5
4	Total aqueous concentration of	
	[Na, K, Li, Ca, Mg, Fe, Al]	7E10.4
5	Total aqueous concentration of	
	[SiO_2, Cl, SO_4, H_2S, HCO_3, CO_3, TIC]	7E10.4
6	Total aqueous concentration of	
	[F, PO_4, NO_3, NH_3, B, Sr, Ba]	7E10.4
7	Total aqueous concentration of	
	[Pb, Zn, Cu, Mn, Hg, Ag]	6E10.4
8	Total aqueous concentration of	
	[As, U, V]	3E10.4
9	Total aqueous concentration of	
	[Acetate, Oxalate, Succinate, CH_4]	4E10.4
10	Carbon, High Temperature Carbon Option	
	ALK, ITIC	2I2
11	Gas Addition Option	
	DCO2, DH2S, DNH3, DCH4	4E10.4
12	pH and CO_2 Saturation Option	
	ICCSAT, IMCO3, FIXIT, FCCSAT	2I2, 2E10.4
13	Gas-Water-Oil Option	
	TCO2M, TCH4M, TH2SM, WROIL,	
	KCO2OL, KCH4OL, KH2SOL, DSEP	8E10.4
14	Ion Exchange Option	
	ADEX	A1
	if ADEX is "E" or "A", then	
	A. CEC, TAREA, SAREA, INSP	3E10.4, I3
	followed by INSP lines of	
	B. ISCHG(I), MBASE(I), SPN(I)	I4, E10.4, A10
	C. KRXN(I), ISCOMP(I),(COEF(I,J),IDN(I,J))	11(E10.4, I3)

15	Precipitation/Mixing/Boiling Options	
	IBMIX, ITMIX	2I2
	Dissolution/Precipitation Option:	
	If IBMIX = 1, then	
	(Dsl/Ppt a specific mineral amount)	
	If IBMIX = 1 and ITMIX < 0, then	
	A. IDDP, AMOL(1)	I4, E10.4
	(Dsl/Ppt a mineral to saturation)	
	Else If IBMIX = 1 and ITMIX = 0, then	
	A. IDSAT, IDDP, DP	2I4, E10.4
	(Add/Subtract aqueous species to saturation with a mineral)	
	If IDDP = 0, then	
	A. ITT	I4
	followed by ITT lines of	
	B. IRXDP(I), RXDP(I)	I4, E10.4
	(Add/Subtract a specific amount of aqueous species)	
	Else If IBMIX = 1 and ITMIX > 0, then	
	followed by ITMIX lines of	
	A. IDMIX(I), AMOL(I)	I4, E10.4
	Mixing Option:	
	Else If IBMIX = 2, then	
	A. INMIX, DFRAC1, DINC, MIXFLE	I4, 2E10.4, A80
	Boiling Option:	
	Else If IBMIX = 3, then	
	A. FBOIL	E10.4
16	Optional User Defined Log K at TEMP	
	A. ODUM(I), NDUM(I), XDUM(I)	6(A1, I4, E10.4)
17	Optional User Defined Log K at HITEMP	
	B. ODUM(I), NDUM(I), XDUM(I)	6(A1, I4, E10.4)

18	Additional Anions Option	
	ANS1, ANS2	2I2
	Skip if both ANS1 = 0 and ANS2 = 0.	
	If ANS1 > 0 or ANS2 > 0, then	
	A. CUNITS, GFW, Z, DHA, PAGE1	2E10.4, I2, E10.4, A8
	followed by ANS1 lines of	
	B. INDEX(I), DHA, LOWKT, HIGHKT, NAME(I)	I2, 3E10.4, A8
	If ANS1 > 0 and ANS2 > 0, then	
	A. CUNITS, GFW, Z, DHA, PAGE1	2E10.4, I2, E10.4, A8
	followed by ANS2 lines of	
	B. INDEX, DHA, LOWKT, HIGHKT, NAME	I2, 3E10.4, A8
19	Additional Cation Option	
	A. NUMCOM, Z, DHA, GFW, CUNITS, NAME	2I2, 3E10.4, A8
	followed by NUMCOM lines of	
	B. INDEX, DHA, LOWKT, HIGHKT, NAME	I2, 3E10.4, A8
20	Additional Minerals Option	
	NUMINS	I2
	followed by NUMINS lines of	
	B. LOWKT, HIGHKT, ADDACT, NAME	5E10.4, A8
	C. (COEFF(I), INDEX(I), I = 1, 8)	8(E10.4, I3)
21	NUFLAG, IPIT, (FLAGS(I), I = 1, 6)	8I2
22	INFORM, RATIO, GEOTH, IPRIN1, IPRIN2, OUTIN	5I2, A80
23	CONV1, CONV2	2E10.4

OUTPUT FROM SOLMINEQ.88

The results of the computations carried out by SOLMINEQ.88 and appearing in the printout (Appendix III) consist of a standard output which is similar to that from the original code and additional output which will depend on the options selected. The standard output consists of items listed below:

1. An input data echo that shows the values and options selected for each sample.

2. A table listing the calculated tolerance factor ($1 - Y_A$) for successive iterations on the anions. Each set of iterations is completed at a fixed pH. At the end of each set or when the tolerance criteria are met, the current hydronium/hydroxyl summation ($m_{H,t,\ T} - m_{OH,t,T}$) is printed out along with the correct (desired) value. The printout of these numbers may be enabled by inputting IPRIN1 = IPRIN2 = 1. These data are used to verify the timely execution of the program and are not normally needed.

3. A list of input to SOLMINEQ.88, including sample description, pH, Eh (measured or computed, a dummy value of 9.0000 is printed when no Eh data are available) temperature, total milliequivalent of cations (MEQ/L CAT) and anions (MEQ/L AN) computed from the analytical data (ANAL...) and from the calculated molalities (CALC...), the true ionic strength of solution (I), the total pressure and the partial pressures, in atmospheres, of H_2O, CO_2, H_2S, CH_4, and NH_3 in the gas phase that is in equilibrium with the solution, the density of the solution, dissolved solids concentration and activity of water. The total hydronium and hydroxyl and their difference; the total alkalinity calculated as HCO_3^-, CO_3^{--} and $CaCO_3$; and the dissolved inorganic carbon (split up into HCO_3^- - alkalinity, H_2CO_3, sum of all HCO_3^- species and the sum of all CO_3^{--} species) and total inorganic carbon are also printed out.

4. A table showing the distribution of species in solution. This consists of the index number (1 to 340) and name of the species which are present, reported and computed ppm, reported and computed mg/l, reported and computed molality, activity, activity coefficient, and -log activity. This table can be used to calculate the degree of complexing in the solution under study.

5. Ratios of a number of cations and anions of importance in geochemical processes. These consist of the mole ratios of cations and anions which may

aid in deciphering the origin of the water samples (White, 1965; Kharaka, 1985) and logs of the activity ratios of a number of cations used to study the stability fields of minerals. The subsurface temperature of a reservoir is computed by 12 different chemical geothermometers (see Table 7 for details of computations). A number of criteria for selecting the most probable temperature are also printed. (Fournier and Truesdell, 1973; Kharaka and Mariner, 1988). The computation and printout of these ratios and temperatures may be suppressed by inputting "RATIO = 0" and "GEOTH = 0" in the INPUT routine.

6. A table showing the states of reactions for minerals considered. The "DELG" column gives the (ΔG_{diff}), in kcal/mole. A positive (DELG) value indicates that the solution is supersaturated with respect to the given mineral; a negative (DELG) value indicates undersaturation with respect to it. This table also shows the mineral name and its ID numbers, log (AP), log (KT), and log (AP/KT). A mineral that contains a species not reported in the chemical analyses of the water sample will not appear in this table. The log (KT) of a number of minerals (for example, kenyaite, magadiite) is known only at 25 °C; it is assumed constant at other temperatures. The "DELG" values obtained for these minerals will not be significant if the temperature of the sample is outside the range of 15°-35 °C.

It is important to repeat here that (DELG) indicates that the reaction can proceed but does not mean that it will proceed in the specified direction. It is possible for a given solution to be supersaturated (unstable but persistent condition) with respect to a mineral by a number of kilocalories without precipitation. It is also important to note here that large uncertainties are involved in the computed log (KT) values for most aqueous complexes at temperatures higher than 200 °C.

Beside the standard output described above, implementation of various options will create additional output. This output is self-explanatory once the standard output format is understood. Selected examples are contained in Appendix III. The total number of possible options is large and could not be illustrated in this report. However, we have input/output from 20 different options that will be mailed, together with the source code, to those willing to implement this program.

REFERENCES

Aggarwal, P. K., Gunter W. D., and Kharaka, Y. K., 1989, The effect of pressure on a aqueous equilibria: American Chemical Society Symposium, Series on Ground Water Modeling, R. L. Bassett and D. C. Melchior, eds., in press.

Aggarwal, P. K., Hull, R. W., Gunter, W. D., and Kharaka, Y. K., 1986, SOLMNEQF: A computer code for geochemical modeling of water-rock interactions in sedimentary basins: Proceedings Third Canadian-American Conference on Hydrogeology-Hydrogeology of Sedimentary Basins. Application to Exploration and Exploitation, B. Hitchon, S. Bachu, and C. M. Sauveplane (editors), National Water Well Association v. 3, p. 196-203.

American Society of Testing and Materials, 1985, Standard method for estimation of solubility of gases in petroleum liquids: Annual Book of ASTM Standards, 05.02, p. 669-673.

Apps, J. A., Neil, J. M., and Chi-Hyuck, J., 1988, Thermochemical properties of gibbsite, boehmite, diaspore and the aluminate ion between 0 and 350°C: Lawrence Berkeley Laboratory Report No. LBL-21482, 98 pp.

Arnorsson, S., Sigurdsson, S., and Svavarsson, H., 1982, The chemistry of geothermal waters in Iceland. I. Calculation of aqueous speciation from 0-370°C: Geochimica et Cosmochimica Acta, v. 46, p. 1513-1532.

Baes, C. F., and Mesmer, R. E., 1981, The thermodynamics of cation hydrolysis: American Journal of Science, v. 281, p. 935-962.

Ball, J. W., Nordstrom, D. K., and Zachmann, D. W., 1987, WATEQ4--A personal computer FORTRAN translation of the geochemical model WATEQ2 with revised data base. U. S. Geological Survey Open-File Report 87-50, 108 p.

Barnes, H. L., Romberger, S. B., and Stemprok, M., 1967, Ore solution chemistry II. Solubility of HgS in sulfide solutions: Economic Geology, v. 62, p. 957-982.

Barnes, I., and Back, W., 1964, Geochemistry of iron-rich ground water of southern Maryland: Journal of Geology, v. 72, p. 435-447.

Barnes, I., and Clarke, F. E., 1969, Chemical properties of ground water and their encrustation effects on wells: U. S. Geological Survey Professional Paper 498-D, 58 p.

Barnes, R. B., 1975, The determination of specific forms of aluminum in natural water: Chemical Geology, v. 15, p. 177-191.

Bassett, R. L., Kharaka, Y. K., and Langmuir, D., 1979, Critical review of the equilibrium constants for kaolinite and sepiolite, in Chemical Modeling in Aqueous Systems, Jenne, E. A., ed., ACS Symposium Series v. 93, p. 389-400.

Beerbower, A., 1980, Estimating the solubility of gases in petroleum and synthetic lubricants: American Society Testing and Materials, Transaction 23, p. 335-342.

Berman, R. G., Brown, T. H., and Greenwood, H. J., 1985, An internally consistent thermodynamic data base for minerals in the system Na_2O-K_2O-CaO-MgO-FeO-Fe_2O_3-Al_2O_3-$SiO_2$$TiO_2$-$H_2O$-$CO_2$: Atomic Energy of Canada Ltd., Technical Record TR-377, 62 p.

Bilinski, H. B., Horvath, L., Ingri, N., and Sjoberg S., 1986, Equilibrium aluminum hydroxo- oxalate phases during initial clay formation; H^+-Al^{3+}-oxalic acid-Na^+ system: Geochimica et Cosmochimica Acta, v. 50, p. 1911-1922.

Bolt, G. H., 1982, Soil Chemistry, B. Physicochemical models: Elsevier Science Publishing Company, New York, 527 p.

Bourcier, W. L., and Barnes, H. L., 1987, Ore solution chemistry--VII. Stabilities of chloride and bisulfide complexes of zinc to 350°C: Economic Geology, v. 82, p. 1839-1863.

Bradley, D. J., and Pitzer, K. S., 1979, Thermodynamics of Electrolytes. 12. Dielectric Properties of Water and Debye-Hückel Parameters to 350 °C and 1 kbar: Journal of Physical Chemistry, v. 83, p. 1599-1603.

Bryzgalin, O. V., and Rafal'ski, R. P., 1982, Estimation of instability constants for ore-element complexes at elevated temperatures: Geochemi. International, v. 19, p. 158-169

Busenberg, E., Plummer, N. L., and Parker, V. B., 1984, The solubility of strontianite ($SrCO_3$) in CO_2-H_2O solutions between 2 and 91°C, the association constant of $SrHCO_3^o$ (aq) between 5 and 80°C, and an evaluation of the thermodynamic properties of Sr^{++}(aq) and $SrCO_3$(cr) at 25°C and 1 atm total pressure: Geochimica et Cosmochimica Acta, v. 48, p.2021-2036.

Busey, R. H., and Mesmer, R. E., 1977, Ionization equilibria of silicic acid and polysilicate formation in aqueous chloride solutions to 300°C: Inorganic Chemistry, v. 16, p. 2444-2450.

Carothers, W. W., and Kharaka, Y. K., 1978, Aliphatic acid anions in oil field waters-Implications for origin of natural gas: American Association Petroleum Geology Bulletin v. 62, p. 2441-2453.

Carothers, W. W., and Kharaka, Y. K., 1980, Stable Carbon Isotopes in Oil Field Waters and the Origin of CO: Geochimica et Cosmochimica Acta, v. 44, p. 323-333.

Chen, C. A., and Marshall, W. M., 1982, Amorphous silica solubility, IV. Behaviour in pure water and aqueous sodium chloride, sodium sulfate, magnesium chloride, and magnesium sulfate solutions up to 350°C: Geochimica et Cosmochimica Acta, v. 46, p. 279-287.

Cho, M., Marayama, S., and Liou, J. G., 1987, An experimental investigation of heulandite-laumontite equilibrium at 1000 to 2000 bar P fluid. Contribution Mineral Petroleum, v. 97, p. 43-50.

Cobble, J. W., Murray, R. C. Jr., Turner, P. J., and Chen, K., 1982, High temperature thermodynamic data for species in aqueous solution: Electric Power Research Institute, EPRI report NP-2400, 165 p.

Conard, B. R., Sridhar, R., and Warner, J. S., 1980, High temperature thermodynamic properties of chalcopyrite: Journal Chemical Thermodynamics, v. 12, p. 817-833.

Crerar, D., E., and Barnes, H. L., 1976, Ore solution chemistry V. Solubilities of chalcopyrite and chalcocite assemblages in hydro-thermal solution at 200° to 350°C. Economic Geology 71, 772-794.

Crerar, D. E., Suzak, N. J., Borszik, M., and Schwartz, S., 1978, Solubility of the buffer assemblage pyrite + phrrhotite + magnetite in NaCl solutions from 200 to 350°C: Geochimica et Cosmochimica Acta, v. 42, p. 1427-1437.

Daniele, P. G., Rigano, C., and Smmartano, S., 1981, The formation of proton and alkali-metal complexes with ligands of biological interest in aqueous solutions. Thermodynamics of H^+, Na^+ and K^+ oxalate complexes: Thermochimica Acta, v. 46, p. 103-116

DeKock, C. W., 1986, Thermodynamic properties of selected metal sulfates and their hydrates. Bureau of Mines Information Circular IC9081, 59 p.

Drummond, S. E. Jr., 1981, Boiling and mixing of hydrothermal fluids: Chemical effects on mineral precipitation: Pennsylvania State University, unpublished Ph.D. thesis.

Ellis, A. J., 1976, The IAGC interlaboratory water analysis comparison programme: Geochimica et Cosmochimica Acta, v. 40, p. 1359-1374.
Ellis, A. J., and Golding, R. M., 1963, The solubility of carbon dioxide above 100 C in water and in sodium chloride solutions: American Journal of Science, v. 261, p. 47-60.
EPRI (Electric Power Research Institute), 1984, Geohydrochemical models for solute migration. Volumes I and II, EPRI Report EA-3417, Palo Alto, California, 120 p.
Felmy, A.R., Girvin, D., and Jenne, E.A., 1984, MINTEQ: a computer program for calculating aqueous geochemical equilibria: U.S. Environmental Protection Agency, Athens, Georgia.
Fournier, R. O., 1981, Application of water chemistry to geothermal exploration and reservoir engineering, in Rybach, Ladislaus, and Muffler, L. J. P., eds., Geothermal Systems: Principles and Case Histories: New York, Wiley, p. 109-143.
Fournier, R. O., and Potter, R. W., 1982, An equation correlating the solubility of quartz in water from 25° to 900°C at pressures up to 10,000 bars: Geochimica et Cosmochimica Acta, v. 46, p. 1969-1974.
Fournier, R. O., and Truesdell, A. H., 1973, An empirical Na-K-Ca geothermometer for natural water: Geochimica et Cosmochimica Acta, v. 37, p. 1255-1276.
Freeze, R. A., and Cherry, J. A., 1979, Ground Water: Englewood Cliffs, New Jersey, Prentice Hall Incorporated, 604 p.
Friedman, L. C., and Erdmann, D. E., 1982, Quality assurance practices for the chemical and biological analyses of water and fluvial sediments: U. S. Geological Survey Professional Paper 750-C, p. c151-c155.
Fuoss, R. M., 1958, Ionic association. III. The equilibrium between ion pairs and free ions: Journal of the American Chemical Society, v. 80, p. 5059-5061.
Garrels, R. M., and Christ, C.L., 1965, Solutions, minerals, and equilibria: Freeman-Cooper, San Francisco, California, 450 p.
Giordano, T. H., and Barnes, H. L., 1981, Lead transport in Mississippi Valley-type ore solutions: Economic Geology, v. 76, p. 2200-2211.
Giordano, T. H., and Drummond, S. E., 1987, Zinc acetate complexing in hydrothermal solutions: (Abs.) Geological Society of American Program, v. 19, p. 677.
Goodwin, B., 1982, Calculated uranium solubility in groundwater: implications for nuclear fuel waste disposal: Canadian Journal of Chemistry, v. 60, p. 1759-1766.
Gueddari, M., Mannin, C., Perret, D., Fritz, B., and Tardy, Y., 1983, Geochemistry of brines of the Chottel Jerid in southern Tunesia -- application of Pitzer's equations: Chemical Geology, v. 39, pp. 165-178.
Harned, H. S., and Owen, B. B., 1958, The physical chemistry of electrolyte solutions: Reinhold, New York, 803 p.
Harvie, C. E., and Weare, J. H., 1980, The prediction of mineral solubilities in natural waters: the Na-K-Mg-Ca-Cl-SO_4-H_2O system from zero to high concentration at 25°C: Geochimica et Cosmochimica Acta., v. 44, p. 981-997.
Harvie, C. E., Møller, N., and Weare, J. H., 1984, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_2-H_2O system to high ionic strengths at 25°C: Geochimica et Cosmochimica Acta, v. 48, p. 723-751.
Healy, T. W., White, L. R., 1978, Ionizable surface group models of aqueous interfaces: Advances in Colloid and Interface Science, v. 9, p. 303-345.

Helgeson, H. C., 1967, Thermodynamics of complex dissociation in aqueous solutions at elevated temperatures: Journal of Physical Chemistry, v. 71, p. 3121-3136

——— 1969, Thermodynamics of hydrothermal systems at elevated temperatures: American Journal of Science, v. 267, p. 729-804.

——— 1971a, KELYCOB, Theoretical geochemistry computer program: Library No. 0802D/E, University of California, Berkeley, California.

——— 1971b, Kinetics of mass transfer among silicates and aqueous solutions: Geochimica et Cosmochimica Acta, v. 34, p. 569-592.

——— 1985, SUPCRT-unpublished thermodynamic data base for minerals, aqueous species and gases. University of California, Berkeley, California.

Helgeson, H. C., Kirkham, D. H., 1974, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: II. Debye-Hückel parameters for activity coefficients and relative partial-molal properties: American Journal of Science, v. 274, p. 1199-1261.

Helgeson, H. C., Brown, T. H., Nigrini, A., and Jones, T. A., 1970, Calculations of mass transfer in geochemical processes involving aqueous solutions. Geochimica et Cosmochimica Acta, v. 34, p. 569-592.

Helgeson, H. C., Delany, J. M., Nesbitt, H. W., and Bird, D. K., 1978, Summary and critique of the thermodynamic properties of rock-forming minerals: American Journal of Science, v. 278A, 229 p.

Helgeson, H. C., Kirkham, D. H., and Flowers, G. C., 1981, Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high temperatures and pressures: IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal properties to 600°C and 5 kb: American Journal of Science, v. 281, p. 1249-1516.

Hem, J. D., 1985, Study and Interpretation of the Chemical Characteristics of Natural Water: U.S. Geological Survey Water-Supply Paper 2254, 253 p.

Hemingway, B. S., 1982, Thermodynamic properties of selected uranium compounds and aqueous species at 298.15 K and at higher temperatures: Preliminary nodels for the origin of coffinite deposits: U.S. Geological Survey Open-File Report 82-619, 90 p.

Hemmes, P., 1972, The volume change of ionic association reactions: Journal of Physical Chemistry, v. 76, p. 895-900.

Hogfeldt, E., 1982, Stability constants of metal-ion complexes. Part A: Inorganic Ligands: Int. Un. of Pure and Appl. Chemical IUPAC Chemical Data Series, No. 21, 310 pp.

Hohl, H., Sigg, L., and Stumm, W., 1980, Characterization of surface chemical properties of oxides in natural waters: in Advances in Chemistry series, Leckie, J., and Kavanaugh, M., eds., American Chemical Society, p. 1-31.

Holmes, H. F., and Mesmer, R. E., 1983, Thermodynamic properties of aqueous solutions of alkali metal chlorides to 250°C. Journal of Physical Chemistry, v. 87, p. 1242-1255.

Holmes, H. F., Bais, C. F., Jr., and Mesmer, R. E., 1978, Isopiestic studies of aqueous solutions at elevated temperatures I. KCl, $CaCl_2$, and $MgCl_2$: Journal of Chemical Thermodynamics, v. 10, p. 983-996.

Holmes, H. F., Bais, C. F., JR., and Mesmer, R. E., 1981, Isopiestic studies of aqueous solutions at elevated temperatures. III. $(1-\gamma)$ NaCl + $\gamma CaCl_2$: Journal of Chemical Thermodynamics, v. 13, p. 101-113.

Hovey, J. K., and Tremaine, P. R., 1986, Thermodynamics of aqueous aluminum standard partial molar heat capacities of Al^{+3} from 10 to 55°C: Geochimica et Cosmochimica Acta, v. 50, p. 453-460.

Hovey, J. K., Hepler, L. G., and Tremaine, P. R., 1988, Thermodynamics of aqueous aluminate ion: standard partial molar heat capacities and volumes of $Al(OH)_4^-(aq)$ from 10 to 55°C: Journal of Physical Chemistry, v. 92, p. 1323-1332.

Hull, R. W., Kharaka, Y. K., Maest, A. S., and Fries, T. L., 1985, Sampling and analysis of subsurface waters. A summary of current methodology: Proceedings Canadian-American Conference on Practical Applications of Groundwater Geo-chemistry, ARC, National Water Well Association, Banff, Canada, p. 117-126.

Hunter, R. J., 1981, Zeta potential in colloid science principles and applications. Academic Press, New York, 386 p.

Jacobson, P. L., and Langmuir, D., 1974, Dissociation constants of calcite and CaHCO for 0° to 50°C: Geochimica et Cosmochimica Acta, v. 38, p. 301-318.

James, R. O., and Parks, G. A., 1982, Characterization of Aqueous Colloids by their electrical double-layer and intrinsic surface chemical properties, in Surface and Colloid Science, Matijevic, E., ed., Plenum Press, New York, v. 12, p. 119-216.

Kalyanaraman, R., Yeatts, L. B., and Marshal, W. L., 1973, Solubility of calcium sulfate and association equilibrium in $CaSO_4$ and $NaSO_4$ and $NaClO_3$ and H_2O at 273 to 623 K: Journal of Chemical Thermodynamics, v. 5, p. 899-909.

Katayama, S., 1976, Conductimetric determination of ion-association constants for calcium, cobalt, zinc, and cadmium sulfates in aqueous solutions at various temperatures between 0° to 45°C: Journal of Solution Chemistry, v. 5, p. 241-248.

Keenan, J. H., Keyes, F. G., Hill, P. G., and Moore, J. G., 1969, Steam Tables: Wiley, New York, p. 162.

Kelly, K. K., 1960, Contributions to the data on theoretical metallurgy. XIII. High temperature heat content, heat capacity and entropy data for the elements and inorganic compounds: U. S. Bureau of Mines Bulletin No. 584, 232 p.

Kennedy, V. C., Zellweger, G. W., and Jones, B. F., 1974, Filter pore-size effects on the analysis of Al, Fe, Mn, and Ti in water: Water Resources Research, v. 10, p. 785-790.

Kerrisk, J. F., 1983, Reaction-path calculations of groundwater chemistry and mineral formation at Rainier Mesa, Nevada: Los Alamos National Laboratory Report #LA.9912-MS, 41 pp.

Kharaka, Y. K., and Barnes, I., 1973, SOLMNEQ: Solution-mineral equilibrium computations: U. S. Geological Survey Computer Contributions, National Technical Information Service, #PB215- 899, 81 p.

Kharaka, Y. K, and Mariner, R. H., 1989, Chemical geothermometers and their application to formation waters from sedimentary basins, in Thermal History of Sedimentary Basins. Naeser, N. D. and McCulloh, T., eds., Springer Verlag, New York, p. 99-117.

Kharaka, Y. K., Lico, M. S., and Carothers, W. W., 1980, Predicted corrosion and scale-formation properties of geopressured-geothermal waters from the Northern Gulf of Mexico Basin: Journal of Petroleum Technology, v. 32, p. 319-324.

Kharaka, Y. K., Hull, R. W., and Carothers, W. W., 1985, Water-rock interactions in sedimentary basins. Chap. 2., in Relationship of Organic Matter and Mineral Diagenesis. SEPM Short Course no. 17, p. 79-176.

Kharaka, Y. K., Law, L. M., Carothers, W. W., and Goerlitz, D. F., 1986, Role of organic species dissolved in formation waters in mineral diagenesis, in Special Vol. on Relationship of Organic Matter and Mineral Diagenesis, (ed D. Gautier), SEPM Special Vol. No. 38, 111-122.

Kielland, J., 1937, Individual activity coefficients of ions in aqueous solutions: American Chemical Society Journal, v. 59, p. 1675-1678.
Kublanovskii, V. S., 1977, Manganese(II) chloride complexes in the manganese(II) chloride-ammonia chloride-water system: Russian Journal of Inorganic Chemistry, v. 22, p. 405-408.
Lafon, G. M., 1969, Some quantitative aspects of the chemical evolution of the oceans: Ph.D. thesis, Northwestern University., Evanston, Illinois.
Lafon, G. M., and Truesdell, A. H., 1971, Temperature dependence of sodium sulfate complexing in aqueous solutions (abs.): American Geophysical Union Transactions, v. 52, p 362.
Langmuir, D., 1978, Uranium solution-mineral equilibria at low temperatures with applications to sedimentary ore deposits: Geochimica et Cosmochimica Acta, v. 42, p. 547-569.
Lemire., R. J., and Tremaine, P. R., 1980, Uranium and plutonium equilibria in aqueous solutions to 200°C: Journal of Chemical Engineering Data, v. 25, p. 361-370.
Lewis, G. N., and Randall, M., 1961, Thermodynamics: McGraw-Hill, New York, 723 p.
Lico, M. S., Kharaka, Y. K., Carothers, W. W., and Wright, V. A., 1982, Methods for collection and analysis of geopressured geothermal and oil-field waters: U. S. Geological Water-Supply Paper 2194, 21 p.
Lindsay, W. T., 1980, Estimation of concentration quotients for ionic equilibria in high temperature water: the model substance approach. Proceedings 41st International Water Conference, Engineering Society of Western Pennsylvania, pp. 284-294.
Lown, D. A., Thirsk, M. R., and Wynn-Jones, L., 1970, Temperature and pressure dependence of the ionization of acetic acid in water from 25° to 225°C and 1 to 3000 bars: Faraday Society Transactions, v. 66, p. 51-73.
Lundegard, P. D., and Land, L. S., 1986, Carbon dioxide and organic acids: Their origin and role in diagenesis, the Texas Gulf Coast Tertiary, in Relationship of Organic Matter and Mineral Diagenesis, Gautier, D.L., ed., SEPM Special Publication No. 38, p. 129-146.
MacGowan, D. B., and Surdam, R. C., 1988, Difunctional carboxylic acids in oilfield waters: Organic Geochemistry, v. 12, pp 245-259.
Marshall, W. M., 1980, Amorphous silica solubility, III. Activity coefficient relationships and prediction of solubility behavior in salt solutions, 0-350°C. Geochimica et Cosmochimica Acta, v. 44, p. 925-931.
Marshall, W. L., and Frank, E. V., 1981, Ion product of water substance, 0-1000°C, 1-10,000 bars, new international formulation and its background: Journal of Physical Chemical Reference Data, v. 10, p. 295-304.
Marshall, W. L., and Mesmer, R. E., 1981, On the pressure effects of ionization constants in aqueous solutions: Journal of Solution Chemistry, v. 10, p. 121-127.
Martell, A. E., and Smith, R. M., 1977, Critical stability constants: New York, Plenum, v. 3, 495 p.
May, H. M., Helmke, P.A., and Jackson, M. L., 1979, gibbsite solubility and thermodynamic properties of hydroxyaluminum ion in aqueous solution at 25°C: Geochimica et Cosmochimica Acta, v. 75, p. 351-361.
May, H. M., Kinniburgh, D. G., Helmke, P. A., and Jackson, M. L., 1986, Aqueous dissolution solubilities and thermodynamic stabilities of common alumino silicate clay minerals: Kaolinite and smectites: Geochimica et Cosmochimica Acta, v. 50, p. 1667-1678.
Merino, E., 1975, Diagenesis in Tertiary Sandstones From Kettleman North Dome, California--I. Diagenetic Mineralogy. Journal of Sedimentary Petrology, v. 45, p. 320-336.

——— , 1979, Internal consistency of a water analysis and uncertainty of the calculated distribution of aqueous species at 25 C: Geochimica et Cosmochimica Acta, v. 43, p. 1533-1542.
Mesmer, R. E., Bates, C. F., and Seeton, F. H., 1972, Acidity measurements at elevated temperatures: VI. Boric acid equilibrium: Inorganic Chemistry, v. 11, p. 536-543.
Meyer, H. J., and McGee, H. W., 1985, Oil and gas fields accompanied by geothermal anomalies in Rocky Mountain Region. American Association of Petroleum Geologists Bulletin, v. 69, p. 933-945.
Millero, F. J., 1972, The partial molal volumes of electrolytes in aqueous solutions, in Water and Aqueous Solutions, Horne, R. A., ed., John Wiley, New York, p. 519-593.
Møller, N., 1988, The prediction of mineral solubilities in natural waters: A chemical equilibrium model for the Na-Ca-Cl-SO_4-H_2O system, to high temperature and concentration: Geochimica et Cosmochimica Acta, v. 52 p. 821-837.
Morel, F. M., 1983, Principles of aqueous geochemistry. Wiley-Interscience, New York, 446 p.
Murray, R. C., and Cobble, J. W., 1980, Chemical equilibria in aqueous systems at high temperatures. Proceedings 41st International Water Conference, Engineering Society of Western Pennsylvania, pp 295-310.
Nancollas, G. H., 1956, Thermodynamics of ion association. II. Alkaline earth acetates and formates: Journal of Chemistry Society, p. 744-749.
Narasimhan, T. N., White, A. F., and Tokunaga, T, 1986, Groundwater contamination from an active uranium mill tailings piles, 2. Application of dynamic mixing model. Water Resources Research, v. 22, p. 1820-1834.
Naumov. G. B., Ryzhenko, B. N., and Khodakouskii, I. L., 1974, Handbook of thermodynamic data: U. S. Geological Survey Water Resources Publication 74-001, 239 p. (translated from Spravochnik Termodinamichesnikh Velichmin, Atomizdat, Moscow).
Navrotsky, A., 1987, Models of crystalline solutions, in Thermodynamic Modeling of Geological Materials: Minerals, Fluids, and Melts, Carmichael, I. S. E., and Eugster, H. P., Mineral Society of America, 17, p. 35-39.
Nordstrom, D. K., and Jenne, E. A., 1977, Fluorite solubility equilibria in selected geothermal waters: Geochimica et Cosmochimica Acta, v. 41, p. 175-188.
Nordstrom, D. K., and Munoz, J. L., 1985, Geochemical thermodynamics. The Benjamin/Cummings Publishing Company, Incorporated, Menlo Park, California, 477 p.
Nordstrom, D. K., Plummer, L. N., Wigley, T. M. L., Wolery, T. J., Ball, J. W., Jenne, E. A., Basset, R. L., Crerar, D. A., Floremce, T. M., Fritz, B., Hoffman, M., Holdren, G. R., Lafon, G. M., Mattigod, S. V., McDuff, R. E., Morel, F., Reddu, M. M., Sposito, G., and Thrailkill, J., (1979), A comparison of computerized chemical models for equilibrium calculations in aqueous systems. In Chemical Modeling in Aqueous Systems, Jenne, E. A., ed., American Chemical Society, Symposium Series 93, p. 857-892.
Pabalan, R. T. and Pitzer, K. S., 1987, Thermodynamics of NaOH(aq) in hydrothermal solutions: Geochimica et Cosmochimica Acta, v. 51, p. 829-838.
Palmer, D. A., and Drummond, S. E., 1988, A potentiometric determination of the molal formation constants of ferrous acetate complexes in aqueous solutions to high temperatures: Journal of Physical Chemistry, v. 92, p. 6795-6800.

Parkhurst, S. L., Thorstenson, C., and Plummer, L.N., 1980, PHREEQE: a computer program for geochemical calculations. U. S. Geological Survey, Report No. PB81-167801.

Parsons, M. L., Major, S., and Forster, A. R., 1983, Trace element determination by atomic spectroscopic methods-state of the art: Applied Spectroscopy, v. 37, no. 5, p. 411-418.

Patterson, C. S., Slocum, G. H., Busey, R. H., and Mesmer, R. E., 1982, Carbonate equilibria in hydrothermal systems: first ionization of carbonic acid in NaCl media to 300°C: Geochimica et Cosmochimica Acta, v. 46, p. 1653-1663.

Perkins, E. H., 1980, A reinvestigation of the theoretical basis of PATHI. University of British Columbia, Unpublished M.Sc. thesis.

Phillips, S. L., 1982, Hydrolysis and formation constants at 25°C: University of California Publication, LBL-14313.

Pitzer, K. S., 1973, Thermodynamics of electrolytes. I. Theoretical basis and general equations: Journal of Physical Chemistry, v. 77, p. 268-277.

———, 1981, Characteristics of very concentrated aqueous solutions, in Chemistry and geochemistry of solutions of high temperatures and pressures. Physics and Chemistry of the Earth, 13-14, p. 249-272.

Plummer, L. N., and Busenberg, Eurybiades, 1982, The solubilities of calcite aragonite and vaterite in CO_2 - H_2O solutions between 0° and 90°C, and an evaluation of the aqueous model for the system $CaCO_3$-CO_2-H_2O: Geochimica et Cosmochimica Acta, v. 46, p. 1011-1040.

Plummer, L. N., Jones, B. F., and Truesdell, A. H., 1976, WATEQF a FORTRAN IV version of WATEQ, a computer program for calculating chemical equilibrium of natural waters: U. S. Geological Survey Water Resource Investigation 76-13, 61 p.

Plummer, L. N., and Busenberg, E., 1984, WATEQF a FORTRAN IV version of WATEQ, a computer program for calculating chemical equilibrium of natural waters. U. S. Geological Survey Water Resources Investigation 76-13, 70 p.

Presser, T. S., and Barnes, I., 1974, Special techniques for determining chemical properties of geothermal waters: U.S. Geological Survey Water Resources Investigation 22-74, 11 p.

Reardon, E. J., 1975, Dissociation constants of some monovalent sulfate ion pairs at 25 form stoichiometric activity coefficients: Journal of Physical Chemistry, v. 79. p. 422-425.

Reed, M. H., 1982, Calculation of multicomponent chemical equilibria and reaction processes involving minerals, gases and an aqueous phase: Geochimica et Cosmochimica Acta, v. 46, p. 513-528.

Richet, P., Bottinga, Y., Denielou, L., Petit, J. P., and Tequi, C., 1982, Thermodynamic properties of quartz, cristobalite and amorphous silicon dioxide: Drop Calorimetry measurements between 1000 and 1800 K and a review from 0 to 2000 K: Geochimica et Cosmochimica Acta, v. 46, p. 2639-2658.

Roberson, C. E., and Barnes, R. B., 1978, Stability of fluoride complex with silica and its distribution in natural water systems: Chemical Geology, v. 21, p. 239-256.

Robie, R. A., Hemingway, B. S., and Fisher, J. R., 1978, Thermodynamic properties of minerals and related substances at 298.15 K and 1 bar pressure and at higher pressures: U. S. Geological Survey Bulletin 1452, 456 p.

Ruaya, J. R., and Seward, T. M., 1986, The stability of chlorozinc (II) complexes of hydrothermal solutions up to 350°C: Geochimica et Cosmochimica Acta, v. 50, p. 651-662.

Schoonen, M. A. A., and Barnes, H. L., 1988, An approximation of the second dissociation constant for H_2S: Geochimica et Cosmochimica Acta, v. 92, p. 649-654.

Seward, T. M., 1976, The stability of chloride complexes of silver in hydrothermal solutions up to 350°C: Geochimica et Cosmochimica Acta, v. 40, p. 1329-1342.

———, 1981, Metal complex formation in aqueous solutions at elevated temperatures and pressures: Physics and Chemistry of the Earth, 13-14, p. 113-128.

———, 1984, The formation of lead(II) chloride complexes to 300°C. A spectrophotometric study: Geochimica et Cosmochimica Acta, v. 48, p. 121-134.

Shanks, W. C., and Bischoff, J. L., 1977, Ore transport and deposition in the Red Sea geothermal system: a geochemical model: Geochimica et Cosmochimica Acta, v. 41, p. 1507-1519.

Siebert, R. M., and Hostetler, P. B., 1977, Stability constants of metal-ion complexes: Chemical Society [London], 745 p.

Sillen, L. G., and Martell, A. E., 1964, Stability constants of metal-ion complexes: Chemical Society [London], 754 p.

Silvester, K. S., and Pitzer, K. S., 1978, Thermodynamics of electrolytes. X. Enthalpy and the effect of temperature on the activity coefficients: Journal of Solution Chemistry, v. 7, p. 327-337.

Smith, R. M., and Martell, A. E., 1976, Critical stability constants: Plenum Press, New York, 4 vols.

Smith, R. W., Popp, C. J., and Norman, D. I., 1986, The dissociation of oxy-acids at elevated temperatures: Geochimica et Cosmochimica Acta, v. 50, p. 137-142.

Smith, W. R., and Missin, R. W., 1982, Chemical reaction equilibrium analysis. Wiley-Interscience, New York.

Sposito, G., 1982, The thermodynamic theory of ion exchange, in Thermodynamics of Ion Exchange, Sposito, G., ed., Wiley, New York, pp. 126-153.

Sposito, G., and Mattigod, S.V., 1980, GEOCHEM: A computer program for the calculation of chemical equilibria in soil solutions and other natural water systems. Report, Kearney Foundation of Soil Science, University of California.

Staples, B. R., and Nuttall, R. L., 1977, The activity and osmotic coefficients of aqueous calcium chloride at 298.15°: Journal of Physical Chemistry Reference Data, v. 6, p. 385-407.

Stoessell, R. K., 1988, 25°C and 1 atm dissolution experiments of sepiolite and kerolite: Geochimica et Cosmochimica Acta, v. 52, p. 365-374.

Swaddle, T. W., and Mak, M. K. S., 1983, The partial molar volumes of aqueous metal cations: their prediction and relation to volumes of activation for water exchange: Canadian Journal of Chemistry, v. 61, p. 473-480.

Tanger, J. C., and Helgeson, H. C., 1988, Calculation of the thermodynamic and transport properties of aqueous species at high pressure and temperatures: Revised equations of state for the standard partial molal properties of ions and electrolytes: American Journal of Science, v. 287, p. 1025-1049.

Tardy, Y., and Garrels, R. M., 1974, A method of estimating the Gibbs energies of formation of layer silicates: Geochimica et Cosmochimica Acta, v. 38, p. 1101-1116.

Thorstenson, D. C., 1984, The concept of electron activity and its relation to redox potentials in aqueous geochemical systems. U.S. Geological Survey Open-File Report 84-072, 45 p.

Thurman, E. M., 1984, Humic Substances I. Geochemistry, Characterization and Isolation. New York, John Wiley and Sons, 380 p.

———, 1985, Organic geochemistry natural waters: Boston Martinus Nijhoff, DRW Junk Publishers, 479 p.

Tremaine, P., 1987, Solubility and hydrolysis of aluminum oxides and hydroxides at elevated temperatures from apparent molar heat capacity and volume measurements near 25°C: Proceedings of Symposium on Chemistry in High Temperature Aqueous Solutions, Provo, Utah, Electric Power Research Institute Report, p. 18.

Tremaine, P. R., Chen, J. D., Wallace, G. J., and Boivin, W. A., 1981, Solubility of Uranium (IV) oxide in alkaline aqueous solutions to 300°C: Journal of Solution Chemistry, v. 10, No. 3, pp. 221-230.

Truesdell, A. H., and Jones, B. F., 1974, WATEQ, a computer program for calculating chemical equilibria of natural waters. Journal of Research, U.S. Geological Survey, v. 2, p. 233-248.

Truesdell, A. H., and Singer W., 1974, The calculation of aquifer chemistry in hot-water geothermal systems: U.S. Geological Survey Journal of Research v. 2, pp. 271-278.

Tugarinov, I. A., Ganeyev, I. G., and Khodakovskiy, I. L., 1975, Experimental determinations of hydrolysis constants of lead ions in aqueous solutions at temperatures up to 300°C: Geochemistry International, v. 12, p. 47- 55.

Vanderzee, C. E., 1982, Thermodynamic relations and equilibria in (Na_2CO_3, $NaHCO_3$, H_2O): Standard Gibbs energies of formation and other properties of sodium hydrogen carbonate, sodium carbonate heptahydrate, sodium carbonate decahydrate, trona: (Na_2CO_3-$NaHCO_3$* $2H_2O$), and wegscheiders salt: (Na_2CO * $3NaHCO_3$): Journal Chemical Termo., v. 14, pp 219-238.

Wagman, D. D., Evans, W. H., Parker, V. B., and Schumm, R. H., 1976, Chemical thermodynamic properties of compounds of sodium, potassium and rubidium: An interm tabulation of selected values: National Technical Information Service (NTIS) report, PB 254-460, 73 pp.

Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H., Harlow, I., Bailey, S. M., Churney, K. L., and Nuttall, R. L., 1982, The NBS tables of chemical thermodynamic properties. Journal of Chemical and Reference Data, vol 11, supplement 2.

Wagman, D. D. and others, 1968 and 1969, Selected values of chemical thermodynamic properties: NBS Technical Note No. 270-3; No. 270-4.

Westall, J., 1980, Chemical equilibrium including adsorption on charged surfaces, in Advances in Chemistry series, Leckie, J., and Kavanaugh, M., eds., American Chemical Society, p. 33-44.

Westall, J., and Hohl, H., 1980, A comparison of electrostatic models for the oxide/solution interface. Advances in Colloid and Interface Science, vol 12, p. 265-294.

Westall, J., Zachary, J. L., and Morel, F. M. M., 1976, MINEQL, a computer program for the calculation of chemical equilibrium composition of aqueous systems. Massachusetts Institute Technical Department of Civil Engineering Technical Note 18, 91 p.

Whitfield, M., 1975, An improved specific interaction model for seawater at 25 C and 1 atmosphere pressure: Mar. Chemical, v. 3, p. 197-205.

Willey, L. M., Kharaka, Y. K., Presser, T. S., Rapp, J. B. and Barmes, I., 1975, Short-chain aliphatic acids in oil field waters of Kettleman Dome oil field, California: Geochimica et Cosmochimica Acta, v. 39, p. 1707-1710.

Williams-Jones, A. E., and Seward, T. M., 1988, The stability of calcium chloro-complexes in aqueous solutions at temperatures between 100° and 360°C: Abstract in proceedings of Experimental investigations of hydrothermal processes: Applications to ore deposit genesis, Montreal, Quebec, Canada.

Wiwchar, B. W., Perkins, E. H., Gunter, W. D., in press, SOLMINEQ.88 PC/SHELL, Alberta Research Council Report, 130 p.

Wolery, T. J., 1979, Calculation of chemical equilibrium between aqueous solution and mineral: the EQ3/EQ6 software package: Lawrence Livermore Laboratory (UCRL-52658), 41 p.

———, 1983, EQ3NR, a computer program for geochemical aqueous speciation-solubility calculations, user's guide and documentation: Lawrence Livermore Laboratory (UCRL-53414), 191 p.

———, 1984, EQ36, a computer program for reaction-path modeling of aqueous geochemical systems: User's guide and documentation, Lawrence Livermore Laboratory UCRL-51 (draft), 251 pp.

———, 1986, unpublished EQ3 data base.

Wolley, E. M., and Hepler, L. G., 1977, Heat capacities of weak electrolytes and ion association reactions: Method and application to aqueous $MgSO_4$ and HIO_3 at 298 K: Canadian Journal of Chemistry, v. 55, p. 158-163.

Wood, S. A., Crerar, D. A., and Borcsik, M. P., 1987, Solubility of the assemblage pyrite-pyrrotite-magnetite-sphalerite-galena-gold-stibnite-dismuthinite-argentite-molybdenite in H_2O-Nacl-CO_2 solutions from 200° to 350°C: Economic Geology, v. 82, p. 1864-1887.

Zen, E-an, 1972, Gibbs free energy, enthalpy and entropy of ten rock-forming minerals: Calculations, discrepancies, implications: American Mineralogist, v. 57, p. 524-553.

APPENDIX I. DATABASE

The database for SOLMINEQ.88 consists of physical parameters of the aqueous species, equilibrium constants (K) of the dissociation, redox, and dissolution reactions, constants for calculating the activity coefficients, and data for the extrapolation of the K values to higher pressures. The physical parameters are listed in Table IA. In this table, the name of the species is followed by its charge, hydrated radius (a^o), and molecular weight.

Tables IB and IC list the equilibrium constants at eleven temperatures from 0° to 350°C for the dissociation of aqueous complexes and redox reactions (IB), and dissolution reactions for the minerals (IC). The eleven constants are arranged in two lines for each of the species; the first line contains data for the temperatures (°C) 0, 25, 50, 75, 100, 125, and 150, and the second line for 200, 250, 300, and 350. The corresponding reactions together with the sources of thermochemical data are listed in Tables 2 and 3 of the main text.

Parameters and equations used for calculating the activity coefficients are given in the main text and Table ID. Table ID contains the $B^{\bullet}$ values for the specific temperatures used to calculate the activity coefficients of charged species by the equation (24).

Data for the pressure effects on K values are given in Tables IE and IF. Table IE contains the fit parameters for adjusting the K values of dissolution reactions of 158 minerals. These parameters have been obtained (see text for details) mainly by the regression of high temperature-high pressure values of K reported by Helgeson and others (1978).

Entries in Table IF consist of three parameters. The first refers to the number of the aqueous dissociation reaction from Table IB, the second to the ΔV of this reaction at 25°C, and the third to the number of water ionization reactions that must be added to convert the dissociation reaction to an "ISOCOULOMBIC" form. Table IG contains the Pitzer Coefficients used to calculate the activity of water and the activity coefficients of charged species. Table IH gives the aqueous species number and stoichiometry involved in the congruent dissolution of minerals. This table is used in the calculation of saturation states of minerals and reactions involving mass transfer between minerals and water.

Table IA. Physical Parameters of Aqueous Species.

	Charge	a^{o}	Molecular Weight		Charge	a^{o}	Molecular Weight
1 Ca ++	2	6.0	40.080	53 Ba(OH) +	1	5.0	154.347
2 Mg ++	2	8.0	24.312	54 BaSO4	0	0.0	233.402
3 Na +	1	4.0	22.990	55 CaCO3	0	0.0	100.089
4 K +	1	3.0	39.102	56 CaHCO3 +	1	6.0	101.097
5 Cl -	-1	3.0	35.453	57 Ca(OH) +	1	6.0	57.087
6 SO4 --	-2	4.0	96.062	58 CaPO4 -	-1	5.4	135.051
7 HCO3 -	-1	4.5	61.017	59 CaHPO4	0	0.0	136.059
8 H +	1	9.0	1.008	60 CaH2PO4+	1	5.4	137.067
9 OH -	-1	3.5	17.007	61 CaSO4	0	0.0	136.142
10 H2O	0	0.0	18.015	62 CuCl	0	0.0	98.993
11 H4SiO4	0	0.0	96.115	63 CuCl2 -	-1	4.0	134.446
12 SiO2	0	0.0	60.085	64 CuCl3 --	-2	5.0	169.899
13 Ag +	1	2.5	107.870	65 CuCl +	1	4.0	98.993
14 Al +3	3	9.0	26.982	66 CuCl2	0	0.0	134.446
15 Ba ++	2	5.0	137.340	67 CuCl3 -	-1	4.0	169.899
16 Cu +	1	2.5	63.540	68 CuCl4 --	-2	5.0	205.352
17 Cu ++	2	6.0	63.540	69 Cu(OH) +	1	4.0	80.547
18 Fe ++	2	6.0	55.847	70 CuSO4	0	0.0	159.602
19 Fe +3	3	9.0	55.847	71 FeCl +	1	4.0	91.300
20 Hg2 ++	2	4.0	401.180	72 FeCl2	0	0.0	126.753
21 Hg ++	2	5.0	200.590	73 FeHPO4	0	0.0	151.826
22 Li +	1	6.0	6.939	74 H3PO4	0	0.0	97.995
23 Mn ++	2	6.0	54.938	75 Fe(OH) +	1	5.0	72.854
24 Mn +3	3	9.0	54.938	76 Fe(OH)2	0	0.0	89.862
25 Pb ++	2	4.5	207.190	77 FeOOH -	-1	5.0	88.854
26 Sr ++	2	5.0	87.620	78 FeSO4	0	0.0	151.909
27 Zn ++	2	6.0	65.370	79 FeCl ++	2	5.0	91.300
28 H2AsO3-	-1	4.0	130.936	80 FeCl2 +	1	5.0	126.753
29 PO4 -3	-3	5.0	94.971	81 FeCl3	0	0.0	162.206
30 F -	-1	3.5	18.998	82 FeCl4 -	-1	4.0	197.659
31 B(OH)3	0	0.0	61.833	83 FeSO4 +	1	5.0	151.909
32 NH3	0	0.0	17.031	84 FeSO4)2-	-1	4.0	247.970
33 H2S	0	0.0	34.080	85 Fe(OH)++	2	5.0	72.854
34 AlF ++	2	5.4	45.980	86 Fe(OH)2+	1	5.4	89.862
35 AlF2 +	1	5.4	64.978	87 Fe(OH)3	0	0.0	106.869
36 AlF3	0	0.0	83.977	88 Fe(OH)4-	-1	5.4	123.877
37 AlF4 -	-1	4.5	102.975	89 B(OH)4 -	-1	2.6	78.840
38 Al(OH)++	2	5.4	43.989	90 H2SiO4--	-2	5.4	94.100
39 Al(OH)2+	1	5.4	60.996	91 H3SiO4 -	-1	4.0	95.108
40 Al(OH)4-	-1	4.5	95.011	92 HAsO3 --	-2	5.0	129.928
41 Al(SO4)+	1	4.5	123.043	93 HAsO4 --	-2	5.0	139.929
42 AlSO4)2-	-1	4.5	219.105	94 H2AsO4 -	-1	4.0	140.936
43 AgCl	0	0.0	143.323	95 H3AsO4	0	0.0	141.944
44 AgCl2 -	-1	4.0	178.776	96 HF	0	0.0	20.006
45 AgCl3 --	-2	5.0	214.229	97 H2CO3	0	0.0	62.025
46 AgCl4 -3	-3	6.0	249.682	98 CO3 --	-2	4.5	60.009
47 Ag(SO4)-	-1	4.0	203.932	99 HPO4 --	-2	5.0	95.979
48 CH3COO -	-1	4.5	59.045	100 H2PO4 -	-1	5.4	96.987
49 H3AsO3	0	0.0	125.944	101 HS -	-1	3.5	33.072
50 AsO4 -3	-3	6.0	138.921	102 S --	-2	5.0	32.064
51 BaCO3	0	0.0	197.349	103 HSO4 -	-1	4.5	97.070
52 BaHCO3 +	1	4.0	198.357	104 HNO3	0	0.0	63.013

		Charge	a^{o}	Molecular Weight			Charge	a^{o}	Molecular Weight
105	HgCl +	1	4.0	236.043	159	ZnCl2	0	0.0	136.276
106	HgCl2	0	0.0	271.496	160	ZnCl3 -	-1	4.0	171.729
107	HgCl3 -	-1	4.0	306.949	161	ZnCl4 --	-2	5.0	207.182
108	HgCl4 --	-2	5.0	342.402	162	ZnSO4	0	0.0	161.432
109	HgSO4	0	0.0	296.652	163	AlF5 --	-2	5.0	121.974
110	HgSH2S)2	0	0.0	300.814	164	AlF6 -3	-3	6.0	140.972
111	Hg(HS)3-	-1	4.0	299.806	165	HgOH +	1	4.0	217.597
112	Hg	0	0.0	200.590	166	Hg(OH)2	0	0.0	234.605
113	KCl	0	0.0	74.555	167	U +4	4	9.9	238.030
114	KCO3 -	-1	3.8	99.111	168	UO2 +	1	2.5	270.030
115	KHSO4	0	0.0	136.172	169	UO2 ++	2	6.0	270.030
116	KSO4 -	-1	5.4	135.164	170	UOH +3	3	9.0	255.040
117	KHPO4 -	-1	5.4	135.081	171	U(OH)2++	2	6.0	272.050
118	LiOH	0	0.0	23.946	172	U(OH)3 +	1	2.5	289.060
119	LiSO4 -	-1	5.0	103.001	173	U(OH)4	0	0.0	306.070
120	MgCO3	0	0.0	84.321	174	U(OH)5 -	-1	3.5	323.080
121	MgHCO3 +	1	4.0	85.329	175	UF +3	3	9.0	257.030
122	MgF +	1	4.5	43.310	176	UF2 ++	2	6.0	276.030
123	MgOH +	1	6.5	41.319	177	UF3 +	1	2.5	295.030
124	MgSO4	0	0.0	120.374	178	UF4	0	0.0	314.030
125	MgPO4 -	-1	5.4	119.283	179	UF5 -	-1	3.5	333.030
126	MgHPO4	0	0.0	120.291	180	UF6 --	-2	4.5	352.030
127	MgH2PO4+	1	5.4	121.299	181	UCl +3	3	9.0	273.480
128	MnCl +	1	4.0	90.391	182	UHPO4 ++	2	6.0	334.010
129	MnCl2	0	0.0	125.844	183	U(HPO4)2	0	0.0	429.990
130	MnCl3 -	-1	4.0	161.297	184	U(HPO4)3	-2	4.5	525.970
131	MnCl4 --	-2	5.0	196.750	185	U(HPO4)4	-4	6.0	621.960
132	MnHCO3 +	1	4.0	115.955	186	USO4 ++	2	6.0	334.090
133	MnSO4	0	0.0	151.000	187	U(SO4)2	0	0.0	430.150
134	MnHPO4	0	0.0	150.917	188	U6(OH)15	9	9.9	1683.330
135	MnOH +	1	4.0	71.945	189	UO2OH +	1	2.5	287.040
136	NO3 -	-1	3.0	62.005	190	UO2(OH)2	0	0.0	304.050
137	NaCl	0	0.0	58.443	191	UO2)2OH2	2	6.0	574.080
138	NaCO3 -	-1	5.4	82.999	192	UO2)3OH5	1	2.5	895.140
139	NaHCO3	0	0.0	84.007	193	UO2)3OH7	-1	3.5	929.160
140	Na2CO3	0	0.0	105.989	194	UO2SO4	0	0.0	366.090
141	Na2SO4	0	0.0	142.041	195	UO2SO4)2	-2	4.5	462.150
142	NaSO4 -	-1	5.4	119.051	196	UO2F +	1	2.5	289.030
143	NaHPO4 -	-1	5.4	118.969	197	UO2F2	0	0.0	308.030
144	NaF	0	0.0	41.988	198	UO2F3 -	-1	3.5	327.030
145	NaHS	0	0.0	56.062	199	UO2F4 --	-2	4.5	346.030
146	NH4 +	1	2.5	18.039	200	UO2Cl +	1	2.5	305.480
147	NH4OH	0	0.0	35.046	201	UH3SiO4+	1	2.5	265.140
148	PbCl +	1	4.0	242.643	202	UO2HPO4	0	0.0	366.010
149	PbCl2	0	0.0	278.096	203	UO2HPO42	-2	4.5	461.990
150	PbCl3 -	-1	4.0	313.549	204	UO2H2PO4	1	2.5	367.080
151	PbCl4 --	-2	5.0	349.002	205	UH2PO4)2	0	0.0	464.130
152	PbSO4	0	0.0	303.252	206	UH2PO4)3	-1	3.5	561.180
153	MnCl ++	2	5.0	90.391	207	UO2CO3	0	0.0	330.040
154	Sr(OH) +	1	5.0	104.627	208	UO2CO3)2	-2	4.5	390.050
155	SrCO3	0	0.0	147.629	209	UO2CO3)3	-4	6.0	450.060
156	SrHCO3 +	1	4.0	148.637	210	VO4 -3	-3	5.2	114.940
157	SrSO4	0	0.0	183.682	211	VO ++	2	5.0	66.940
158	ZnCl +	1	4.0	100.823	212	V +3	3	9.0	50.940

		Charge	a°	Molecular Weight
213	HVO4 --	-2	5.2	115.950
214	H2VO4 -	-1	5.6	116.960
215	H3VO4	0	0.0	117.970
216	H4VO4 +	1	4.0	118.980
217	NaHVO4 -	-1	4.0	138.940
218	VO2F	0	0.0	101.940
219	VO2F2 -	-1	4.0	120.940
220	VOH ++	2	5.0	67.950
221	V(OH)2 +	1	5.4	84.960
222	V(OH)3	0	0.0	101.970
223	VOOH +	1	2.5	83.950
224	VOSO4	0	0.0	163.000
225	VOCl +	1	2.5	102.390
226	VOF +	1	2.5	85.940
227	VOF2	0	0.0	104.940
228	CH3COOH	0	0.0	60.053
229	AlAce ++	2	4.5	86.027
230	BaAce +	1	4.5	196.385
231	CaAce +	1	4.5	99.125
232	CuAce +	1	4.5	122.585
233	FeAce +	1	4.5	114.892
234	Fe(Ace)2	0	0.0	173.937
235	KAce	0	0.0	98.147
236	MgAce +	1	4.5	83.357
237	NaAce	0	0.0	82.035
238	PbAce +	1	4.5	266.235
239	Pb(Ace)2	0	0.0	325.280
240	Pb(Ace)3	-1	4.5	384.325
241	SrAce +	1	4.5	146.665
242	UO2Ace +	1	3.5	329.075
243	UO2Ace2	0	0.0	338.120
244	ZnAce +	1	4.5	124.415
245	Zn(Ace)2	0	0.0	183.460
246	C2O4 --	-2	5.4	88.018
247	HC2O4 -	-1	4.5	89.026
248	H2C2O4	0	0.0	90.034
249	AlOxy +	1	4.5	115.000
250	AlOxy)2-	-1	4.5	203.018
251	BaOxy	0	0.0	225.358
252	CaOxy	0	0.0	128.098
253	FeOxy	0	0.0	143.865
254	FeOxy +	1	4.5	143.865
255	KOxy -	-1	4.5	127.120
256	MgOxy	0	0.0	112.330
257	MnOxy	0	0.0	142.956
258	MnOxy)2	-2	5.4	197.894
259	MnOxy)3	-4	5.4	252.832
260	MnOxy +	1	4.5	142.956
261	NaOxy -	-1	4.5	111.008
262	PbOxy	0	0.0	295.208
263	SrOxy	0	0.0	175.638
264	ZnOxy	0	0.0	153.388
265	C4H4O4--	-2	5.4	116.072
266	HC4H4O4-	-1	4.5	117.080
267	H2C4H4O4	0	0.0	118.088
268	AlSuc +	1	4.5	143.054
269	AlSuc)2-	-1	4.5	143.054
270	BaSuc	0	0.0	253.412
271	CaSuc	0	0.0	156.152
272	FeSuc	0	0.0	171.919
273	FeSuc +	1	4.5	171.919
274	KSuc -	-1	4.5	155.174
275	MgSuc	0	0.0	140.384
276	MnSuc	0	0.0	171.010
277	NaSuc -	-1	4.5	139.062
278	PbSuc	0	0.0	323.262
279	SrSuc	0	0.0	203.692
280	ZnSuc	0	0.0	181.442
281	CaCl +	1	4.0	75.533
282	CaCl2	0	0.0	110.986
283	FeF ++	2	5.0	74.845
284	SiF6 --	-2	5.0	142.076
285	CH4 Gas	0	0.0	16.043
286	Pb(HS)2	0	0.0	273.334
287	Pb(HS)3-	-1	4.0	306.416
288	PbCO3	0	0.0	267.199
289	PbOH +	1	4.0	224.197
290	Zn(HS)2	0	0.0	131.514
291	Zn(HS)3-	-1	4.0	164.596
292	ZnHCO3 +	1	4.0	126.387
293	ZnOH +	1	4.0	82.377
294	Zn(OH)2	0	0.0	99.385
295	ZnHSOH	0	0.0	115.449

Table IB. Equilibrium Constants of Dissociation, and Redox Reactions at 0°to 350°C.

	0/200	25/250	50/300	75/350	100	125	150
1 HCO3 -	-10.63	-10.33	-10.17	-10.13	-10.16	-10.25	-10.39
	-10.78	-11.29	-11.88	-12.53			
2 H2O	-14.94	-13.99	-13.27	-12.71	-12.26	-11.91	-11.64
	-11.31	-11.20	-11.33	-11.88			
3 H4SiO4	-10.28	-9.83	-9.49	-9.26	-9.09	-8.97	-8.90
	-8.87	-8.96	-9.20	-9.36			
4 Cu ++	-11.09	-10.35	-9.72	-9.16	-8.68	-8.25	-7.86
	-7.21	-6.66	-6.20	-5.80			
5 Fe +3	8.96	8.80	8.64	8.48	8.33	8.20	8.09
	7.92	7.84	7.85	7.94			
6 Hg ++	6.11	4.67	3.46	2.44	1.56	0.80	0.13
	-0.97	-1.85	-2.56	-3.14			
7 Mn +3	13.23	11.95	10.86	9.94	9.14	8.44	7.83
	6.80	5.98	5.31	4.74			
8 H2AsO3 -	-12.68	-12.13	-11.74	-11.47	-11.30	-11.23	-11.20
	-11.35	-11.70	-12.10	-12.60			
9 AlF5 --	-20.39	-20.40	-20.61	-20.99	-21.54	-22.26	-23.16
	-25.20	-27.77	-30.86	-34.72			
10 H2S	-7.40	-7.00	-6.75	-6.63	-6.61	-6.61	-6.75
	-7.17	-7.72	-8.43	-9.23			
11 AlF ++	-6.94	-6.97	-7.07	-7.22	-7.43	-7.71	-8.04
	-8.78	-9.69	-10.94	-11.93			
12 AlF2 +	-12.52	-12.57	-12.76	-13.05	-13.45	-13.93	-14.51
	-15.88	-17.53	-19.64	-21.60			
13 AlF3	-16.61	-16.65	-16.86	-17.22	-17.72	-18.34	-19.06
	-20.82	-22.94	-25.42	-28.21			
14 AlF4 -	-19.00	-19.04	-19.26	-19.64	-20.18	-20.88	-21.75
	-23.89	-26.08	-28.87	-32.02			
15 Al(OH)++	-9.17	-9.04	-8.96	-8.97	-9.00	-9.05	-9.13
	-9.32	-9.54	-9.86	-10.49			
16 Al(OH)2+	-18.08	-18.06	-18.22	-18.57	-19.05	-19.66	-20.40
	-22.19	-24.38	-26.92	-29.81			
17 Al(OH)4-	-33.72	-32.77	-32.20	-31.84	-31.67	-31.58	-31.59
	-31.88	-32.40	-33.10	-34.20			
18 Al(SO4)+	-2.88	-3.00	-3.16	-3.34	-3.54	-3.76	-4.01
	-4.55	-5.18	-5.88	-6.65			
19 AlSO4)2-	-4.72	-4.89	-5.10	-5.35	-5.64	-5.96	-6.32
	-7.13	-8.06	-9.01	-10.27			
20 AgCl	-3.70	-3.32	-3.07	-2.94	-2.88	-2.88	-2.88
	-2.90	-3.07	-3.54	-4.22			
21 AgCl2 -	-5.80	-5.32	-4.74	-4.52	-4.46	-4.46	-4.45
	-4.58	-4.86	-5.42	-6.52			
22 AgCl3 --	-6.30	-5.10	-4.40	-4.00	-3.85	-3.77	-3.73
	-3.66	-3.70	-3.85	-4.10			
23 AgCl4 -3	-5.80	-3.90	-3.10	-2.40	-1.94	-1.70	-1.60
	-1.40	-1.50	-1.70	-2.10			
24 Ag(SO4)-	-1.22	-1.31	-1.41	-1.51	-1.62	-1.75	-1.89
	-2.23	-2.69	-3.44	-5.02			
25 CH3COOH	-4.77	-4.76	-4.78	-4.85	-4.79	-5.12	-5.31
	-5.58	-6.10	-6.80	-7.68			
26 BaCO3	-2.40	-2.50	-2.60	-2.70	-2.85	-3.00	-3.20
	-3.60	-4.10	-4.70	-5.30			

	0/200	25/250	50/300	75/350	100	125	150
27 BaHCO3)+	-1.18	-1.44	-1.70	-2.00	-2.27	-2.60	-2.88
	-3.62	-4.60	-5.60	-6.80			
28 Ba(OH)+	-0.43	-0.53	-0.65	-0.83	-1.03	-1.22	-1.43
	-1.86	-2.30	-2.83	-3.68			
29 BaSO4	-2.39	-2.31	-2.26	-2.23	-2.23	-2.24	-2.26
	-2.38	-2.59	-3.01	-3.60			
30 CaCO3	-3.14	-3.22	-3.51	-3.86	-4.17	-4.32	-4.67
	-5.44	-6.30	-7.24	-8.28			
31 CaHCO3)+	-0.82	-1.11	-1.28	-1.47	-1.66	-1.83	-2.00
	-2.33	-2.64	-2.90	-3.10			
32 Ca(OH)+	-1.03	-1.14	-1.28	-1.47	-1.67	-1.87	-2.08
	-2.51	-2.91	-3.44	-4.24			
33 CaPO4 -	-6.31	-6.47	-6.69	-6.95	-7.23	-7.65	-8.09
	-9.19	-10.77	-13.41	-19.11			
34 CaHPO4	-2.41	-2.61	-2.82	-3.05	-3.29	-3.57	-3.87
	-4.58	-5.56	-7.13	-10.46			
35 CaH2PO4+	-1.23	-1.44	-1.65	-1.87	-2.10	-2.34	-2.60
	-3.21	-4.01	-5.27	-7.90			
36 CaSO4	-2.30	-2.30	-2.40	-2.55	-2.70	-2.90	-3.10
	-3.60	-4.10	-4.50	-5.00			
37 CuCl	-2.80	-2.70	-2.65	-2.60	-2.50	-2.45	-2.35
	-2.25	-2.20	-2.40	-2.70			
38 CuCl2 -	-4.99	-4.94	-4.94	-4.98	-5.06	-5.19	-5.35
	-5.82	-6.57	-7.40	-8.80			
39 CuCl3 --	-5.15	-5.14	-5.18	-5.27	-5.39	-5.56	-5.78
	-6.36	-7.25	-8.30	-10.50			
40 CuCl +	-0.53	-0.02	-0.54	-1.04	-1.54	-2.05	-2.58
	-3.73	-4.80	-6.00	-7.30			
41 CuCl2	1.38	0.71	0.08	-0.53	-1.13	-1.73	-2.34
	-3.67	-4.90	-6.50	-8.50			
42 CuCl3 -	3.18	2.30	1.49	0.72	-0.02	-0.76	-1.50
	-3.08	-4.60	-6.50	-9.00			
43 CuCl4 --	5.75	4.60	3.56	2.58	1.65	0.74	-0.16
	-2.04	-3.90	-6.10	-8.70			
44 Cu(OH)+	-6.19	-6.06	-6.06	-6.02	-6.08	-6.18	-6.30
	-6.57	-6.89	-7.32	-8.06			
45 CuSO4	-2.19	-2.25	-2.34	-2.44	-2.56	-2.70	-2.86
	-3.26	-3.84	-4.79	-6.84			
46 FeCl +	1.06	0.53	0.08	-0.31	-0.66	-0.69	-1.23
	-1.58	-2.34	-2.33	-2.00			
47 FeCl2	9.19	8.21	7.23	6.25	5.27	4.29	3.31
	1.35	-0.61	-2.57	-4.53			
48 FeHPO4	-3.49	-3.60	-3.72	-3.89	-4.09	-4.30	-4.56
	-5.00	-5.60	-6.30	-7.10			
49 H3PO4	-21.97	-21.69	-21.63	-21.80	-22.02	-22.34	-22.73
	-23.71	-24.97	-26.60	-29.15			
50 Fe(OH) +	-4.54	-4.50	-4.50	-4.57	-4.66	-4.77	-4.90
	-5.19	-5.49	-5.87	-6.54			
51 Fe(OH)2	-7.28	-7.39	-7.57	-7.87	-8.20	-8.55	-8.94
	-9.73	-10.54	-11.50	-13.04			
52 FeOOH -	31.22	29.00	27.22	25.76	24.55	23.54	22.68
	21.36	20.41	19.77	19.36			
53 FeSO4	-2.41	-2.43	-2.48	-2.54	-2.63	-2.73	-2.86
	-3.19	-3.69	-4.53	-6.37			
54 FeCl ++	-0.98	-1.47	-1.96	-2.45	-2.94	-3.45	-3.97
	-5.06	-6.20	-7.50	-8.80			

	0/200	25/250	50/300	75/350	100	125	150
55 FeCl2 +	-1.64	-2.13	-2.62	-3.12	-3.62	-4.16	-4.72
	-5.87	-7.11	-8.46	-9.89			
56 FeCl3	-0.48	-1.13	-1.75	-2.37	-2.99	-3.63	-4.30
	-5.64	-7.06	-8.59	-10.19			
57 FeCl4 -	1.67	0.79	-0.04	-0.84	-1.63	-2.42	-3.23
	-4.83	-6.49	-8.24	-10.05			
58 FeSO4 +	-3.77	-4.14	-4.54	-4.96	-5.42	-5.91	-6.42
	-7.54	-8.79	-10.16	-11.64			
59 FeSO4)2-	5.16	5.42	5.72	6.07	6.45	6.89	7.38
	8.61	10.40	13.40	20.89			
60 Fe(OH)++	-12.10	-11.86	-11.69	-11.60	-11.55	-11.56	-11.58
	-11.68	-11.82	-12.08	-12.66			
61 Fe(OH)2+	-21.14	-20.88	-20.75	-20.89	-21.17	-21.61	-22.19
	-23.71	-25.66	-28.01	-30.70			
62 Fe(OH)3	-30.28	-28.50	-27.01	-25.90	-24.97	-24.28	-23.79
	-23.31	-23.60	-25.06	-30.05			
63 Fe(OH)4-	-34.92	-34.06	-33.70	-33.64	-33.83	-34.28	-34.95
	-36.95	-39.47	-42.68	-46.43			
64 H4(BO4)-	-5.45	-4.77	-4.20	-3.72	-3.32	-2.99	-2.71
	-2.27	-1.98	-1.80	-1.70			
65 AlF6 -3	-20.97	-20.88	-21.00	-21.30	-21.18	-22.42	-23.25
	-25.14	-27.54	-30.39	-33.81			
66 H3SiO4)-	-12.20	-11.70	-11.30	-11.10	-11.00	-11.00	-11.00
	-11.00	-11.50	-12.00	-13.00			
67 H3AsO3	-9.70	-9.29	-8.94	-8.67	-8.49	-8.35	-8.27
	-8.22	-8.29	-8.51	-8.59			
68 HAsO4 --	-11.85	-11.52	-11.30	-11.20	-11.15	-11.20	-11.25
	-11.50	-11.90	-12.40	-12.90			
69 H2AsO4 -	-18.79	-18.46	-18.24	-18.20	-18.24	-18.40	-18.61
	-19.19	-20.01	-21.12	-22.40			
70 H3AsO4	-20.95	-20.70	-20.60	-20.71	-20.90	-21.23	-21.63
	-22.60	-23.57	-25.49	-27.40			
71 HF	-2.99	-3.18	-3.38	-3.61	-3.84	-4.09	-4.33
	-4.86	-5.40	-5.95	-6.50			
72 H2CO3	-6.58	-6.35	-6.29	-6.32	-6.43	-6.58	-6.77
	-7.23	-7.79	-8.40	-8.26			
73 HPO4 --	-12.62	-12.34	-12.18	-12.14	-12.10	-12.14	-12.20
	-12.45	-12.80	-13.30	-13.80			
74 H2PO4 -	-19.93	-19.54	-19.36	-19.38	-19.43	-19.58	-19.77
	-20.35	-21.16	-22.26	-24.20			
75 HS -	-17.50	-17.00	-16.70	-16.30	-16.10	-15.80	-15.40
	-15.10	-14.80	-14.60	-14.40			
76 HSO4 -	-1.63	-1.95	-2.29	-2.64	-3.00	-3.37	-3.74
	-4.51	-5.29	-6.08	-6.88			
77 HNO3	1.67	1.43	1.13	0.85	0.59	0.30	0.05
	-0.49	-1.04	-1.66	-2.25			
78 HgCl +	-6.59	-6.25	-5.99	-5.80	-5.65	-5.56	-5.51
	-5.54	-5.78	-6.39	-8.00			
79 HgCl2	-14.18	-13.26	-12.51	-11.91	-11.42	-11.03	-10.73
	-10.36	-10.34	-10.84	-12.63			
80 HgCl3 -	-16.40	-15.35	-14.50	-13.81	-13.26	-12.82	-12.48
	-12.09	-12.10	-12.73	-14.91			
81 HgCl4 --	-15.85	-14.92	-14.18	-13.59	-13.13	-12.79	-12.54
	-12.34	-12.58	-13.53	-16.35			
82 HgSO4	-1.20	-1.40	-1.60	-1.90	-2.10	-2.30	-2.60
	-3.20	-4.00	-5.10	-6.05			

	0/200	25/250	50/300	75/350	100	125	150
83 HgSH2S)2	-38.50	-35.65	-33.25	-31.26	-29.58	-28.16	-26.97
	-25.15	-24.04	-23.83	-25.50			
84 Hg(HS)3-	-24.41	-22.03	-19.90	-18.13	-16.13	-14.43	-12.79
	-9.79	-7.15	-5.31	-6.16			
85 Hg	-3.28	-4.06	-5.61	-6.42	-7.28	-8.20	-9.19
	-10.30	-13.04	-17.31	-26.18			
86 KCl	1.00	0.88	0.77	0.67	0.57	0.46	0.34
	-0.06	-0.34	-0.95	-1.90			
87 KCO3 -	-1.04	-1.07	-1.14	-1.24	-1.37	-1.52	-1.96
	-2.10	-2.67	-3.64	-5.80			
88 KHSO4	-0.65	-0.85	-1.05	-1.15	-1.29	-1.39	-1.41
	-1.80	-2.20	-2.60	-3.20			
89 KSO4 -	-0.87	-0.89	-0.95	-1.04	-1.14	-1.27	-1.41
	-1.74	-2.21	-3.00	-4.78			
90 KHPO4 -	-0.11	-0.29	-0.51	-0.77	-1.05	-1.47	-1.91
	-3.01	-4.59	-7.23	-12.42			
91 LiOH	-0.26	-0.18	-0.20	-0.26	-0.34	-0.42	-0.50
	-0.68	-0.87	-1.07	-1.30			
92 Li(SO4)-	-0.64	-0.64	-0.64	-0.64	-0.64	-0.64	-0.64
	-0.64	-0.64	-0.64	-0.64			
93 MgCO3	-2.87	-2.98	-3.11	-3.27	-3.46	-3.66	-3.89
	-4.40	-4.98	-5.65	-6.37			
94 MgHCO3)+	-1.00	-1.07	-1.14	-1.23	-1.32	-1.42	-1.53
	-1.77	-2.04	-2.34	-2.67			
95 MgF +	-1.54	-1.82	-2.11	-2.41	-2.72	-3.00	-3.20
	-3.70	-4.40	-5.29	-6.27			
96 Mg(OH) +	-2.55	-2.60	-2.71	-2.89	-3.09	-3.32	-3.56
	-4.04	-4.59	-5.03	-5.82			
97 MgSO4	-2.34	-2.40	-2.49	-2.60	-2.73	-2.87	-3.02
	-3.32	-3.64	-3.96	-4.27			
98 MgPO4 -	-6.31	-6.47	-6.69	-6.95	-7.23	-7.65	-8.09
	-9.19	-10.77	-13.41	-19.11			
99 MgHPO4	-2.91	-3.11	-3.32	-3.55	-3.79	-4.07	-4.37
	-5.08	-6.06	-7.63	-11.00			
100 MgH2PO4+	-1.23	-1.44	-1.65	-1.87	-2.10	-2.34	-2.60
	-3.21	-4.01	-5.27	-7.90			
101 MnCl +	6.50	6.50	6.45	6.40	6.35	6.30	6.20
	6.00	5.70	5.20	4.00			
102 MnCl2	3.15	3.10	3.00	2.95	2.90	2.80	2.65
	2.25	1.80	1.00	-0.70			
103 MnCl3 -	1.80	1.70	1.60	1.50	1.30	1.15	0.95
	0.40	-0.20	-1.20	-3.40			
104 MnCl4 --	1.05	0.80	0.60	0.40	0.15	-0.15	-0.40
	-1.00	-1.80	-3.10	-5.80			
105 MnHCO3 +	-1.25	-1.27	-1.36	-1.50	-1.68	-1.87	-2.08
	-2.54	-3.02	-3.51	-4.00			
106 MnSO4	-2.03	-2.26	-2.40	-2.56	-2.74	-2.93	-3.15
	-3.70	-4.49	-5.85	-9.10			
107 MnCl ++	-2.12	-2.61	-3.10	-3.59	-4.08	-4.59	-5.11
	-6.20	-7.34	-8.64	-9.94			
108 MnHPO4	-3.47	-3.58	-3.70	-3.87	-4.07	-4.28	-4.55
	-4.98	-5.60	-6.30	-7.10			
109 MnOH +	-3.41	-3.44	-3.52	-3.66	-3.82	-4.00	-4.20
	-4.64	-5.17	-5.91	-7.24			
110 NaCl	1.00	0.85	0.80	0.70	0.65	0.55	0.45
	0.15	-0.25	-0.95	-2.00			

	0/200	25/250	50/300	75/350	100	125	150
111 NaCO3 -	-0.71	-1.27	-1.81	-2.35	-2.89	-3.45	-4.04
	-5.10	-6.15	-7.20	-8.30			
112 NaHCO3	0.39	0.25	0.12	-0.01	-0.13	-0.25	-0.38
	-0.68	-0.96	-1.40	-1.80			
113 Na2CO3	1.00	0.68	0.40	0.20	-0.05	-0.40	-0.70
	-1.40	-2.20	-3.20	-4.30			
114 Na2SO4	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
115 NaSO4 -	-1.00	-1.20	-1.30	-1.50	-1.64	-1.80	-1.90
	-2.20	-2.60	-3.00	-3.80			
116 NaHPO4 -	-0.11	-0.29	-0.51	-0.77	-1.05	-1.47	-1.91
	-3.01	-4.59	-7.23	-12.42			
117 Hg(OH) +	-10.90	-10.46	-10.14	-9.92	-9.79	-9.74	-9.77
	-10.08	-10.79	-12.29	-15.93			
118 NH4OH	-4.87	-4.75	-4.70	-4.75	-4.85	-4.95	-5.10
	-5.53	-6.00	-6.75	-8.00			
119 NaHS	0.90	0.83	0.77	0.69	0.57	0.47	0.34
	-0.06	-0.34	-0.95	-1.90			
120 NaF	1.06	0.88	0.70	0.54	0.38	0.23	0.08
	-0.22	-0.55	-0.93	-1.45			
121 PbCl +	-1.39	-1.41	-1.47	-1.55	-1.67	-1.85	-2.09
	-2.55	-3.18	-3.89	-4.80			
122 PbCl2	-1.80	-1.97	-2.17	-2.39	-2.62	-2.89	-3.18
	-4.00	-4.98	-6.26	-8.20			
123 PbCl3 -	-1.64	-1.66	-1.70	-1.91	-2.21	-2.50	-2.84
	-3.81	-5.03	-6.76	-9.50			
124 PbCl4 --	-1.40	-1.46	-1.56	-1.73	-1.93	-2.14	-2.36
	-2.14	-2.14	-2.14	-2.14			
125 PbSO4	-2.75	-2.75	-2.75	-2.75	-2.75	-2.75	-2.75
	-2.75	-2.75	-2.75	-2.75			
126 Zn(AC)2	-1.02	-1.35	-1.72	-2.04	-2.33	-2.70	-3.07
	-3.96	-5.07	-7.02	-11.55			
127 Sr(OH) +	-0.57	-0.69	-0.83	-0.99	-1.22	-1.42	-1.63
	-2.07	-2.52	-3.06	-3.92			
128 SrCO3	-2.48	-2.82	-3.13	-3.45	-3.77	-4.18	-4.72
	-5.90	-7.40	-9.24	-11.65			
129 SrHCO3 +	-0.82	-1.19	-1.56	-1.93	-2.31	-2.70	-3.12
	-4.14	-5.35	-6.88	-8.86			
130 SrSO4	-2.12	-2.20	-2.29	-2.40	-2.52	-2.67	-2.84
	-3.25	-3.84	-4.81	-6.30			
131 ZnCl +	0.07	-0.42	-0.88	-1.35	-1.80	-2.34	-2.89
	-4.01	-5.21	-6.55	-8.00			
132 ZnCl2	-0.13	-0.62	-1.04	-1.45	-1.92	-2.37	-2.96
	-3.98	-5.70	-7.51	-9.54			
133 ZnCl3 -	-0.11	-0.34	-0.62	-0.94	-1.36	-1.69	-2.02
	-3.00	-3.89	-4.86	-5.85			
134 ZnCl4 --	1.07	-0.18	-1.03	-1.63	-2.04	-2.57	-3.21
	-4.23	-6.24	-9.00	-12.70			
135 ZnSO4	-2.10	-2.21	-2.35	-2.50	-2.67	-2.86	-3.07
	-3.60	-4.36	-5.68	-6.85			
136 AsO4 -3	6.05	5.21	4.62	4.53	4.73	5.00	5.30
	6.33	7.75	9.80	12.60			
137 Hg(OH)2	-22.99	-21.87	-21.02	-20.38	-19.94	-19.66	-19.54
	-19.77	-20.77	-23.14	-29.13			
138 Fe2-Fe3	17.10	17.75	18.38	19.01	19.64	20.29	20.94
	22.33	23.92	26.01	29.87			

	0/200	25/250	50/300	75/350	100	125	150
139 Cu+-Cu2	3.77	4.25	4.65	5.00	5.32	5.61	5.89
	6.41	6.93	7.52	8.49			
140 Hg2-2Hg2	20.90	20.95	21.01	21.07	21.15	21.23	21.32
	21.56	21.90	22.47	23.78			
141 Mn2-Mn3	34.00	34.48	34.97	35.47	36.49	37.00	38.06
	28.80	28.60	28.50	28.30			
142 U4-UO2+	10.62	8.74	6.87	4.99	3.12	1.25	-0.61
	-4.35	-8.07	-11.79	-15.51			
143 UO2+-++	-3.76	-3.77	-3.83	-3.94	-4.08	-4.26	-4.48
	-5.01	-5.66	-6.42	-7.27			
144 V - VO	-6.72	-5.71	-4.87	-4.15	-3.53	-3.00	-2.53
	-1.74	-1.12	-0.61	-0.19			
145 VO - VO4	-48.37	-45.34	-42.90	-40.92	-39.45	-38.12	-37.19
	-36.21	-36.58	-39.28	-48.59			
146 CaCl +	-0.12	-0.42	-0.65	-0.87	-1.08	-1.25	-1.49
	-1.88	-2.04	-2.59	-2.91			
147 CaCl2	0.30	0.15	-0.02	-0.25	-0.51	-0.83	-1.15
	-1.82	-2.58	-3.44	-4.81			
148 UOH +3	-13.41	-13.27	-13.21	-13.19	-13.19	-13.21	-13.25
	-13.41	-13.69	-14.10	-14.66			
149 U(OH)2++	-26.29	-25.65	-25.24	-24.96	-24.78	-24.67	-24.64
	-24.78	-25.23	-25.99	-27.07			
150 U(OH)3 +	5.54	5.00	3.69	2.64	1.77	1.01	0.37
	-0.74	-1.60	-2.01	-0.93			
151 U(OH)4	10.25	8.57	7.13	6.05	5.18	4.47	3.88
	2.94	2.27	1.17	4.03			
152 U(OH)5 -	17.28	15.09	13.30	11.86	10.65	9.63	8.77
	7.44	6.57	6.14	10.06			
153 UF +3	-8.35	-8.66	-9.24	-9.51	-9.78	-10.03	-10.57
	-10.57	-11.16	-11.96	-13.55			
154 UF2 ++	-14.08	-14.49	-14.94	-15.40	-15.86	-16.33	-16.81
	-17.83	-19.01	-20.62	-23.85			
155 UF3 +	-18.86	-19.10	-19.48	-19.94	-20.45	-21.01	-21.63
	-23.07	-24.92	-27.71	-33.83			
156 UF4	-23.56	-23.72	-24.07	-24.54	-25.11	-25.72	-26.48
	-28.23	-30.57	-34.17	-42.23			
157 UF5 -	-25.19	-25.35	-25.72	-26.21	-26.78	-27.45	-28.21
	-30.09	-32.68	-36.85	-46.59			
158 UF6 --	-27.64	-27.68	-27.99	-28.45	-29.02	-29.69	-30.46
	-32.34	-34.88	-38.84	-47.78			
159 UCl +3	-2.58	-2.59	-2.76	-3.03	-3.38	-3.79	-4.25
	-5.28	-6.45	-7.73	-9.12			
160 UHPO4 ++	-11.39	-12.06	-12.73	-13.41	-14.09	-14.75	-15.40
	-16.66	-17.86	-19.00	-20.08			
161 U(HPO4)2	-21.53	-21.99	-22.59	-23.29	-24.06	-24.88	-25.72
	-27.44	-29.18	-30.90	-32.57			
162 U(HPO4)3	-8.81	-9.06	-9.43	-9.79	-10.33	-10.74	-11.23
	-11.99	-12.67	-13.27	-13.63			
163 U(HPO4)4	-10.56	-9.86	-9.50	-9.24	-9.33	-9.34	-9.52
	-9.76	-10.05	-10.55	-10.54			
164 USO4 ++	-5.56	-5.54	-5.68	-5.92	-6.23	-6.59	-7.01
	-8.00	-9.21	-10.65	-12.34			
165 U(SO4)2	-9.61	-9.84	-10.25	-10.76	-11.32	-11.95	-12.63
	-14.22	-16.17	-18.55	-21.39			
166 U6(OH)15	-31.52	-24.80	-18.42	-12.06	-5.90	-0.09	5.55
	16.47	27.80	38.00	38.00			

	0/200	25/250	50/300	75/350	100	125	150
167 UO2OH +	-8.42	-8.23	-8.10	-8.01	-7.94	-7.89	-7.85
	-7.86	-7.98	-8.24	-8.65			
168 UO2(OH)2	-16.71	-16.05	-15.54	-15.11	-14.74	-14.41	-14.14
	-13.76	-13.65	-13.84	-14.37			
169 UO2)2OH2	-23.42	-22.43	-21.68	-21.08	-20.60	-20.21	-19.91
	-19.56	-19.55	-19.89	-20.58			
170 UO2)3OH5	17.35	15.64	14.18	13.14	12.35	11.73	11.20
	10.51	10.09	10.33	12.98			
171 UO2)3OH7	33.97	30.80	27.84	25.36	23.14	21.10	19.24
	15.81	12.82	10.00	12.22			
172 UO2SO4	-2.72	-2.93	-3.33	-3.84	-4.43	-5.08	-5.78
	-7.34	-9.10	-11.09	-13.29			
173 UO2SO4)2	-3.81	-4.18	-4.57	-4.99	-5.43	-5.92	-6.46
	-7.75	-9.57	-12.69	-20.01			
174 UO2F +	-5.27	-5.19	-5.19	-5.24	-5.33	-5.46	-5.62
	-6.01	-6.54	-7.32	-8.94			
175 UO2F2	-9.04	-8.92	-8.91	-8.96	-9.06	-9.19	-9.37
	-9.86	-10.58	-11.80	-14.68			
176 UO2F3 -	-11.53	-11.43	-11.39	-11.38	-11.38	-11.40	-11.46
	-11.72	-12.29	-13.57	-17.36			
177 UO2F4 --	-12.71	-12.54	-12.55	-12.66	-12.85	-13.11	-13.45
	-14.36	-15.73	-18.07	-23.75			
178 UO2Cl +	-1.71	-2.10	-2.62	-3.22	-3.88	-4.57	-5.30
	-6.83	-8.45	-10.14	-11.91			
179 UH3SiO6+	2.62	2.40	2.21	2.06	1.92	1.80	1.69
	1.51	1.37	1.25	1.15			
180 UO2HPO4	-8.37	-8.41	-8.53	-8.73	-8.97	-9.24	-9.54
	-10.19	-10.86	-11.55	-12.23			
181 UO2HPO42	-18.73	-18.25	-18.16	-18.36	-18.77	-19.34	-20.02
	-21.62	-23.41	-25.30	-27.23			
182 UO2H2PO4	-10.22	-10.15	-10.20	-10.44	-10.54	-10.79	-11.07
	-11.70	-12.39	-13.10	-13.82			
183 UH4P2O10	-20.68	-19.92	-19.48	-19.27	-19.24	-19.34	-19.54
	-20.17	-20.99	-21.92	-22.92			
184 UH6P3O14	-30.18	-28.80	-27.94	-27.48	-27.32	-27.37	-27.61
	-28.45	-29.62	-30.99	-32.48			
185 UO2CO3	-10.41	-10.04	-10.00	-10.20	-10.55	-11.04	-11.65
	-13.11	-14.84	-16.87	-19.59			
186 UO2CO3)2	4.31	3.60	3.11	2.77	2.56	2.43	2.37
	2.36	2.35	2.10	0.67			
187 UO2CO3)3	9.42	9.55	9.51	9.36	9.12	8.81	8.45
	7.54	6.36	4.62	1.03			
188 HVO4 -3	-13.62	-13.27	-13.02	-12.98	-12.95	-13.21	-13.32
	-14.14	-15.53	-17.60	-20.48			
189 H2VO4 --	-21.92	-21.33	-20.94	-20.73	-20.74	-20.86	-21.24
	-22.47	-24.58	-27.76	-32.22			
190 H3VO4 -	-26.55	-25.16	-24.11	-23.25	-22.83	-22.55	-22.47
	-22.93	-25.94	-28.85	-32.85			
191 H4VO4	-29.76	-28.38	-27.33	-26.57	-26.06	-25.77	-25.69
	-26.16	-27.54	-29.94	-33.48			
192 NaHVO4 --	-0.20	-0.30	-0.40	-0.40	-0.50	-0.60	-0.70
	-0.90	-1.10	-1.40	-1.70			
193 VO2F	-27.17	-24.96	-23.10	-21.51	-20.16	-18.98	-17.95
	-16.25	-14.94	-13.99	-13.55			
194 VO2F2 -	-22.78	-21.10	-19.73	-18.56	-17.63	-16.82	-16.15
	-15.13	-14.55	-14.48	-15.70			

	0/200	25/250	50/300	75/350	100	125	150
195 V(OH) ++	-11.88	-11.73	-11.48	-11.40	-11.32	-11.32	-11.38
	-11.52	-11.83	-12.03	-12.60			
196 V(OH)2 +	-23.48	-22.13	-21.07	-20.18	-19.62	-19.15	-18.83
	-18.62	-19.00	-20.00	-21.67			
197 V(OH)3	-32.69	-30.92	-29.55	-28.40	-27.73	-27.18	-26.85
	-26.76	-27.61	-29.60	-33.30			
198 VOOH +	-8.52	-8.32	-8.29	-8.23	-8.28	-8.38	-8.50
	-8.87	-9.31	-9.82	-10.57			
199 VOSO4	2.72	2.48	2.18	1.88	1.57	1.23	0.92
	0.24	-0.69	-2.00	-3.10			
200 VOCl +	0.13	-0.04	-0.21	-0.36	-0.54	-0.70	-0.87
	-1.25	-1.69	-2.34	-3.74			
201 VOF +	-3.39	-3.30	-3.28	-3.43	-3.56	-3.68	-3.86
	-4.25	-4.85	-6.40	-6.95			
202 VOF2	-5.61	-5.46	-5.37	-5.30	-5.34	-5.40	-5.50
	-5.82	-6.35	-7.10	-8.10			
203 UO2 Ace+	-2.23	-2.39	-2.57	-2.76	-2.96	-3.20	-3.46
	-4.09	-4.99	-6.55	-10.24			
204 UO2(Ace2	-4.41	-4.51	-4.64	-4.81	-5.03	-5.28	-5.57
	-6.33	-7.47	-9.51	-14.44			
205 UO2 +	10.66	10.24	9.87	8.53	9.22	8.95	8.71
	8.33	8.10	8.00	8.04			
206 U +4	5.19	6.62	7.84	8.89	9.81	10.62	11.37
	12.68	13.86	14.96	16.04			
207 VO ++	-7.11	-7.44	-7.73	-7.94	-8.20	-8.40	-8.60
	-9.00	-9.42	-9.91	-10.46			
208 VO4 -3	34.98	32.33	30.13	28.27	26.71	25.38	24.25
	22.51	21.43	21.21	22.99			
209 AlAce +	-2.86	-2.86	-2.86	-2.86	-2.86	-2.86	-2.86
	-2.86	-2.86	-2.86	-2.86			
210 BaAce +	-1.08	-1.13	-1.19	-1.26	-1.40	-1.40	-1.53
	-1.80	-2.20	-2.85	-3.60			
211 CaAce +	-1.18	-1.23	-1.29	-1.36	-1.44	-1.54	-1.64
	-1.90	-2.30	-2.92	-3.73			
212 CuAce +	-1.84	-1.89	-1.96	-2.04	-2.14	-2.26	-2.40
	-2.74	-3.25	-4.17	-6.36			
213 FeAce +	-0.60	-0.87	-1.10	-1.38	-1.60	-1.79	-2.00
	-2.40	-3.00	-3.70	-4.80			
214 FeAce)2	-1.70	-1.89	-2.10	-2.34	-2.60	-2.90	-3.20
	-4.00	-5.27	-6.82	-8.90			
215 KAce	0.31	0.39	0.13	0.13	0.13	0.13	0.13
	0.13	0.13	0.13	0.13			
216 MgAce +	-1.35	-1.25	-1.16	-1.09	-1.03	-0.97	-0.93
	-0.86	-0.82	-0.80	-0.81			
217 NaAce	0.33	0.23	0.11	0.11	0.11	0.11	0.11
	0.11	0.11	0.11	0.11			
218 PbAce +	-2.28	-2.26	-2.26	-2.29	-2.33	-2.39	-2.47
	-2.71	-3.10	-3.83	-5.63			
219 PbAce)2	-3.67	-3.64	-3.65	-3.68	-3.75	-3.85	-3.98
	-4.36	-4.98	-6.14	-9.02			
220 PbAce)3-	-3.82	-3.72	-3.67	-3.65	-3.66	-3.70	-3.77
	-4.02	-4.48	-5.38	-7.69			
221 SrAce +	-1.12	-1.16	-1.21	-1.27	-1.34	-1.42	-1.51
	-1.70	-2.10	-2.64	-3.37			
222 ZnAce +	-5.40	-4.91	-4.83	-4.76	-4.75	-4.78	-4.84
	-5.10	-5.53	-6.53	-9.19			

	0/200	25/250	50/300	75/350	100	125	150
223 HC2O4 -	-1.32	-1.25	-1.20	-1.17	-1.14	-1.13	-1.12
	-1.13	-1.18	-1.27	-1.39			
224 H2C2O4	-4.23	-4.31	-4.43	-4.58	-4.77	-4.99	-5.26
	-5.90	-6.82	-7.96	-9.35			
225 AlOxy +	-6.00	-6.00	-6.00	-6.00	-6.00	-6.00	-6.00
	-6.00	-6.00	-6.00	-6.00			
226 AlOxy)2-	-11.00	-11.00	-11.00	-11.00	-11.00	-11.00	-11.00
	-11.00	-11.00	-11.00	-11.00			
227 BaOxy	-1.57	-1.57	-1.57	-1.57	-1.57	-1.57	-1.57
	-1.57	-1.57	-1.57	-1.57			
228 CaOxy	-3.00	-3.00	-3.00	-3.00	-3.00	-3.00	-3.00
	-3.00	-3.00	-3.00	-3.00			
229 FeOxy	-4.30	-4.40	-4.50	-4.60	-4.90	-5.00	-5.20
	-5.80	-6.70	-7.70	-9.00			
230 FeOxy +	-7.74	-7.74	-7.74	-7.74	-7.74	-7.74	-7.74
	-7.74	-7.74	-7.74	-7.74			
231 KOxy -	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
	-0.70	-0.70	-0.70	-0.70			
232 MgOxy	-3.47	-3.47	-3.47	-3.47	-3.47	-3.47	-3.47
	-3.47	-3.47	-3.47	-3.47			
233 MnOxy	-3.93	-4.00	-4.10	-4.29	-4.41	-4.61	-4.86
	-5.49	-6.45	-8.18	-12.37			
234 MnOxy)2	-17.70	-17.70	-17.70	-17.80	-17.90	-18.00	-18.20
	-18.70	-19.20	-20.20	-22.70			
235 MnOxy)3	-19.50	-19.50	-19.50	-19.60	-19.70	-19.80	-20.00
	-20.50	-21.00	-22.00	-24.50			
236 MnOxy +	-11.00	-11.10	-11.10	-11.20	-11.30	-11.40	-11.60
	-12.10	-12.60	-13.60	-16.10			
237 NaOxy -	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
	-0.90	-0.90	-0.90	-0.90			
238 PbOxy	-4.90	-4.74	-4.65	-4.59	-4.58	-4.61	-4.66
	-4.90	-5.31	-5.89	-6.62			
239 SrOxy	-2.54	-2.54	-2.54	-2.54	-2.54	-2.54	-2.54
	-2.54	-2.54	-2.54	-2.54			
240 ZnOxy	-4.78	-4.90	-4.90	-5.00	-5.10	-5.20	-5.40
	-5.90	-6.40	-7.40	-9.90			
241 HC4H4O4-	-4.27	-4.21	-4.18	-4.20	-4.25	-4.34	-4.44
	-4.80	-5.33	-6.04	-6.92			
242 H2C4H4O4	-5.67	-5.64	-5.68	-5.76	-5.89	-6.07	-6.26
	-6.89	-7.77	-8.91	-10.31			
243 AlSuc +	-5.30	-5.30	-5.30	-5.30	-5.30	-5.30	-5.30
	-5.30	-5.30	-5.30	-5.30			
244 AlSuc)2-	-10.00	-10.00	-10.00	-10.00	-10.00	-10.00	-10.00
	-10.00	-10.00	-10.00	-10.00			
245 BaSuc	-2.02	-2.02	-2.02	-2.02	-2.02	-2.02	-2.02
	-2.02	-2.02	-2.02	-2.02			
246 CaSuc	-2.00	-2.00	-2.00	-2.00	-2.00	-2.00	-2.00
	-2.00	-2.00	-2.00	-2.00			
247 FeSuc	-2.00	-2.20	-2.40	-2.60	-2.80	-3.00	-3.30
	-3.90	-4.70	-5.70	-6.80			
248 FeSuc +	-7.00	-7.00	-7.00	-7.00	-7.00	-7.00	-7.00
	-7.00	-7.00	-7.00	-7.00			
249 KSuc -	-0.30	-0.30	-0.30	-0.30	-0.30	-0.30	-0.30
	-0.30	-0.30	-0.30	-0.30			
250 MgSuc	-2.05	-2.05	-2.05	-2.05	-2.05	-2.05	-2.05
	-2.05	-2.05	-2.05	-2.05			

	0/200	25/250	50/300	75/350	100	125	150
251 MnSuc	-1.99	-2.17	-2.36	-2.57	-2.79	-3.03	-3.28
	-3.91	-4.71	-5.69	-6.84			
252 NaSuc +	-0.30	-0.30	-0.30	-0.30	-0.30	-0.30	-0.30
	-0.30	-0.30	-0.30	-0.30			
253 PbSuc	-3.20	-3.50	-3.70	-4.00	-4.30	-4.70	-5.00
	-5.90	-6.90	-8.20	-9.70			
254 SrSuc	-2.00	-2.00	-2.00	-2.00	-2.00	-2.00	-2.00
	-2.00	-2.00	-2.00	-2.00			
255 ZnSuc	-2.19	-2.46	-2.73	-3.02	-3.33	-3.67	-4.02
	-4.85	-5.92	-7.20	-8.72			
256 FeF ++	-5.82	-6.00	-6.20	-6.48	-6.81	-7.18	-7.60
	-8.50	-9.60	-10.70	-12.00			
257 SiF6 --	28.30	25.72	23.60	21.90	20.42	19.06	17.92
	15.41	12.92	10.75	10.33			
258 Pb(HS)2	-16.80	-15.90	-15.10	-14.50	-14.00	-13.50	-13.30
	-13.00	-13.40	-14.20	-15.30			
259 Pb(HS)3-	-18.58	-16.66	-15.23	-14.19	-13.46	-12.98	-12.71
	-12.66	-13.11	-13.93	-15.03			
260 PbCO3	-6.00	-7.00	-8.00	-8.80	-9.60	-10.30	-10.80
	-11.70	-12.40	-13.00	-13.51			
261 PbOH +	-8.00	-7.82	-7.68	-7.57	-7.48	-7.44	-7.42
	-7.51	-7.79	-8.33	-9.49			
262 Zn(HS)2	-14.14	-13.78	-12.75	-12.20	-12.30	-12.30	-12.30
	-12.90	-13.80	-15.00	-16.30			
263 Zn(HS)3-	-17.01	-15.95	-15.10	-14.50	-14.20	-14.20	-14.20
	-14.60	-15.30	-16.20	-17.10			
264 ZnHCO3 +	-1.35	-1.42	-1.55	-1.68	-1.82	-1.98	-2.20
	-2.71	-3.41	-4.55	-6.03			
265 ZnOH +	-5.14	-5.04	-5.06	-5.12	-5.27	-5.41	-5.58
	-5.96	-6.45	-7.16	-8.46			
266 Zn(OH)2	-10.50	-9.58	-8.96	-8.54	-8.32	-8.20	-8.13
	-8.25	-8.71	-9.70	-11.91			
267 ZnHSOH	-19.20	-18.40	-17.80	-17.30	-16.80	-16.30	-16.00
	-16.00	-16.40	-17.00	-17.80			

Table IC. Equilibrium Constants of Dissolution Reactions at 0° to 350°C

	0/200	25/250	50/300	75/350	100	125	150
1 ADULARIA	2.16	1.26	0.54	-0.35	-0.51	-0.91	-1.24
	-1.76	-2.14	-2.43	-2.65			
2 AKERMANITE	50.13	45.46	41.41	37.93	34.94	32.35	30.10
	26.35	23.28	20.58	19.03			
3 ALBITE	3.63	2.50	1.75	1.02	0.46	-0.05	-0.48
	-1.16	-1.75	-3.45	-4.90			
4 ALBITE LOW	3.93	3.11	2.30	1.58	0.96	0.43	-0.02
	-0.76	-1.39	-2.11	-2.58			
5 ALBITE HIGH	5.42	4.43	3.47	2.62	1.89	1.27	0.73
	-0.15	-0.90	-1.72	-2.27			
6 ALUNITE	0.11	-2.79	-5.53	-7.84	-9.89	-11.80	-13.59
	-17.11	-20.99	-26.54	-40.08			
7 AMESI14A	44.87	38.63	33.50	29.00	25.20	22.30	19.24
	14.55	10.46	6.00	3.00			
8 ANALCIME	7.33	6.05	4.91	3.93	3.11	2.41	1.81
	0.83	-0.03	-1.15	-3.65			
9 ANDALUSITE	20.16	16.57	13.53	10.97	8.78	6.90	5.23
	2.42	-0.09	-2.89	-6.79			
10 ANDESITE	15.12	12.73	10.64	8.85	7.30	5.97	4.82
	2.91	1.28	-0.37	-1.61			
11 ANHYDRITE	-4.14	-4.33	-4.64	-5.00	-5.40	-5.82	-6.26
	-7.26	-8.48	-9.26	-12.06			
12 ANNITE	33.22	29.14	25.48	22.39	19.74	17.47	15.49
	12.16	9.22	5.88	-0.60			
13 ANORTHITE	30.54	25.83	21.81	18.38	15.44	12.91	10.69
	6.93	3.63	0.02	-6.45			
14 APATCHLR	-64.90	-66.15	-67.40	-68.65	-69.90	-71.15	-72.40
	-74.90	-77.40	-79.80	-82.40			
15 APATFLUR	-68.56	-68.34	-68.74	-69.50	-70.50	-71.70	-73.04
	-76.13	-79.82	-84.61	-93.10			
16 APATHYDX	-59.89	-60.39	-61.41	-62.70	-64.15	-65.73	-67.41
	-71.03	-75.13	-80.22	-88.93			
17 ARAGONITE	-8.22	-8.34	-8.54	-8.81	-9.17	-9.59	-10.08
	-11.23	-12.59	-14.14	-15.84			
18 AUGITE	37.91	32.56	28.04	24.22	20.96	18.14	15.68
	11.51	7.88	4.00	-2.66			
19 AZURITE	-39.86	-39.46	-39.36	-39.38	-39.50	-39.68	-39.94
	-40.68	-41.89	-44.14	-50.00			
20 BARITE	-10.50	-9.96	-9.69	-9.58	-9.59	-9.69	-9.88
	-10.31	-10.80	-11.57	-13.00			
21 BOEHMITE	8.70	6.95	5.50	4.27	3.24	2.35	1.56
	0.23	-0.96	-2.33	-4.85			
22 BRUCITE	-11.54	-11.47	-11.53	-11.65	-11.85	-12.00	-12.24
	-12.89	-13.83	-15.12	-16.79			
23 BYTOWNITE	22.18	18.60	15.51	12.89	10.62	8.69	6.97
	4.20	2.96	-0.60	-2.44			
24 CALCITE	-8.38	-8.48	-8.66	-8.93	-9.27	-9.68	-10.16
	-11.29	-12.64	-14.18	-15.84			
25 CELESTITE	-6.51	-6.43	-6.53	-6.71	-6.95	-7.23	-7.56
	-8.35	-9.41	-10.30	-12.15			
26 CHALCEDONY	-4.21	-3.73	-3.38	-3.10	-2.88	-2.69	-2.53
	-2.26	-2.05	-1.88	-1.80			
27 CHAM, 7A	34.60	29.03	24.50	20.05	17.00	14.00	11.54
	7.23	3.43	-0.80	-3.50			

	0/200	25/250	50/300	75/350	100	125	150
28 CHLOR, 7A	81.86	71.94	63.47	56.30	50.24	45.06	40.53
	32.96	26.43	19.41	9.99			
29 CHLOR, 14A	78.30	68.57	60.28	53.70	47.32	42.25	37.80
	30.39	23.97	17.04	7.70			
30 CRYSOTIL	35.65	32.03	28.89	26.23	23.97	22.04	20.39
	17.68	15.53	13.74	14.50			
31 C-ENSTATIT	12.63	11.29	10.10	9.08	8.20	7.44	6.77
	5.67	4.75	3.91	3.32			
32 C-PTIL,Na	-8.10	-7.90	-8.10	-8.55	-9.00	-9.35	-9.70
	-10.20	-10.70	-11.90	-13.80			
33 C-PTIL,K	-16.00	-15.00	-14.55	-14.25	-14.10	-13.95	-13.90
	-13.80	-14.00	-15.00	-16.90			
34 C-PTIL,Ca	-9.20	-9.30	-9.60	-10.10	-10.60	-11.10	-11.70
	-13.10	-14.40	-15.50	-16.80			
35 C-PTIL,Mg	-4.20	-5.00	-5.80	-7.00	-8.10	-9.10	-10.00
	-11.50	-13.00	-15.30	-18.00			
36 CORUNDUM	25.60	21.40	17.91	15.00	12.53	10.40	8.53
	5.37	2.58	-0.45	-4.47			
37 CRISTOBA	-3.80	-3.54	-3.27	-3.01	-2.80	-2.61	-2.43
	-2.13	-1.91	-1.77	-1.76			
38 CRISTOBB	-3.13	-2.94	-2.76	-2.59	-2.54	-2.34	-2.23
	-2.09	-1.90	-1.79	-1.78			
39 DICKITE	8.34	6.17	4.32	2.78	1.48	0.38	-0.54
	-2.07	-3.35	-4.61	-3.98			
40 DIOPSIDE	21.69	19.63	17.79	16.19	14.81	13.63	12.59
	10.88	9.47	8.16	7.45			
41 DOLOMITE	-17.75	-18.06	-18.68	-19.50	-20.42	-21.45	-22.60
	-25.19	-28.36	-32.77	-39.61			
42 DSORD	-16.01	-16.52	-17.30	-18.26	-19.31	-20.45	-21.69
	-24.44	-27.74	-32.26	-39.18			
43 ENSTATITE	12.82	11.47	10.27	9.23	8.34	7.57	6.90
	5.77	4.85	4.00	3.40			
44 EPIDOTE	38.04	31.99	26.79	22.37	18.61	15.37	12.54
	7.74	3.45	-1.47	-10.99			
45 FAYALITE	21.91	19.43	17.27	15.42	13.84	12.47	11.27
	9.28	7.61	6.10	5.19			
46 FLUORITE	-11.32	-10.96	-10.73	-10.59	-10.53	-10.52	-10.55
	-10.71	-10.95	-11.24	-11.57			
47 FORSTERITE	32.49	29.07	26.13	23.63	21.48	19.62	18.00
	15.30	13.08	11.07	9.69			
48 GIBBS AM	-34.29	-34.42	-32.41	-31.80	-31.23	-30.89	-30.60
	-30.70	-31.29	-32.60	-36.22			
49 GIBBSITE	-34.95	-34.92	-32.70	-32.09	-31.64	-31.31	-31.13
	-31.11	-31.75	-33.22	-37.00			
50 GREENALITE	25.28	22.58	20.21	18.16	16.41	14.89	13.56
	11.34	9.42	7.30	4.36			
51 GYPSUM	-4.65	-4.60	-4.70	-4.85	-4.98	-5.16	-5.37
	-5.88	-6.50	-7.67	-8.48			
52 HALITE	1.50	1.59	1.62	1.62	1.57	1.52	1.44
	1.24	0.89	-0.41	-0.20			
53 HALLOYSITE	11.35	8.91	6.83	5.08	3.61	2.36	1.29
	-0.46	-1.93	-3.33	-2.84			
54 HEULANDITE	3.00	1.41	-0.20	-1.63	-2.86	-3.91	-4.80
	-6.26	-7.61	-9.57	-14.80			
55 HUNTITE	-28.79	-30.62	-32.33	-33.88	-35.26	-36.53	-37.08
	-39.91	-42.13	-44.85	-50.13			

	0/200	25/250	50/300	75/350	100	125	150
56 HYDRMAGN	-36.72	-38.53	-40.34	-41.99	-43.49	-44.89	-45.21
	-48.79	-51.65	-55.68	-64.64			
57 HYPHILIT	13.03	11.80	10.64	9.56	8.55	7.60	6.69
	4.92	3.09	0.86	-3.18			
58 ILLITE	13.52	10.34	7.75	5.61	3.82	2.31	1.03
	-1.03	-2.59	-3.79	-4.74			
59 KAOLINITE	8.55	6.23	4.25	2.58	1.17	-0.03	-1.07
	-2.82	-4.44	-6.50	-11.08			
60 KENYAITE	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00
	-25.00	-25.00	-25.00	-25.00			
61 K-SPAR	-0.18	-0.55	-0.99	-1.40	-1.76	-2.07	-2.34
	-2.82	-3.31	-4.12	-6.42			
62 KYANITE	17.85	14.48	11.64	9.24	7.21	5.46	3.93
	1.36	-0.87	-3.13	-5.12			
63 LABRADOR	19.29	16.25	14.28	11.31	9.43	7.77	6.32
	3.92	2.26	-0.18	-1.89			
64 LARNITE	42.58	38.88	35.71	32.99	30.66	28.64	26.87
	23.94	21.56	19.51	18.38			
65 LAUMONTITE	17.05	14.17	11.63	9.46	7.63	6.08	4.76
	2.66	0.99	-0.39	-2.20			
66 LEUCITE	7.75	6.52	5.42	4.46	3.64	2.93	2.32
	1.31	0.44	-0.46	-0.97			
67 LIME	35.76	32.66	30.04	27.81	25.89	24.23	22.78
	20.34	18.38	16.72	15.65			
68 MAGADITE	-14.34	-14.34	-14.34	-14.34	-14.34	-14.34	-14.34
	-14.34	-14.34	-14.34	-14.34			
69 MgFe2O4	25.60	21.10	17.31	14.12	11.39	9.04	6.97
	3.48	0.46	-2.51	-4.75			
70 MAGNESITE	-7.58	-8.05	-8.50	-8.89	-9.25	-9.57	-9.87
	-10.43	-11.00	-11.71	-13.07			
71 MgCl2	24.57	22.15	20.00	18.09	16.34	14.76	13.30
	10.70	8.44	6.44	4.65			
72 MARIALITE	4.05	1.71	-0.45	-2.25	-3.63	-5.15	-6.37
	-8.04	-9.57	-11.28	-13.80			
73 MERWINITE	75.05	68.17	62.24	57.17	52.82	49.05	45.77
	40.31	35.86	31.97	29.75			
74 MICROCLN	-0.18	-0.55	-0.99	-1.41	-1.77	-2.09	-2.36
	-2.84	-3.33	-4.13	-6.41			
75 MIEONITE	83.98	69.95	57.12	45.48	34.86	25.08	15.99
	-0.78	-16.72	-34.00	-60.60			
76 MIRABILT	-2.36	-1.09	-0.02	0.92	1.76	2.53	3.24
	4.52	5.73	7.33	15.95			
77 MONTICEL	33.28	30.15	27.40	25.02	22.96	21.14	19.54
	16.81	14.51	12.42	11.07			
78 MORD, Na	-4.00	-3.90	-4.04	-4.22	-4.40	-4.60	-4.80
	-5.10	-5.50	-6.00	-6.60			
79 MORD, K	-8.00	-7.60	-7.30	-7.13	-7.10	-7.03	-7.00
	-6.90	-7.00	-7.30	-7.80			
80 MUSCOVITE	16.51	12.88	9.76	7.12	4.89	3.00	1.37
	-1.34	-3.68	-6.10	-7.07			
81 NACHOLIT	-0.71	-0.43	-0.16	0.10	0.35	0.59	0.82
	1.23	1.53	1.60	0.87			
82 NATRTHRM	0.08	-0.01	-0.21	-0.48	-0.80	-1.17	-1.56
	-2.39	-3.26	-4.14	-5.02			
83 NATRON	-1.93	-0.88	0.01	0.76	1.47	2.10	2.66
	3.70	4.74	6.38	15.88			

	0/200	25/250	50/300	75/350	100	125	150
84 NEPHALINE	15.63	13.52	11.73	10.21	8.92	7.82	6.87
	5.28	3.89	2.37	-0.47			
85 NESQUHON	-4.14	-5.35	-5.32	-5.22	-5.04	-4.96	-4.90
	-4.86	-4.86	-5.07	-6.01			
86 NONT, Na	-10.88	-11.48	-11.90	-13.17	-13.18	-13.58	-13.95
	-14.59	-15.35	-16.83	-19.90			
87 NONT, K	-11.30	-11.81	-12.17	-13.38	-13.35	-13.72	-14.06
	-14.66	-15.40	-16.85	-19.90			
88 NONT, H	-11.94	-12.50	-12.92	-14.21	-14.26	-14.73	-15.16
	-15.95	-16.90	-18.54	-21.76			
89 NONT, Ca	-10.84	-11.54	-12.05	-13.40	-13.48	-13.96	-14.38
	-15.13	-16.00	-17.58	-20.77			
90 NONT, Mg	-10.81	-11.56	-12.12	-13.49	-13.61	-14.11	-14.56
	-15.35	-16.25	-17.87	-21.10			
91 OLDHAMIT	13.19	11.90	10.75	9.71	8.77	7.90	7.10
	5.66	4.40	3.27	2.26			
92 OLIGOCLA	10.40	8.73	7.22	5.91	4.79	3.82	2.99
	1.63	0.47	0.44	-1.46			
93 PARAGONI	18.42	14.39	10.95	8.03	5.57	3.47	1.65
	-1.41	-4.20	-7.61	-14.89			
94 PARAGASI	114.71	100.79	88.81	78.61	69.89	62.38	55.83
	44.82	35.35	25.38	8.34			
95 PERICLAS	23.92	21.51	19.46	17.74	16.26	14.98	13.86
	12.00	10.48	9.14	8.19			
96 PHILLIPS	3.30	3.30	3.30	3.30	3.30	3.30	3.30
	3.30	3.30	3.30	3.30			
97 PHLOGPITE	42.10	37.22	32.91	29.21	26.09	23.41	21.06
	17.25	13.75	10.11	3.20			
98 PHLOGPTF	20.52	16.73	13.25	10.19	7.49	5.10	2.94
	-0.91	-4.59	-8.84	-14.53			
99 PORTLAN	-5.25	-5.42	-5.71	-6.04	-6.38	-6.73	-7.09
	-7.90	-8.92	-10.51	-14.25			
100 POTASSI	90.96	84.12	78.33	73.39	69.13	65.41	62.15
	56.69	52.32	48.79	46.58			
101 PREHNITE	36.87	32.02	27.82	24.24	21.19	18.56	16.27
	12.41	9.00	5.16	-2.13			
102 PYROPHYL	1.42	-0.10	-1.61	-2.90	-4.02	-4.98	-5.82
	-7.27	-8.65	-10.54	-15.09			
103 QUARTZ	-4.24	-3.93	-3.63	-3.35	-3.10	-2.88	-2.68
	-2.36	-2.11	-1.94	-1.90			
104 SANIDINE	1.74	1.18	0.58	0.03	-0.45	-0.86	-1.22
	-1.82	-2.36	-3.00	-3.35			
105 SAPO, Na	30.19	26.88	23.91	21.32	19.14	17.26	15.61
	12.87	10.50	7.85	4.07			
106 SAPO, K	29.78	26.55	23.65	21.11	18.97	17.12	15.50
	12.80	10.45	7.82	4.08			
107 SAPO, H	28.16	25.85	22.91	20.33	18.15	16.26	14.61
	11.84	9.43	6.75	2.97			
108 SAPO, Ca	30.23	26.82	23.76	21.09	18.84	16.89	15.18
	12.33	9.85	7.09	3.20			
109 SAPO, Mg	30.26	26.80	23.71	21.00	18.72	16.74	15.01
	12.12	9.61	6.82	2.89			
110 SEPIOLITE	34.56	31.52	28.70	26.60	25.00	23.60	22.20
	20.10	18.36	17.10	16.40			
111 SILICAAM	-2.88	-2.70	-2.52	-2.37	-2.23	-2.10	-1.99
	-1.81	-1.67	-1.59	-1.54			

	0/200	25/250	50/300	75/350	100	125	150
112 SILICGEL	-2.94	-2.71	-2.52	-2.36	-2.20	-2.06	-1.93
	-1.74	-1.53	-1.30	-0.95			
113 SILLIMAN	19.39	15.73	12.63	10.02	7.79	5.86	4.18
	1.31	-1.24	-4.09	-9.28			
114 SMEC Ca	9.14	6.14	3.70	1.68	-0.01	-1.44	-2.65
	-4.60	-6.07	-7.20	-8.10			
115 SMEC K	8.67	5.86	3.57	1.69	0.12	-1.21	-2.33
	-4.12	-5.47	-6.51	-7.32			
116 SMEC Mg	9.08	6.04	3.57	1.51	-0.02	-1.64	-2.87
	-4.83	-6.32	-7.47	-8.36			
117 SMEC Na	9.01	6.12	3.77	1.83	0.22	-1.14	-2.29
	-4.13	-5.51	-6.57	-7.39			
118 Na2O	73.09	67.43	62.69	58.65	55.20	52.25	49.59
	45.27	41.86	39.12	37.47			
119 SPINEL	42.49	36.46	31.44	27.24	23.68	20.63	17.99
	13.58	9.88	6.36	3.56			
120 STILBITE	3.00	1.41	-0.20	-1.63	-2.86	-3.91	-4.80
	-6.26	-7.61	-9.57	-14.80			
121 STRENGIT	-27.31	-27.20	-27.41	-27.76	-28.22	-28.69	-29.36
	-30.66	-32.03	-33.43	-34.84			
122 SrCO3	-9.34	-9.27	-9.37	-9.59	-9.90	-10.28	-10.70
	-11.64	-12.65	-13.70	-14.72			
123 SYLVITE	0.60	0.91	1.12	1.26	1.35	1.39	1.40
	1.29	1.02	0.61	0.04			
124 TALC	23.59	21.13	18.83	16.84	15.11	13.62	12.32
	10.16	8.27	6.14	1.98			
125 THENARDI	-0.33	-0.29	-0.37	-0.52	-0.71	-0.94	-1.19
	-1.84	-2.71	-4.09	-7.25			
126 TREMOLITE	67.53	60.89	54.87	49.62	45.10	41.19	37.78
	32.06	27.15	21.83	12.15			
127 TRONA	-0.65	-0.63	-1.56	-2.21	-2.70	-3.04	-3.23
	-3.29	-2.92	-2.16	-1.32			
128 VIVIANIT	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00
	-36.00	-36.00	-36.00	-36.00			
129 WAIRAKITE	21.05	17.33	14.05	11.22	8.79	6.70	4.87
	1.80	-0.92	-4.04	-10.17			
130 WITHERITE	-8.96	-8.63	-8.78	-9.05	-9.42	-9.88	-10.41
	-11.70	-13.31	-15.25	-17.55			
131 WOLLASTO	14.82	12.60	12.50	11.55	10.73	10.01	9.39
	8.34	7.79	6.58	5.21			
132 ZOISITE	49.21	42.10	36.03	30.89	26.46	22.66	19.39
	13.76	8.83	3.37	-6.69			
133 SILVER	-1.53	-0.50	0.35	1.09	1.73	2.31	2.83
	2.75	4.58	5.43	6.69			
134 AgCl	-10.82	-9.73	-8.86	-8.15	-7.65	-7.19	-6.81
	-6.33	-6.10	-6.43	-6.97			
135 Ag2S	-39.90	-36.26	-33.18	-30.52	-28.20	-26.16	-24.35
	-21.30	-18.89	-16.99	-15.53			
136 COPPER	3.78	4.25	4.65	5.00	5.31	5.61	5.89
	6.41	6.93	7.52	8.49			
137 MALACHITE	-33.55	-33.58	-32.03	-31.76	-31.65	-31.70	-31.90
	-32.71	-34.16	-36.77	-43.08			
138 CuO	8.70	7.67	6.80	6.07	5.44	4.91	4.44
	3.66	2.98	2.23	0.90			
139 Cu2O	-2.35	-1.90	-1.50	-1.11	-0.73	-0.36	-0.01
	0.65	1.25	1.72	1.86			

	0/200	25/250	50/300	75/350	100	125	150
140 CuS	-24.48	-22.83	-21.50	-20.41	-19.50	-18.75	-18.10
	-17.16	-16.64	-16.70	-18.15			
141 Cu2S	-38.29	-34.95	-32.17	-29.79	-27.74	-25.96	-24.39
	-21.82	-19.86	-18.40	-17.38			
142 CuFeS2	-36.32	-34.07	-32.32	-30.90	-29.76	-28.83	-28.08
	-27.09	-26.77	-27.45	-30.99			
143 BORNITE	-111.09	-102.51	-95.49	-89.60	-84.60	-80.33	-76.67
	-70.88	-67.01	-65.43	-69.17			
144 FeCl2	9.12	7.90	6.76	5.70	4.70	3.76	2.88
	1.24	-0.24	-1.60	-2.55			
145 FeCl3	14.65	12.34	10.23	8.30	6.51	4.84	3.28
	0.42	-2.13	-4.45	-6.57			
146 FeCO3	-10.34	-10.54	-10.84	-11.21	-11.57	-11.96	-12.38
	-13.27	-14.28	-15.48	-17.32			
147 FeO	15.19	13.50	12.07	10.15	9.81	8.91	8.91
	6.79	5.66	4.55	2.93			
148 Fe2O3HEM	2.14	0.04	-1.69	-3.13	-4.34	-5.37	-6.28
	-7.85	-9.36	-11.30	-15.55			
149 Fe2O3MGH	6.40	6.40	6.40	6.40	6.40	6.40	6.40
	6.40	6.40	6.40	6.40			
150 Fe3O4	14.28	10.75	7.82	5.36	3.28	1.51	-0.04
	-2.64	-4.92	-7.26	-8.92			
151 Fe(OH)3	-38.67	-37.20	-36.10	-35.30	-34.73	-34.34	-34.10
	-33.92	-34.04	-34.35	-34.79			
152 GOETHITE	1.49	0.48	-0.33	-1.00	-1.60	-2.08	-2.50
	-3.20	-3.83	-4.47	-4.50			
153 FeSPYRHO	-3.69	-3.76	-3.90	-4.06	-4.24	-4.44	-4.66
	-5.19	-5.86	-6.89	-9.24			
154 FeSTROLT	-3.78	-3.87	-4.02	-4.20	-4.38	-4.59	-4.81
	-5.33	-5.99	-7.01	-9.36			
155 FeS2PYR	-26.54	-24.71	-23.34	-22.28	-21.46	-20.82	-20.36
	-19.88	-20.00	-21.05	-25.35			
156 GREIGITE	-45.00	-45.00	-45.00	-45.00	-45.00	-45.00	-45.00
	-45.00	-45.00	-45.00	-45.00			
157 Hg(L)	-4.25	-2.84	-1.69	-0.70	0.18	0.96	1.68
	2.98	4.16	5.38	7.11			
158 HgCl2(C)	-15.11	-14.11	-13.30	-12.64	-12.10	-11.66	-11.32
	-10.88	-10.79	-11.25	-12.99			
159 Hg2Cl2(C	-19.49	-17.84	-16.43	-15.23	-14.19	-14.27	-12.46
	-11.08	-9.95	-8.97	-8.04			
160 HgO	2.83	2.44	2.11	1.86	1.67	1.53	1.43
	1.31	1.25	1.19	1.53			
161 CINNABAR	-43.32	-39.86	-37.02	-34.64	-32.62	-30.90	-29.44
	-27.14	-25.53	-24.94	-23.94			
162 CINABMET	-41.84	-38.58	-35.89	-33.64	-31.74	-30.12	-28.75
	-26.60	-25.11	-25.26	-23.25			
163 MnCl2	9.89	8.79	7.75	6.77	5.85	4.99	4.16
	2.54	0.84	-1.30	-5.35			
164 MnCO3	-10.52	-10.54	-10.70	-10.94	-11.21	-11.54	-11.92
	-12.81	-13.91	-15.43	-18.26			
165 MnO	19.62	17.70	16.08	14.72	13.56	12.56	11.70
	10.28	9.13	8.13	7.56			
166 MnO2	-7.79	-8.33	-8.75	-9.11	-9.42	-9.68	-9.90
	-10.23	-10.36	-10.06	-7.29			
167 MnS	-0.13	-0.47	-0.82	-1.16	-1.50	-1.82	-2.16
	-2.87	-3.70	-4.67	-5.82			

	0/200	25/250	50/300	75/350	100	125	150
168 PbC12	-5.31	-4.82	-4.51	-4.31	-4.19	-4.14	-4.15
	-4.35	-4.86	-5.94	-8.92			
169 PbCO3	-13.37	-12.89	-12.62	-12.48	-12.40	-12.42	-12.51
	-12.88	-13.52	-14.58	-16.85			
170 PbOLITHR	13.60	12.55	11.67	10.90	10.25	9.66	9.18
	8.62	8.33	7.64	8.97			
171 PbOMASIC	13.76	12.69	11.80	11.07	10.48	9.99	9.59
	8.98	8.53	8.19	8.34			
172 PbS GALN	-16.30	-14.78	-13.59	-12.90	-12.34	-11.83	-11.42
	-10.93	-10.72	-10.82	-11.10			
173 PbSO4	-8.07	-7.80	-7.70	-7.69	-7.74	-7.84	-7.98
	-8.43	-9.15	-10.45	-13.74			
174 ZnCO3	-9.20	-9.87	-10.50	-10.15	-11.72	-12.22	-12.66
	-13.34	-13.83	-14.22	-14.63			
175 ZnO	12.90	11.20	9.70	8.30	7.17	6.10	5.38
	4.42	4.02	4.02	4.23			
176 ZnS	-12.42	-11.79	-11.32	-11.00	-10.82	-10.65	-10.54
	-10.60	-10.83	-11.05	-10.95			
177 ZnSO4	4.71	3.54	2.38	1.30	0.30	-0.66	-1.58
	-3.36	-5.23	-7.57	-11.95			
178 RUTHERFO	-17.11	-16.88	-16.81	-16.89	-17.03	-17.26	-17.57
	-18.33	-19.31	-20.54	-22.47			
179 URAMPHIT	-27.44	-27.07	-27.04	-27.25	-27.64	-28.17	-28.80
	-30.26	-31.89	-33.62	-35.39			
180 PRZHEVAL	-18.49	-19.52	-20.62	-21.75	-22.89	-24.03	-25.17
	-27.42	-29.65	-31.86	-34.06			
181 TOBERNIT	-19.02	-20.37	-21.82	-23.33	-24.87	-26.41	-27.96
	-31.04	-34.09	-37.11	-40.13			
182 SALEEITE	-16.92	-18.73	-20.28	-21.62	-22.80	-23.83	-24.76
	-26.36	-27.81	-29.16	-30.47			
183 SR AUTUN	-18.31	-19.52	-20.77	-22.02	-23.26	-24.48	-25.69
	-28.06	-30.38	-32.69	-34.99			
184 URANOCIR	-18.77	-19.70	-20.84	-22.12	-23.49	-24.90	-26.34
	-29.29	-32.27	-35.27	-38.28			
185 BASSETIT	-17.94	-19.55	-21.23	-22.94	-24.64	-26.33	-28.00
	-31.30	-34.53	-37.72	-40.87			
186 UO3 (C)	9.05	7.76	6.66	5.71	4.88	4.16	3.51
	2.41	1.50	0.75	0.11			
187 UO3 (AM)	10.99	10.45	9.14	8.01	7.02	6.16	5.39
	4.09	3.02	2.13	1.38			
188 UO2(OH)2	-23.06	-22.12	-21.47	-21.00	-20.68	-20.47	-20.36
	-20.38	-20.78	-21.54	-22.64			
189 UF4*2.5W	-27.66	-27.61	-27.70	-27.89	-28.15	-28.48	-28.89
	-29.96	-31.41	-33.29	-35.61			
190 UHP)2*4W	-26.69	-26.74	-27.06	-27.56	-28.19	-28.92	-29.71
	-31.40	-33.09	-34.41	-32.18			
191 NINGYOIT	-28.73	-29.19	-29.85	-30.63	-31.50	-32.42	-33.38
	-35.39	-37.49	-39.66	-41.89			
192 U3O8	0.30	-1.00	-2.08	-2.99	-3.76	-4.42	-5.00
	-5.93	-6.67	-7.26	-7.73			
193 UO2(AM)	2.81	0.92	-0.68	-2.05	-3.22	-4.25	-5.15
	-6.66	-7.87	-8.85	-9.68			
194 UO2(C)	-3.40	-4.66	-5.72	-6.61	-7.39	-8.06	-8.65
	-9.64	-10.42	-11.07	-11.60			
195 U4O9	-13.61	-16.33	-18.54	-20.36	-21.86	-23.11	-24.16
	-25.79	-26.95	-27.78	-28.37			

	0/200	25/250	50/300	75/350	100	125	150
196 USIO4	-7.44	-8.30	-9.06	-9.72	-10.31	-10.81	-11.05
	-11.96	-12.51	-12.95	-13.33			
197 H AUTUNI	-22.78	-23.40	-24.01	-24.64	-25.24	-25.83	-26.41
	-27.52	-28.58	-29.57	-30.51			
198 NA AUTUN	-22.04	-22.49	-22.95	-23.41	-23.85	-24.29	-24.71
	-25.51	-26.29	-27.06	-27.83			
199 K AUTUNI	-23.27	-23.28	-23.40	-23.58	-23.81	-24.07	-24.35
	-24.94	-25.58	-26.25	-26.95			
200 AUTUNITE	-18.30	-19.62	-20.85	-22.00	-23.05	-24.03	-24.96
	-26.69	-28.31	-29.86	-31.40			
201 K2U2V2Ox	-57.98	-56.45	-55.26	-54.32	-53.58	-52.99	-52.51
	-51.87	-51.51	-51.39	-51.58			
202 CAU2V2OX	-53.28	-53.02	-52.94	-52.97	-53.08	-53.25	-53.47
	-54.03	-54.72	-55.62	-57.11			
203 URANOPHA	17.38	17.38	17.38	17.38	17.38	17.38	17.38
	17.38	17.38	17.38	17.38			
204 SCHOEPIT	-24.46	-23.38	-22.60	-22.02	-21.59	-21.28	-21.07
	-20.91	-21.07	-21.72	-23.17			
205 MGUO4	26.42	23.22	20.51	18.21	16.23	14.51	13.01
	10.51	8.49	6.85	6.56			
206 CAUO4	17.01	14.89	13.12	11.63	10.38	9.32	8.41
	6.94	5.82	5.00	5.58			
207 BAUO4	19.75	17.64	15.88	14.41	13.16	12.09	11.18
	9.71	8.60	7.83	8.56			
208 UO2F2	-6.79	-7.30	-7.82	-8.33	-8.83	-9.33	-10.87
	-10.78	-12.05	-13.66	-16.88			
209 US3	-19.33	-18.41	-17.83	-17.53	-17.41	-17.45	-17.63
	-18.32	-19.51	-21.59	-27.48			
210 V2O3	12.50	9.83	7.61	5.74	4.16	2.80	1.62
	-0.30	-1.80	-2.99	-3.94			
211 V2O4	10.47	8.53	6.98	5.73	4.71	3.88	3.20
	2.19	1.51	1.06	0.78			
212 V2O5	-33.26	-31.82	-30.60	-29.55	-28.64	-27.85	-27.15
	-25.98	-25.03	-24.24	-23.58			
213 VOSO4*6W	-5.10	-4.68	-4.64	-4.85	-5.26	-5.81	-6.49
	-8.14	-10.13	-12.14	-15.01			
214 PB3VO4)2	-52.49	-50.84	-49.52	-48.39	-47.39	-46.51	-45.72
	-44.41	-43.47	-43.11	-44.37			

Table ID. Parameters for Calculating Activity Coefficients by the $B^{\bullet}$ Method (Helgeson, 1969).

Temperature	$B^{\bullet}$	Temperature	$B^{\bullet}$
0.0	0.038	200.0	0.047
25.0	0.041	250.0	0.034
50.0	0.043	270.0	0.015
100.0	0.046	300.0	0.000
150.0	0.047	350.0	0.000

Table IE. Fit Parameters for Calculating the Equilibrium Constants of Dissolution Reactions at Higher Pressures.

	500 bars			1000 bars		
	A	$Bx10^4$	$Cx10^{16}$	A	$Bx10^4$	$Cx10^{16}$
1	0.623	-5.380	12.260	2.275	-22.600	16.490
2	0.038	17.930	10.050	0.059	28.706	12.710
3	0.584	-4.260	11.170	1.057	-1.960	14.986
4	0.705	-10.557	15.702	1.388	-24.487	24.043
5	0.709	-10.696	15.144	1.390	-24.371	24.005
6	1.847	32.520	75.360	3.717	42.296	96.763
7	1.603	-20.100	59.016	2.810	-14.920	80.253
8	0.491	-2.578	12.683	0.869	-1.719	15.855
9	0.537	-0.576	21.450	0.930	3.320	26.929
10	0.769	-7.714	20.010	1.441	-14.938	27.290
11	0.423	-1.000	16.176	0.729	1.576	20.302
12	0.871	-3.512	28.668	1.506	0.512	35.887
13	0.865	-3.449	26.480	1.520	-0.614	32.160
14	1.380	0.000	0.000	2.750	0.000	0.000
15	1.380	0.000	0.000	2.750	0.000	0.000
16	1.380	0.000	0.000	2.750	0.000	0.000
17	0.473	-1.575	17.190	0.846	0.108	21.650
18	0.000	0.000	0.000	0.000	0.000	0.000
19	1.701	-28.676	27.076	3.206	-44.737	38.138
20	0.394	-1.119	15.305	0.674	1.229	19.202
21	0.193	-0.145	10.250	0.288	3.732	13.108
22	0.484	-1.633	18.297	0.840	0.681	23.004
23	0.833	-4.871	24.320	1.494	-5.389	30.540
24	0.514	-1.970	17.096	0.928	-0.790	21.485
25	0.417	-1.015	15.819	0.720	1.324	19.876
26	0.111	-0.963	0.435	0.210	-1.617	0.575
27	0.913	-13.266	29.151	1.646	-14.039	39.787
28	0.000	0.000	0.000	0.000	0.000	0.000
29	0.000	0.000	0.000	0.000	0.000	0.000
30	0.432	1.186	17.613	0.661	7.287	21.954
31	0.188	0.084	6.001	0.313	1.520	7.530
32	0.000	0.000	0.000	0.000	0.000	0.000
33	0.000	0.000	0.000	0.000	0.000	0.000
34	0.000	0.000	0.000	0.000	0.000	0.000
35	0.000	0.000	0.000	0.000	0.000	0.000
36	0.413	0.634	20.940	0.690	5.624	26.290
37	0.135	-1.345	0.584	0.268	-2.402	0.583
38	0.150	-1.600	0.480	0.288	-2.940	0.621
39	0.162	28.640	16.790	0.900	5.826	27.260
40	0.422	-0.558	21.130	0.638	1.832	13.700
41	0.982	-3.101	35.360	1.749	0.756	44.430
42	0.921	-15.653	9.425	1.747	-26.193	13.480
43	0.188	0.084	6.001	0.313	1.520	7.530
44	1.221	-12.484	36.876	2.180	-8.362	50.108
45	0.349	-1.967	11.190	0.610	-0.943	14.060
46	0.399	-0.047	17.580	0.682	3.602	22.020
47	0.302	0.224	11.630	0.476	3.687	14.510
48	0.773	-2.712	29.530	1.373	0.453	37.140
49	0.773	-2.712	29.530	1.373	0.453	37.140
50	0.645	-7.980	14.829	1.156	-7.986	20.008

	500 bars			1000 bars		
	A	$Bx10^4$	$Cx10^{16}$	A	$Bx10^4$	$Cx10^{16}$
51	0.328	0.589	16.120	0.553	4.785	20.180
52	0.120	-2.333	6.703	0.192	-2.372	10.020
53	0.540	0.126	21.850	0.897	5.936	27.290
54	1.282	-10.518	23.935	2.343	-7.283	31.729
55	1.942	-5.414	71.810	3.447	3.294	90.210
56	2.218	10.018	73.150	3.960	-5.114	92.040
57	0.301	0.321	15.168	0.514	3.745	19.007
58	1.195	-3.120	27.430	2.167	0.492	33.510
59	0.540	0.139	21.840	0.902	5.834	27.290
60	0.000	0.000	0.000	0.000	0.000	0.000
61	0.572	-3.745	10.640	1.037	-1.236	14.246
62	0.494	-0.082	21.500	0.839	4.588	27.000
63	0.801	-6.292	22.170	1.467	-10.163	28.910
64	0.313	-0.730	9.450	0.521	-0.985	11.843
65	0.848	-2.231	27.360	1.545	2.523	34.230
66	0.506	-2.701	12.135	0.907	-2.396	12.230
67	0.122	-0.348	4.519	0.196	0.548	5.695
68	0.000	0.000	0.000	0.000	0.000	0.000
69	1.175	-10.520	25.750	2.165	-15.470	32.590
70	0.464	-0.684	18.160	-0.198	79.600	10.345
71	0.243	1.783	16.182	0.405	6.100	20.350
72	0.000	0.000	0.000	0.000	0.000	0.000
73	0.665	-1.940	20.071	2.013	-42.620	29.840
74	0.600	-3.402	12.610	1.080	-3.414	15.770
75	3.298	-40.570	75.131	6.054	-46.600	102.888
76	0.010	4.441	13.900	-0.118	12.740	17.310
77	0.340	-0.910	10.583	0.559	1.329	13.210
78	0.000	0.000	0.000	0.000	0.000	0.000
79	0.000	0.000	0.000	0.000	0.000	0.000
80	0.897	-0.853	33.490	1.532	-0.853	33.490
81	0.270	0.000	0.000	0.540	0.000	0.000
82	1.790	-6.960	15.300	3.470	-9.280	22.520
83	1.790	-6.960	15.310	3.470	-9.280	22.520
84	0.381	-1.777	12.251	0.660	-0.203	15.327
85	0.690	-4.549	18.330	0.476	54.330	12.490
86	0.000	0.000	0.000	0.000	0.000	0.000
87	0.000	0.000	0.000	0.000	0.000	0.000
88	0.000	0.000	0.000	0.000	0.000	0.000
89	0.000	0.000	0.000	0.000	0.000	0.000
90	0.000	0.000	0.000	0.000	0.000	0.000
91	0.256	-3.080	9.658	0.419	1.628	12.010
92	0.737	-9.135	17.860	1.414	-19.712	25.670
93	0.994	-10.189	30.429	1.786	-6.568	41.289
94	1.963	-17.122	59.240	3.416	-5.334	80.087
95	0.232	-1.814	5.702	0.404	-1.879	7.131
96	0.933	-7.970	13.700	2.097	-23.500	20.250
97	0.846	-6.644	25.840	1.449	-10.942	34.783
98	1.570	-10.500	42.430	3.903	-25.200	54.210
99	0.528	-2.789	17.224	0.935	-1.821	21.710
100	1.659	-86.100	11.590	-0.030	1.101	1.788

	500 bars			1000 bars		
	A	$Bx10^4$	$Cx10^{16}$	A	$Bx10^4$	$Cx10^{16}$
101	1.435	-32.900	38.060	1.932	-7.150	39.750
102	0.783	-1.869	22.750	1.374	1.858	28.420
103	0.111	-0.936	0.453	0.208	-1.530	0.559
104	0.632	-5.382	12.265	2.275	-22.630	16.490
105	0.000	0.000	0.000	0.000	0.000	0.000
106	0.000	0.000	0.000	0.000	0.000	0.000
107	0.000	0.000	0.000	0.000	0.000	0.000
108	0.000	0.000	0.000	0.000	0.000	0.000
109	0.000	0.000	0.000	0.000	0.000	0.000
110	0.164	-1.848	0.495	0.313	3.366	0.634
111	0.118	-0.936	0.453	0.216	-1.530	0.559
112	0.000	0.000	0.000	0.000	0.000	0.000
113	0.537	-0.576	21.450	0.926	3.447	26.880
114	1.687	-2.840	26.970	3.160	0.915	33.390
115	1.430	11.450	25.790	1.700	8.230	34.040
116	1.420	11.690	25.690	1.600	1.216	34.260
117	1.420	10.620	25.500	1.600	-5.920	34.210
118	0.111	-5.330	2.757	-0.066	-7.940	6.728
119	0.540	0.599	26.580	0.884	7.127	33.330
120	2.591	-24.662	58.576	4.697	-18.025	78.189
121	0.560	0.000	0.000	1.130	0.000	0.000
122	0.528	-2.590	16.820	0.951	-1.671	21.140
123	0.919	-42.710	11.120	0.144	2.149	7.550
124	0.682	-1.479	18.610	1.125	3.350	23.110
125	0.313	-0.813	14.140	0.524	1.988	17.690
126	1.644	-4.370	40.530	2.790	2.628	50.680
127	0.770	0.000	0.000	1.550	0.000	0.000
128	0.000	0.000	0.000	0.000	0.000	0.000
129	1.522	32.050	33.180	0.793	82.000	19.150
130	0.523	-3.039	16.310	0.936	-2.343	20.500
131	0.237	-1.350	4.990	0.317	4.920	7.330
132	1.090	-1.000	41.850	1.815	8.850	52.300
133	0.000	0.000	0.000	0.000	0.000	0.000
134	0.055	0.658	6.124	0.081	2.613	7.689
135	0.075	-0.017	6.804	0.108	1.843	8.524
136	-0.056	-1.220	-3.224	-0.095	-2.810	-4.000
137	0.866	2.034	35.420	1.887	-4.074	45.700
138	0.413	-6.360	5.423	0.754	-9.060	7.200
139	0.481	-23.710	8.307	0.600	-25.920	-9.942
140	0.213	-0.334	10.590	0.331	3.695	13.060
141	0.183	-1.730	7.770	0.316	-1.113	9.756
142	0.422	-0.588	21.130	0.737	3.213	26.530
143	0.810	-3.689	36.971	1.423	0.869	46.525
144	0.247	0.130	16.070	0.340	-2.840	19.790
145	0.429	0.547	25.870	0.734	6.011	32.390
146	0.495	-2.141	18.000	0.897	-7.380	22.640
147	0.123	-0.665	5.394	0.202	0.330	6.734
148	0.472	-0.912	19.790	0.813	2.430	24.840
149	0.427	-0.912	19.790	0.813	2.430	24.840
150	0.610	-1.692	25.150	1.054	2.029	31.620

	500 bars			1000 bars		
	A	$Bx10^4$	$Cx10^{16}$	A	$Bx10^4$	$Cx10^{16}$
151	0.000	0.000	0.000	0.000	0.000	0.000
152	0.266	-0.456	9.895	0.468	1.215	12.420
153	0.200	-0.500	10.440	0.570	-13.900	16.150
154	0.200	-0.500	10.440	0.570	-13.900	16.150
155	0.257	0.376	16.920	0.390	6.890	21.580
156	0.000	0.000	0.000	0.000	0.000	0.000
157	-0.174	4.580	-7.010	-0.263	4.295	-8.800
158	0.000	0.000	0.000	0.000	0.000	0.000
159	0.000	0.000	0.000	0.000	0.000	0.000
160	0.134	-1.463	4.317	0.282	-4.143	5.732
161	0.210	-0.849	9.432	0.372	0.173	11.897
162	0.218	-1.114	9.478	0.382	0.026	11.920
163	0.217	1.652	15.730	0.354	6.450	19.660
164	0.482	-2.991	18.350	0.853	-1.391	23.100
165	0.082	0.153	5.148	0.122	1.805	6.407
166	0.000	0.000	0.000	0.000	0.000	0.000
167	0.150	0.954	10.255	0.224	4.054	12.830
168	0.226	0.812	14.580	0.417	2.367	17.990
169	0.507	-2.940	16.660	0.924	-2.370	20.970
170	0.137	-1.400	4.039	0.034	14.200	2.259
171	0.123	-0.828	4.090	0.015	14.870	2.083
172	0.202	-0.663	9.142	0.359	0.548	11.497
173	0.398	-1.417	15.660	0.699	0.496	19.700
174	0.468	-1.760	18.010	0.833	4.472	22.620
175	0.339	-2.930	4.950	0.663	-4.240	5.850
176	0.198	0.094	10.490	0.340	2.350	13.170
177	0.409	-1.110	17.050	0.699	2.090	21.330

Table IF. Data for Calculating the Effect of Pressure on Aqueous Dissociation Reactions.

	ΔV @25°C	# Water Ionization Reactions
1	-28.7	1.0
3	-37.9	1.0
10	-13.0	1.0
15	-22.4	1.0
16	-43.2	2.0
17	-64.3	3.0
25	-11.2	1.0
26	-7.5	2.0
27	-34.3	1.0
28	-19.74	1.0
29	-7.1	2.0
30	-10.6	2.0
31	-31.6	1.0
32	-19.74	1.0
36	-25.0	2.0
44	-19.74	1.0
45	-7.1	2.0
50	-19.74	1.0
51	-5.7	2.0
53	-7.1	2.0
54	-4.6	1.0
60	-22.4	1.0
61	-43.5	2.0
62	-64.6	3.0
63	-85.7	4.0
64	-35.5	0.0
72	-27.2	1.0
73	-35.96	1.0
74	-25.85	1.0
76	-14.81	1.0
87	-19.8	1.0
93	-9.8	2.0
94	-31.5	1.0
96	-19.74	1.0
97	-7.4	2.0
105	-34.0	1.0
106	-7.1	2.0
110	-13.7	1.0
111	-23.1	1.0
112	-13.8	1.0
114	-7.1	2.0
115	-15.8	1.0
118	-28.8	1.0
127	-19.74	1.0
128	-9.12	2.0
129	-31.5	1.0
130	-7.1	2.0
135	-7.6	2.0

Table IG. Pitzer Coefficients

M	X	t	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}	M	X	t	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Na	Cl	0	0.0532	0.2496	0.00441	K	Cl	0	0.0296	0.1621	0.00119
		25	0.0765	0.2664	0.00127			25	0.0485	0.2122	-0.00084
		50	0.0903	0.2846	-0.00095			50	0.0596	0.2429	-0.00205
		75	0.0978	0.3041	-0.00250			75	0.0662	0.2705	-0.00277
		100	0.1012	0.3250	-0.00354			100	0.0698	0.2977	-0.00318
		125	0.1017	0.3472	-0.00420			125	0.0715	0.3250	-0.00340
		150	0.1003	0.3707	-0.00457			150	0.0721	0.3527	-0.00350
		200	0.0938	0.4218	-0.00469			200	0.0710	0.4084	-0.00349
		250	0.0838	0.4738	-0.00429			250	0.0677	0.4640	-0.00322
		300	0.0708	0.5401	-0.00357			300	0.0621	0.5188	-0.00264
		350	0.0546	0.6073	-0.00268			350	0.0534	0.5724	-0.00162
Na	SO_4	0	-0.08601	0.892	0.0353	K	SO_4	0	-0.04138	0.7830	0.0172
		25	0.01864	1.096	0.00555			25	0.00000	1.1023	0.0188
		50	0.06264	1.213	-0.00303			50	0.02771	1.2578	0.0174
		75	0.0888	1.285	-0.00839			75	0.04888	0.3704	0.0137
		100	0.1057	1.330	-0.0123			100	0.06819	0.4637	0.00811
		125	0.1175	1.357	-0.0153			125	0.0887	1.5510	0.00098
		150	0.1266	1.374	-0.0178			150	0.1124	1.6415	-0.00741
		200	0.1415	1.444	-0.0213			200	0.1743	1.8578	-0.0271
		250	0.1546	1.856	-0.0235			250	0.2596	2.1511	-0.0499
		300	0.1656	3.730	-0.0249			300	0.3701	2.5460	-0.0749
		350	0.1723	12.550	-0.0256			350	0.5058	3.0590	-0.1015
Na	HCO_3	25	0.0277	0.0411	0.0000	K	HCO_3	25	0.0296	-0.013	-0.0080
Na	CO_3	25	0.0399	1.389	0.0044	K	CO_3	25	0.1488	1.430	-0.0015
Ca	SO_4	25	0.200	3.1973	0.0000	H	Cl	25	0.1775	0.2945	0.0008
Ca	HCO_3	25	0.400	2.977	0.0000	H	SO_4	25	0.0298	0.000	0.0438
Zn	Cl	25	0.2602	1.6425	-0.08798	Al	Cl	25	0.6993	5.845	0.00273

M X	t	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Ca Cl	0	0.318	1.500	0.00155
	25	0.3159	1.6140	-0.00034
	50	0.313	1.800	-0.0033
	75	0.310	1.980	-0.0058
	100	0.305	2.170	-0.0080
	125	0.299	2.400	-0.0098
	150	0.291	2.600	-0.0113
	200	0.272	3.100	-0.0138
	250	0.230	3.830	-0.0133
	300	0.244	5.250	-0.0143
	350	0.369	8.300	-0.0232
Ba Cl	0	0.385	2.10	-0.0154
	25	0.350	2.00	-0.0193
	50	0.314	1.92	-0.0222
	75	0.292	1.90	-0.247
	100	0.276	1.92	-0.261
	125	0.263	2.00	-0.263
	150	0.252	2.22	-0.258
	200	0.235	2.87	-0.229
	250	0.219	3.83	-0.0168
	300	0.210	5.25	-0.0122
	350	0.206	8.30	-0.0067
Sr Cl	0	0.460	2.35	0.0100
	25	0.381	2.22	-0.0013
	50	0.344	2.20	-0.0080
	75	0.320	2.13	-0.0115
	100	0.302	2.10	-0.0139
	125	0.290	2.16	-0.0156
	150	0.278	2.30	-0.0167
	200	0.264	2.90	-0.0180
	250	0.258	3.83	-0.0191
	300	0.256	5.25	-0.0198
	350	0.2555	8.30	-0.0203

M X	t	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Mg Cl	0	0.368	1.55	0.00700
	25	0.3524	1.682	0.00519
	50	0.338	1.85	0.00325
	75	0.324	2.03	0.00125
	100	0.311	2.23	-0.00025
	125	0.300	2.45	-0.00138
	150	0.289	2.65	-0.00238
	200	0.269	3.15	-0.00388
	250	0.230	3.88	-0.00513
	300	0.244	5.30	-0.00613
	350	0.369	8.35	-0.00700
Mg SO_4	0	0.1866	3.039	0.00979
	25	0.2150	3.365	0.00699
	50	0.2275	3.163	0.00494
	75	0.2372	3.843	0.00290
	100	0.2489	4.410	0.00079
	125	0.2640	4.805	-0.00130
	150	0.2856	5.912	-0.00353
	200	0.3785	9.736	-0.0115
	250	0.6489	7.532	-0.0364
	300	1.334	9.736	-0.1046
	350	2.806	12.57	-0.2575
Mg HCO_3	25	0.329	0.6072	0.0000
Mn SO_4	25	0.201	2.98	0.0182

i	j	t	θ
Na	Ca	0	-0.0085
		25	-0.0078
		50	-0.00726
		75	-0.00696
		100	-0.0068
		125	-0.0069
		150	-0.0074
		200	-0.0099
		250	-0.0128
		300	-0.0155
		350	-0.0180
Na	K	25	-0.012
Na	Mg	25	0.070
Na	H	25	0.036
K	Ca	25	0.032
K	H	25	0.005
Ca	Mg	25	0.007
Ca	H	25	0.092
Mg	H	25	0.100

k	l	t	θ
Cl	SO_4	25	0.02
Cl	HCO_3	25	0.03
Cl	CO_3	25	-0.02
Cl	OH	25	-0.05
SO_4	HCO_3	25	0.01
SO_4	CO_3	25	0.02
SO_4	OH	25	-0.01
HCO_3	CO_3	25	-0.04
CO_3	OH	25	0.01

i	j	k	t	ψ
Na	Ca	Cl	0	0.0044
			25	0.0029
			50	0.0015
			75	0.00066
			100	0.00042
			125	0.00035
			150	0.00035
			200	0.00035
			250	0.00035
			300	0.00035
			350	0.00035
Na	K	Cl	25	-0.0018
Na	K	SO_4	25	-0.01
Na	K	HCO_3	25	-0.003
Na	K	CO_3	25	0.003
Na	Ca	SO_4	25	-0.055
Na	Mg	Cl	25	-0.012
Na	Mg	SO_4	25	-0.015
Na	H	Cl	25	-0.004
Na	H	SO_4	25	-0.012
K	Ca	Cl	25	-0.025
K	Mg	Cl	25	-0.022
K	Mg	SO_4	25	-0.048

k	l	i	t	ψ
Cl	SO_4	Na	25	0.0014
Cl	SO_4	Ca	25	-0.018
Cl	SO_4	Mg	25	-0.004
Cl	HCO_3	Na	25	-0.015
Cl	HCO_3	Mg	25	-0.096
Cl	CO_3	Na	25	0.0085
Cl	CO_3	K	25	0.004
Cl	OH	Na	25	-0.006
Cl	OH	K	25	-0.006
Cl	OH	Ca	25	-0.025
SO_4	HCO_3	Na	25	-0.005
SO_4	HCO_3	Mg	25	-0.161
SO_4	CO_3	Na	25	-0.005
SO_4	CO_3	K	25	-0.009
SO_4	OH	Na	25	-0.009
SO_4	OH	K	25	-0.05
HCO_3	CO_3	Na	25	0.002
HCO_3	CO_3	K	25	0.0129

i	j	k	t	ψ
K	H	Cl	25	-0.011
K	H	SO_4	25	0.197
Ca	Mg	Cl	25	-0.012
Ca	Mg	SO_4	25	0.024
Ca	H	Cl	25	-0.015
Mg	H	Cl	25	-0.011

k	l	i	t	ψ
CO_3	OH	Na	25	-0.017
CO_3	OH	K	25	-0.01

Table IH. Table of congruent dissolution of minerals listing the aqueous species number and stoichiometry.

```
1,    1.0,4,1.0,14,3.0,11,-4.0,8,-4.0,10,
2,    2.0,1,1.0,2,2.0,11,-6.0,8,-1.0,10,
3,    1.0,3,1.0,14,3.0,11,-4.0,8,-4.0,10,
4,    1.0,3,1.0,14,3.0,11,-4.0,8,-4.0,10,
5,    1.0,3,1.0,14,3.0,11,-4.0,8,-4.0,10,
6,    1.0,4,3.0,14,2.0,6,-6.0,8,6.0,10,
7,    2.0,2,2.0,14,1.0,11,-10.0,8,5.0,10,
8,    1.0,3,1.0,14,2.0,11,-4.0,8,-1.0,10,
9,    2.0,14,1.0,11,-6.0,8,1.0,10,
10,   0.4,1,0.6,3,1.4,14,2.6,11,-5.6,8,-2.4,10,
11,   1.0,1,1.0,6,
12,   1.0,4,3.0,18,1.0,14,3.0,11,-10.0,8,
13,   1.0,1,2.0,14,2.0,11,-8.0,8,
14,   5.0,1,3.0,29,1.0,5,
15,   5.0,1,3.0,29,1.0,30,
16,   5.0,1,3.0,29,1.0,9,
17,   1.0,1,1.0,98,
18,   1.0,1,2.0,14,1.0,11,-8.0,8,2.0,10,
19,   3.0,17,2.0,98,2.0,9,
20,   1.0,15,1.0,6,
21,   1.0,14,2.0,10,-3.0,8,
22,   1.0,2,2.0,9,
23,   0.8,1,0.2,3,1.8,14,2.2,11,-7.2,8,-0.8,10,
24,   1.0,1,1.0,98,
25,   1.0,26,1.0,6,
26,   1.0,11,-2.0,10,
27,   2.0,18,2.0,14,1.0,11,-10.0,8,5.0,10,
28,   5.0,2,2.0,14,3.0,11,6.0,10,-16.0,8,
29,   5.0,2,2.0,14,3.0,11,6.0,10,-16.0,8,
30,   3.0,2,2.0,11,-6.0,8,1.0,10,
31,   1.0,2,1.0,11,-2.0,8,-1.0,10,
32,   2.0,3,2.0,14,10.0,11,-8.0,8,-8.0,10,
33,   2.0,4,2.0,14,10.0,11,-8.0,8,-8.0,10,
34,   1.0,1,2.0,14,10.0,11,-8.0,8,-8.0,10,
35,   1.0,2,2.0,14,10.0,11,-8.0,8,-8.0,10,
36,   2.0,14,3.0,10,-6.0,8,
37,   1.0,11,-2.0,10,
38,   1.0,11,-2.0,10,
39,   2.0,14,2.0,11,-6.0,8,1.0,10,
40,   1.0,1,1.0,2,2.0,11,-4.0,8,-2.0,10,
41,   1.0,1,1.0,2,2.0,98,
42,   1.0,1,1.0,2,2.0,98,
43,   1.0,2,1.0,11,-2.0,8,-1.0,10,
44,   2.0,1,1.0,19,2.0,14,3.0,11,-13.0,8,1.0,10,
45,   2.0,18,1.0,11,-4.0,8,
46,   1.0,1,2.0,30,
47,   2.0,2,1.0,11,-4.0,8,
48,   1.0,14,3.0,9,
49,   1.0,14,3.0,9,
50,   3.0,18,2.0,11,-6.0,8,1.0,10,
51,   1.0,1,1.0,6,2.0,10,
52,   1.0,3,1.0,5,
53,   2.0,14,2.0,11,-6.0,8,1.0,10,
54,   1.0,1,2.0,14,7.0,11,-8.0,8,-4.0,10,
55,   1.0,1,3.0,2,4.0,98,
```

```
56,   5.0,2,4.0,98,2.0,9,3.0,10,
57,   1.0,1,2.0,5,
58,   0.6,4,0.25,2,2.3,14,3.5,11,-8.0,8,-2.0,10,
59,   2.0,14,2.0,11,-6.0,8,1.0,10,
60,   1.0,3,11.0,11,-1.0,8,-16.5,10,
61,   1.0,4,1.0,14,3.0,11,-4.0,8,-4.0,10,
62,   2.0,14,1.0,11,-6.0,8,1.0,10,
63,   0.6,1,0.4,3,1.6,14,2.4,11,-6.6,8,-1.6,10,
64,   2.0,1,1.0,11,-4.0,8,
65,   1.0,1,2.0,14,4.0,11,-8.0,8,
66,   1.0,4,1.0,14,2.0,11,-4.0,8,-2.0,10,
67,   1.0,1,1.0,10,-2.0,8,
68,   1.0,3,7.0,11,-1.0,8,-9.0,10,
69,   1.0,2,2.0,19,4.0,10,-8.0,8,
70,   1.0,2,1.0,98,
71,   1.0,2,2.0,5,
72,   4.0,3,3.0,14,9.0,11,1.0,5,-12.0,8,-12.0,10,
73,   3.0,1,1.0,2,2.0,11,-8.0,8,
74,   1.0,4,1.0,14,3.0,11,-4.0,8,-4.0,10,
75,   4.0,1,6.0,14,6.0,11,1.0,98,-24.0,8,
76,   2.0,3,1.0,6,10.0,10,
77,   1.0,1,1.0,2,1.0,11,-4.0,8,
78,   1.0,3,1.0,14,5.0,11,-4.0,8,-5.0,10,
79,   1.0,4,1.0,14,5.0,11,-4.0,8,-5.0,10,
80,   1.0,4,3.0,14,3.0,11,-10.0,8,
81,   1.0,3,1.0,7,
82,   2.0,3,1.0,98,1.0,10,
83,   2.0,3,1.0,98,10.0,10,
84,   1.0,3,1.0,14,1.0,11,-4.0,8,
85,   1.0,2,1.0,98,3.0,10,
86,   0.33,3,2.0,19,0.33,14,3.67,11,-7.32,8,-2.68,10,
87,   0.33,4,2.0,19,0.33,14,3.67,11,-7.32,8,-2.68,10,
88,   2.0,19,0.33,14,3.67,11,-6.99,8,-2.68,10,
89,   0.165,1,2.0,19,0.33,14,3.67,11,-7.32,8,-2.68,10,
90,   0.165,2,2.0,19,0.33,14,3.67,11,-7.32,8,-2.68,10,
91,   1.0,1,1.0,101,-1.0,8,
92,   0.2,1,0.8,3,1.2,14,2.8,11,-4.8,8,-3.2,10,
93,   1.0,3,3.0,14,3.0,11,-10.0,8,
94,   1.0,3,2.0,1,4.0,2,3.0,14,6.0,11,-22.0,8,
95,   1.0,2,-2.0,8,1.0,10,
96,   0.5,3,0.5,4,1.0,14,3.0,11,-4.0,8,-3.0,10,
97,   1.0,4,3.0,2,1.0,14,3.0,11,-10.0,8,
98,   1.0,4,3.0,2,1.0,14,3.0,11,2.0,30,-8.0,8,-2.0,10,
99,   1.0,1,2.0,9,
100,  2.0,4,-2.0,8,1.0,10,
101,  2.0,1,2.0,14,3.0,11,-10.0,8,
102,  2.0,14,4.0,11,-6.0,8,-4.0,10,
103,  1.0,11,-2.0,10,
104,  1.0,4,1.0,14,3.0,11,-4.0,8,-4.0,10,
105,  0.33,3,3.0,2,0.33,14,3.67,11,-7.32,8,-2.68,10,
106,  0.33,4,3.0,2,0.33,14,3.67,11,-7.32,8,-2.68,10,
107,  3.0,2,0.33,14,3.67,11,-6.99,8,-2.68,10,
108,  0.165,1,3.0,2,0.33,14,3.67,11,-7.32,8,-2.68,10,
109,  0.165,2,3.0,2,0.33,14,3.67,11,-7.32,8,-2.68,10,
110,  4.0,2,6.0,11,-8.0,8,-1.0,10,
111,  1.0,11,-2.0,10,
112,  1.0,11,-2.0,10,
113,  2.0,14,1.0,11,-6.0,8,1.0,10,
```

```
114,  0.167,1,2.33,14,3.67,11,-7.32,8,-2.68,10,
115,  0.33,4,2.33,14,3.67,11,-7.32,8,-2.68,10,
116,  0.167,2,2.33,14,3.67,11,-7.32,8,-2.68,10,
117,  0.33,3,2.33,14,3.67,11,-7.32,8,-2.68,10,
118,  2.0,3,-2.0,8,1.0,10,
119,  1.0,2,2.0,14,4.0,10,-8.0,8,
120,  1.0,1,2.0,14,7.0,11,-8.0,8,-3.0,10,
121,  1.0,19,1.0,29,2.0,10,
122,  1.0,26,1.0,98,
123,  1.0,4,1.0,5,
124,  3.0,2,4.0,11,-6.0,8,-4.0,10,
125,  2.0,3,1.0,6,
126,  2.0,1,5.0,2,8.0,11,-14.0,8,-8.0,10,
127,  3.0,3,1.0,7,1.0,98,2.0,10,
128,  3.0,18,2.0,29,8.0,10,
129,  1.0,1,2.0,14,4.0,11,-8.0,8,-2.0,10,
130,  1.0,15,1.0,98,
131,  1.0,1,1.0,11,-2.0,8,-1.0,10,
132,  2.0,1,3.0,14,3.0,11,-13.0,8,1.0,10,
133,  1.0,13,1.0,18,-1.0,19,
134,  1.0,13,1.0,5,
135,  2.0,13,1.0,101,-1.0,8,
136,  1.0,16,1.0,18,-1.0,19,
137,  2.0,17,1.0,98,2.0,9,
138,  1.0,17,-2.0,8,1.0,10,
139,  2.0,16,-2.0,8,1.0,10,
140,  1.0,17,1.0,101,-1.0,8,
141,  2.0,16,1.0,101,-1.0,8,
142,  1.0,17,1.0,18,2.0,101,-2.0,8,
143,  4.0,16,1.0,17,1.0,18,4.0,101,-4.0,8,
144,  1.0,18,2.0,5,
145,  1.0,19,3.0,5,
146,  1.0,18,1.0,98,
147,  1.0,18,-2.0,8,1.0,10,
148,  2.0,19,3.0,10,-6.0,8,
149,  2.0,19,3.0,10,-6.0,8,
150,  2.0,19,1.0,18,4.0,10,-8.0,8,
151,  1.0,19,3.0,9,
152,  1.0,19,2.0,10,-3.0,8,
153,  1.0,18,1.0,101,-1.0,8,
154,  1.0,18,1.0,101,-1.0,8,
155,  1.0,18,1.75,101,0.25,6,0.25,8,-1.0,10,
156,  2.0,19,1.0,18,4.0,101,-4.0,8,
157,  1.0,21,2.0,18,-2.0,19,
158,  1.0,21,2.0,5,
159,  1.0,20,2.0,5,
160,  1.0,21,-2.0,8,1.0,10,
161,  1.0,21,1.0,101,-1.0,8,
162,  1.0,21,1.0,101,-1.0,8,
163,  1.0,23,2.0,5,
164,  1.0,23,1.0,98,
165,  1.0,23,-2.0,8,1.0,10,
166,  2.0,24,2.0,10,-1.0,23,-4.0,8,
167,  1.0,23,1.0,101,-1.0,8,
168,  1.0,25,2.0,5,
169,  1.0,25,1.0,98,
170,  1.0,25,-2.0,8,1.0,10,
171,  1.0,25,-2.0,8,1.0,10,
```

```
172,  1.0,25,1.0,101,-1.0,8,
173,  1.0,25,1.0,6,
174,  1.0,27,1.0,98,
175,  1.0,27,-2.0,8,1.0,10,
176,  1.0,27,1.0,101,-1.0,8,
177,  1.0,27,1.0,6,
178,  1.0,169,1.0,98,
179,  -2.0,8,2.0,169,2.0,99,2.0,146,
180,  -2.0,8,2.0,169,2.0,99,1.0,25,
181,  -2.0,8,2.0,169,2.0,99,1.0,17,
182,  -2.0,8,2.0,169,2.0,99,1.0,2,
183,  -2.0,8,2.0,169,2.0,99,1.0,26,
184,  -2.0,8,2.0,169,2.0,99,1.0,15,
185,  -2.0,8,2.0,169,2.0,99,1.0,18,
186,  1.0,169,-2.0,8,1.0,10,
187,  1.0,169,-2.0,8,1.0,10,
188,  1.0,169,2.0,9,
189,  1.0,167,2.5,10,4.0,30,
190,  2.0,99,1.0,167,4.0,10,
191,  -2.0,8,1.0,167,2.0,99,2.0,10,1.0,1,
192,  1.0,169,2.0,168,-4.0,8,2.0,10,
193,  1.0,167,-4.0,8,2.0,10,
194,  1.0,167,-4.0,8,2.0,10,
195,  2.0,167,2.0,168,-10.0,8,5.0,10,
196,  -4.0,8,1.0,167,1.0,11,
197,  2.0,169,2.0,99,
198,  -2.0,8,2.0,3,2.0,169,2.0,99,
199,  -2.0,8,2.0,4,2.0,169,2.0,99,
200,  -2.0,8,1.0,1,2.0,169,2.0,99,
201,  2.0,4,2.0,169,2.0,210,
202,  1.0,1,2.0,169,2.0,210,
203,  -6.0,8,1.0,1,2.0,169,2.0,11,
204,  1.0,169,2.0,9,1.0,10,
205,  1.0,169,1.0,2,-4.0,8,2.0,10,
206,  1.0,169,1.0,1,-4.0,8,2.0,10,
207,  1.0,169,1.0,15,-4.0,8,2.0,10,
208,  1.0,169,2.0,30,
209,  1.0,169,3.0,101,1.0,8,-2.0,10,
210,  2.0,212,3.0,10,-6.0,8,
211,  2.0,211,-4.0,8,2.0,10,
212,  2.0,210,6.0,8,-3.0,10,
213,  1.0,211,1.0,6,6.0,10,
214,  2.0,210,3.0,25,
```

APPENDIX II. An abbreviated version of the interactive input routine SOLINPUT

SOLMINEQ_88 Input Data File Creation Program

Sample 1

MAIN MENU

1) Create/Edit Current Sample Data
2) Read an Existing Input File
3) Go to Next Sample
4) Go to Previous Sample
5) Write All Samples to an Input File
6) Exit Program

Enter Choice (1-6)

1

OPTIONS MENU

1) Enter Basic Parameters
2) Enter Program Option Flags
3) Enter Gas, pH, and CO2 Options
4) Enter Gas Distribution Option
5) Enter Ion Exchange or Adsorption Option
6) Enter Precipitation/Mixing/Boiling Option
7) Enter User Log K Option
8) Enter Additional Anions/Cation/Minerals Option
9) Return to Main Menu

Enter Choice (1-9)

1

BASIC PARAMETERS MENU

1) Enter Title and Units
2) Enter Temperatures, Density, and Pressure
3) Enter pH, and Eh
4) Enter Concentrations for Major Species
5) Enter Concentrations for Minor Species
6) Enter Concentrations for Organic Species
7) Return to Options Menu

Enter Choice (1-7)

```
 Enter the title of this sample
 [SAMPLE #  1]
Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C

 Enter Concentration Units (Mg/l, PPM, Mol/l, Mol/K, Meq/l)
 [MG/L ]
ppm

 Enter the pH                                    [Current =  7.0000]
8.2
 Enter Eh in Volts                               [Current =  9.0000]
0.5

          1)  ENTER: Na, K, Li, Ca, Mg, Fe, Al
          2)  ENTER: SiO2, Cl, SO4, H2S, HCO3, CO3, TIC
          3)  Return to Basic Parameters Menu
              Enter Choice (1-3)

 Enter Concentration of Na  [Current = 0.0000E-01]
10770
 Enter Concentration of K   [Current = 0.0000E-01]
399.1
 Enter Concentration of Li  [Current = 0.0000E-01]
0.181
 Enter Concentration of Ca  [Current = 0.0000E-01]
412.3
 Enter Concentration of Mg  [Current = 0.0000E-01]
1292
 Enter Concentration of Fe  [Current = 0.0000E-01]
0.002
 Enter Concentration of Al  [Current = 0.0000E-01]
0.002
 Enter Concentration of SiO2 [Current = 0.0000E-01]
4.28
 Enter Concentration of Cl   [Current = 0.0000E-01]
0.1935E+05
 Enter Concentration of SO4  [Current = 0.0000E-01]
2712
```

```
 Enter Concentration of H2S  [Current = 0.0000E-01]

 Enter Alkalinity as HCO3    [Current = 0.0000E-01]
123.4
 Enter Alkalinity as CO3     [Current = 0.0000E-01]

 Enter TIC                   [Current = 0.0000E-01]


          1)  ENTER: F, PO4, NO3, NH3, B, Sr, Ba
          2)  ENTER: Pb, Zn, Cu, Mn, Hg, Ag
          3)  ENTER: As, U, V
          4)  Return to Basic Parameters Menu
              Enter Choice (1-4)

 Enter Concentration of F   [Current = 0.0000E-01]
1.39
 Enter Concentration of PO4 [Current = 0.0000E-01]
0.06
 Enter Concentration of NO3 [Current = 0.0000E-01]
.29
 Enter Concentration of NH3 [Current = 0.0000E-01]
.03
 Enter Concentration of B   [Current = 0.0000E-01]
4.45
 Enter Concentration of Sr  [Current = 0.0000E-01]
8.14
 Enter Concentration of Ba  [Current = 0.0000E-01]
.02
 Enter Concentration of Pb   [Current = 0.0000E-01]
0.5E-4
 Enter Concentration of Zn   [Current = 0.0000E-01]
0.0049
 Enter Concentration of Cu   [Current = 0.0000E-01]
0.0007
 Enter Concentration of Mn   [Current = 0.0000E-01]
0.0002
```

```
 Enter Concentration of Hg   [Current = 0.0000E-01]

 Enter Concentration of Ag   [Current = 0.0000E-01]
0.004

              OPTIONS MENU
          1)  Enter Basic Parameters
          2)  Enter Program Option Flags
          3)  Enter Gas, pH, and CO2 Options
          4)  Enter Gas Distribution Option
          5)  Enter Ion Exchange or Adsorption Option
          6)  Enter Precipitation/Mixing/Boiling Option
          7)  Enter User Log K Option
          8)  Enter Additional Anions/Cation/Minerals Option
          9)  Return to Main Menu
              Enter Choice (1-9)
2

              FLAGS MENU
          1)  Enter Carbonate Distribution
          2)  Enter Activity Coefficient Control
          3)  Enter Redox Equilibria
          4)  Enter Printout Control
          5)  Enter Tolerance Control
          6)  Return to Options Menu
              Enter Choice (1-6)

 What does the concentration of bicarbonate/carbonate
 refer to:
      0 = Total Alkalinity as HCO3/CO3?
      1 = Carbonate Alkalinity as HCO3/CO3?
      2 = Total Inorganic Carbon (TIC)?
           [Current =  0]
2

 Do you wish to use TIC for the distribution of
 carbonate species at high temperature? (Y/N)
      [Current =  N]
```

```
 Do you want to distribute Fe using Eh? (Y/N)
           [Current =  N]
y
 Do you want to distribute Cu using Eh? (Y/N)
           [Current =  N]
y
 Do you want to distribute Hg using Eh? (Y/N)
           [Current =  N]
y
 Do you want to distribute Mn using Eh? (Y/N)
           [Current =  N]
y
 Do you want to distribute U  using Eh? (Y/N)
           [Current =  N]

 Do you want to distribute V  using Eh? (Y/N)
           [Current =  N]

 Do you want to print the aqueous log K values in the
  data base at the temperatures of interest ? (Y/N)
      [Current =  N]

 Do you want to print out the analytical and calculated
  activity ratios of the major elements? (Y/N)
      [Current =  N]
y
 Do you want to print out the temperature estimates
  from the chemical geothermometers? (Y/N)
      [Current =  N]
y
 Do you want to print out the data on the iteration
  of the anions? (Y/N)
      [Current =  N]

 Do you want to print out the data on the mass balance
  on Hydrogen whenever a new pH is calculated? (Y/N)
      [Current =  N]
```

```
 Name of a new input file to be created based upon
  the output of this sample.
      [Current =  ]

                                                          Sample  1

              MAIN MENU
          1)  Create/Edit Current Sample Data
          2)  Read an Existing Input File
          3)  Go to Next Sample
          4)  Go to Previous Sample
          5)  Write All Samples to an Input File
          6)  Exit Program
              Enter Choice (1-6)
5

 What do you want to call this file?
      [Current = SOLMINEQ.IN]

 SOLMINEQ.IN
  already exists.  Do you wish to overwrite?
y
 Will write out  1 sample(s).
 Enter a <CR> for ok or a number indicating how many
  samples you want written out.

 Writing file ...

                                                          Sample  1

              MAIN MENU
          1)  Create/Edit Current Sample Data
          2)  Read an Existing Input File
          3)  Go to Next Sample
          4)  Go to Previous Sample
          5)  Write All Samples to an Input File
          6)  Exit Program
              Enter Choice (1-6)
6
**** STOP
```

```
Input File Created
Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C
0.2500E+020.0000E+000.0000E+000.0000E+00
0.8200E+010.5000E+000.9000E+010.9000E+01PPM
0.1077E+050.3991E+030.1810E+000.4123E+030.1292E+040.2000E-020.2000E-02
0.4280E+010.1935E+050.2712E+040.0000E+000.1234E+030.0000E+000.0000E+00
0.1390E+010.6000E-010.2900E+000.3000E-010.4450E+010.8140E+010.2000E-01
0.5000E-040.4900E-020.7000E-030.2000E-030.3000E-040.4000E-04
0.4000E-020.0000E+000.0000E+00
0.0000E+000.0000E+000.0000E+000.0000E+00
 2 0
0.0000E+000.0000E+000.0000E+000.0000E+00
 0 00.0000E+000.5000E-01
0.0000E+000.0000E+000.0000E+000.0000E+000.0000E+000.0000E+000.0000E+000.0000E+00

 0 0
    00.0000E+00    00.0000E+00    00.0000E+00    00.0000E+00    00.0000E+00
00.0000E+00
    00.0000E+00    00.0000E+00    00.0000E+00    00.0000E+00    00.0000E+00
00.0000E+00
 0 0
 0
 0
 1 0 1 1 1 1 0 0
 0 1 1 0 0
0.5000E-040.5000E-04
```

APPENDIX III. Output Examples

The output from four test cases are given below. These cases were selected to illustrate several of the main options in this code and to be used for comparison of results by those who acquire and implement this program. The number of possible options in this code is extremely large and can not be adequately illustrated in this report.

Test sample #1 gives the chemical composition of modified sea water (Nordstrom and others, 1979) to which has been added 0.1 ppm acetate, oxalate, and succinate. The output gives the distribution of all the inorganic and organic species and the saturation states of all the minerals in the database with the exception of those for U and V. The activity coefficients for the charged species are calculated using the $B^{\bullet}$ method and those for neutral species are made equal to the activity coefficient of dissolved CO_2. The printing options selected display the iterations for anions (total = 6), the ratios for cations and anions, and the chemical geothermometers.

The mixing option in SOLMINEQ.88 is illustrated with the test sample #2. This case is a real world test involving the mixing of formation water from the McMurray formation, Alberta, Canada, and high pH flood water. The mixing proportions specified in this case are 50/50%, but the number of the mixtures and the mixing proportions can be varied by the user for any one run. Speciation and saturation computations are carried out and results are listed for each end member as well as for the specified mixture or mixtures.

Test sample #3 illustrates one of the dissolution/precipitation options in SOLMINEQ.88. In this case the mineral anorthite (index number = 13) is to be dissolved/precipitated until the sea water of test sample #1 is at equilibrium with the mineral gibbsite (index number = 49). The program initially carries out speciation and saturation computations for sea water (printout not shown, but is similar to that shown on pages 2-10 of test sample #1). Results of speciation and saturation computations after equilibration with gibbsite are then printed.

The amount of anorthite precipitated to achieve equilibrium with gibbsite ($SI \leq 0.05$) is -3.076×10^{-8} moles. The "thinking" geochemist should realize that the program (which obeys all commands!) is performing an impossible task. The saturation states of anorthite and gibbsite in sea water are -6.782 and 0.917 kcal/mole, respectively. Thus, in order to equilibrate with gibbsite, anorthite must precipitate form this sea water sample. Precipitation of

anorthite from a solution that is undersaturated with respect to it is, of course, thermodynamically impossible. This example illustrates the fact that the user (not the code) is responsible for all the results of computations carried out by this program.

The ion exchange option is illustrated with the test sample #4. In this case 100 g of smectite, with cation exchange capacity (CEC) of 100 meq per 100 g and with its sites filled with an equal amount of Ca and Mg, is added to one liter of sea water. We assume that the selectivity constant of smectite for divalent cations relative to monovalent cations is so high that we can neglect any exchange with monovalent cations in sea water. We assume, also, that the selectivity of smectite for Ca and Mg is equal to one.

The program initially computes the distribution of species and the saturation states of minerals (printout deleted as it is similar to that of test sample #1). The program then computes the final distribution of Ca and Mg on the smectite surface and the new distribution of species and saturation state of minerals in the resulting sea water sample. The output shows that 424 ppm Ca has been transferred from the smectite surface to the sea water and 257 ppm Mg from sea water to the smectite surface. The saturation states of all the Ca and Mg minerals, of course, are changed from the initial conditions.

```
****** INPUT DATA ECHO ******

TITLE : Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C
      TEMP       HITEMP        DENS       PRESS
0.2500E+02  0.0000E+00  0.1023E+01  0.0000E+00
        PH         EHM        EHMC      EMFZSC
0.8200E+01  0.5000E+00  0.9000E+01  0.9000E+01
CONCENTRATION UNITS :  PPM
  Na          K           Li          Ca          Mg          Fe          Al
0.1077E+05  0.3991E+03  0.1810E+00  0.4123E+03  0.1292E+04  0.2000E-02  0.2000E-02
  SiO2        Cl          SO4         H2S         HCO3        CO3         TIC
0.4280E+01  0.1935E+05  0.2712E+04  0.0000E+00  0.1234E+03  0.0000E+00  0.0000E+00
  F           PO4         NO3         NH3         B           Sr          Ba
0.1390E+01  0.6000E-01  0.2900E+00  0.3000E-01  0.4450E+01  0.8140E+01  0.2000E-01
  Pb          Zn          Cu          Mn          Hg          Ag
0.5000E-04  0.4900E-02  0.7000E-03  0.2000E-03  0.3000E-04  0.4000E-04
  As          U           V
0.4000E-02  0.0000E+00  0.0000E+00
  Acetate     Oxalate     Succinate   CH4
0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00
      ALK      ITIC
     2          0
    DCO2         DH2S        DNH3        DCH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   ICCSAT      IMCO3        FIXIT       FCCSAT
     0          0      0.00000E+00       0.0500
  TCO2M       TCH4M       TH2SM       WROIL       KCO2OL      KCH4OL      KH2SOL      DSEP
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
Adsorption/Exchange option (N=no) = N
      IBMIX      ITMIX
      0          0
LOG KT TO BE CHANGED AT TEMP =  25.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
LOG KT TO BE CHANGED AT TEMP =   0.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
       ANS1       ANS2
     0          0
Number of Additional Minerals =           0
FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    1
FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS:  0
FLAGS FOR CALCULATING REDOX SPECIES:
Fe  Cu  Hg  Mn   U   V
 1   1   1   1   0   0
PRINTING OPTIONS:
   INFORM       RATIO       GEOTH       IPRIN1      IPRIN2
     0           1           1           1           1
TOLERANCE FACTORS:  CONV1 =   0.5000E-04  CONV2 =   0.5000E-04
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SOLMINEQ.87 (VERSION: USGS-ARC-88-8) - SOLUTION-MINERAL-EQUILIBRIUM COMPUTATIONS

SAMPLE IDENT:- Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C

ITERATIVE CONVERGENCE TEST AT TEMPERATURE = 25.00

ITER	CARBONATE	SULFATE	FLUORIDE	PHOSPHATE	CHLORIDE	ACETATE	SULFIDE	OXYLATE	SUCCINATE	USR-DEF #1	USR-DEF #2
1	3.442E-01	1.131E+00	6.964E-01	3.761E+00	3.108E-02	3.447E-01	0.000E+00	8.063E+00	4.936E-01	0.000E+00	0.000E+00
6	5.388E-06	1.801E-05	1.245E-05	2.843E-05	2.752E-07	5.398E-06	0.000E+00	3.134E-05	9.374E-06	0.000E+00	0.000E+00

Total number of iterations = 6 at pH = 8.20

SAMPLE IDENT:- Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C

PH	EH	TEMP		CATIONS	ANIONS	DIFFERENCE (MEQ/L)
8.20	0.5000	25.00	ANAL=	619.6747	618.2648	1.4099
			CALC=	577.6364	569.7726	7.8638

--- H - OH BALANCE (MOLES) -------

HTOT	OHTOT	DIFFERENCE
0.2198E-02	0.1351E-02	0.8477E-03

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER	PRESSURE P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0230	35906.34	0.64945	0.9809	1.0000	0.3169E-01	0.4782E-03	0.0000E+00	0.5252E-02	0.1644E-08

	Total Alkalinity as HCO3-	CO3=	CaCO3	Dissolved Inorganic Carbon as TIC	HCO3- Alkalinity	H2CO3 species	Sum of HCO3-	Sum of CO3=
(MG/L)=	0.1423E+03	0.6999E+02	0.1167E+03	0.2485E+02	0.1373E+03	0.8648E+00	0.1130E+03	0.1216E+02
(PPM)=	0.1391E+03	0.6842E+02	0.1141E+03	0.2429E+02	0.1343E+03	0.8454E+00	0.1105E+03	0.1188E+02
(MOLALITY)=	0.2363E-02	0.1182E-02	0.1182E-02	0.2096E-02	0.2287E-02	0.1413E-04	0.1877E-02	0.2052E-03

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
1	Ca ++	412.3000	421.7829	0.1066E-01	0.2844E+03	0.2909E+03	0.7353E-02	0.1807E-02	0.2458	2.7429
2	Mg ++	1292.0000	1321.7160	0.5508E-01	0.1121E+04	0.1147E+04	0.4779E-01	0.1261E-01	0.2640	1.8992
3	Na +	10770.0000	11017.7100	0.4855E+00	0.1024E+05	0.1048E+05	0.4618E+00	0.3099E+00	0.6710	0.5088
4	K +	399.1000	408.2793	0.1058E-01	0.3825E+03	0.3913E+03	0.1014E-01	0.6357E-02	0.6269	2.1968
5	Cl -	19350.0000	19795.0500	0.5656E+00	0.1874E+05	0.1917E+05	0.5478E+00	0.3434E+00	0.6269	0.4641
6	SO4 --	2712.0000	2774.3760	0.2926E-01	0.1203E+04	0.1231E+04	0.1298E-01	0.2189E-02	0.1687	2.6598
7	HCO3 -	123.4000	126.2382	0.2096E-02	0.8534E+02	0.8730E+02	0.1449E-02	0.1000E-02	0.6899	3.0000
8	H +				0.7638E-05	0.7814E-05	0.7853E-08	0.6310E-08	0.8034	8.2000
9	OH -				0.4016E-01	0.4108E-01	0.2447E-05	0.1591E-05	0.6501	5.7984
11	H4SiO4				0.6615E+01	0.6767E+01	0.7133E-04	0.7133E-04	1.0000	4.1467
12	SiO2	4.2800	4.3784	0.7382E-04						
13	Ag +	0.0000	0.0000	0.3843E-09	0.1039E-08	0.1063E-08	0.9982E-14	0.6000E-14	0.6011	14.2219
14	Al +3	0.0020	0.0020	0.7682E-07	0.4280E-11	0.4379E-11	0.1644E-15	0.1404E-16	0.0854	16.8525
15	Ba ++	0.0200	0.0205	0.1509E-06	0.1815E-01	0.1857E-01	0.1370E-06	0.2849E-07	0.2080	7.5453
16	Cu +	0.0007	0.0007	0.1142E-07	0.2395E-09	0.2450E-09	0.3906E-14	0.2348E-14	0.6011	14.6294
17	Cu ++				0.3648E-03	0.3732E-03	0.5950E-08	0.1462E-08	0.2458	8.8349
18	Fe ++	0.0020	0.0020	0.3711E-07	0.1268E-08	0.1297E-08	0.2353E-13	0.5784E-14	0.2458	14.2378
19	Fe +3				0.1009E-12	0.1032E-12	0.1872E-17	0.1599E-18	0.0854	18.7962
21	Hg ++	0.0000	0.0000	0.1550E-09	0.7474E-18	0.7646E-18	0.3861E-23	0.8033E-24	0.2080	24.0951
22	Li +	0.1810	0.1852	0.2703E-04	0.1792E+00	0.1833E+00	0.2677E-04	0.1973E-04	0.7373	4.7048
23	Mn ++	0.0002	0.0002	0.3773E-08	0.5864E-06	0.5999E-06	0.1106E-10	0.2719E-11	0.2458	11.5656
24	Mn +3				0.8887E-23	0.9092E-23	0.1677E-27	0.1432E-28	0.0854	28.8440
25	Pb ++	0.0001	0.0001	0.2501E-09	0.9966E-06	0.1020E-05	0.4985E-11	0.9397E-12	0.1885	12.0270
26	Sr ++	8.1400	8.3272	0.9628E-04	0.7551E+01	0.7725E+01	0.8931E-04	0.1858E-04	0.2080	4.7310
27	Zn ++	0.0049	0.0050	0.7768E-07	0.2886E-02	0.2952E-02	0.4575E-07	0.1124E-07	0.2458	7.9490
28	H2AsO3-	0.0067	0.0068	0.5281E-07	0.7209E-03	0.7375E-03	0.5706E-08	0.3829E-08	0.6710	8.4169
29	PO4 -3	0.0600	0.0614	0.6548E-06	0.5919E-05	0.6055E-05	0.6459E-10	0.1748E-11	0.0271	11.7573
30	F -	1.3900	1.4220	0.7583E-04	0.7672E+00	0.7848E+00	0.4185E-04	0.2721E-04	0.6501	4.5653
31	B(OH)3	25.4540	26.0394	0.4266E-03	0.2205E+02	0.2256E+02	0.3696E-03	0.3696E-03	1.0000	3.4323
32	NH3	0.0300	0.0307	0.1826E-05						
34	AlF ++				0.7083E-09	0.7246E-09	0.1597E-13	0.3566E-14	0.2234	14.4478
35	AlF2 +				0.3364E-08	0.3442E-08	0.5366E-13	0.3863E-13	0.7198	13.4131
36	AlF3				0.1024E-08	0.1047E-08	0.1263E-13	0.1263E-13	1.0000	13.8984
37	AlF4 -				0.1215E-10	0.1243E-10	0.1223E-15	0.8438E-16	0.6899	16.0737

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
38	Al(OH)++				0.4655E-08	0.4762E-08	0.1097E-12	0.2450E-13	0.2234	13.6109
39	Al(OH)2+				0.3336E-05	0.3413E-05	0.5669E-10	0.4081E-10	0.7198	10.3893
40	Al(OH)4-				0.7037E-02	0.7199E-02	0.7676E-07	0.5296E-07	0.6899	7.2761
41	AlSO4 +				0.5289E-11	0.5411E-11	0.4455E-16	0.3074E-16	0.6899	16.5123
42	AlSO4)2-				0.1600E-11	0.1637E-11	0.7569E-17	0.5222E-17	0.6899	17.2822
43	AgCl				0.5954E-06	0.6091E-06	0.4305E-11	0.4305E-11	1.0000	11.3660
44	AgCl2 -				0.3801E-04	0.3889E-04	0.2204E-09	0.1479E-09	0.6710	9.8301
45	AgCl3 --				0.3041E-04	0.3111E-04	0.1471E-09	0.3060E-10	0.2080	10.5143
46	AgCl4 -3				0.4054E-05	0.4148E-05	0.1683E-10	0.6631E-12	0.0394	12.1784
47	AgSO4 -				0.7863E-10	0.8044E-10	0.3996E-15	0.2681E-15	0.6710	15.5717
48	CH3COO -	0.1000	0.1023	0.1755E-05	0.7225E-01	0.7391E-01	0.1268E-05	0.8749E-06	0.6899	6.0580
49	H3AsO3				0.5724E-02	0.5856E-02	0.4710E-07	0.4710E-07	1.0000	7.3269
51	BaCO3				0.1272E-04	0.1301E-04	0.6679E-10	0.6679E-10	1.0000	10.1753
52	BaHCO3 +				0.2238E-03	0.2290E-03	0.1169E-08	0.7847E-09	0.6710	9.1053
53	BaOH +				0.3234E-07	0.3309E-07	0.2172E-12	0.1536E-12	0.7071	12.8137
54	BaSO4				0.2867E-02	0.2933E-02	0.1273E-07	0.1273E-07	1.0000	7.8951
55	CaCO3				0.2147E+01	0.2197E+01	0.2224E-04	0.2224E-04	1.0000	4.6529
56	CaHCO3 +				0.3081E+01	0.3152E+01	0.3158E-04	0.2328E-04	0.7373	4.6329
57	CaOH +				0.2965E-02	0.3034E-02	0.5383E-07	0.3969E-07	0.7373	7.4013
58	CaPO4 -				0.1688E-02	0.1727E-02	0.1296E-07	0.9326E-08	0.7198	8.0303
59	CaHPO4				0.2333E-02	0.2387E-02	0.1777E-07	0.1777E-07	1.0000	7.7503
60	CaH2PO4+				0.2207E-04	0.2258E-04	0.1669E-09	0.1201E-09	0.7198	9.9203
61	CaSO4				0.1037E+03	0.1061E+03	0.7893E-03	0.7893E-03	1.0000	3.1028
62	CuCl				0.3860E-07	0.3949E-07	0.4041E-12	0.4041E-12	1.0000	12.3935
63	CuCl2 -				0.4663E-05	0.4770E-05	0.3594E-10	0.2412E-10	0.6710	10.6177
64	CuCl3 --				0.1035E-04	0.1058E-04	0.6311E-10	0.1313E-10	0.2080	10.8818
65	CuCl +				0.7487E-04	0.7659E-04	0.7839E-09	0.5260E-09	0.6710	9.2790
66	CuCl2				0.4364E-05	0.4464E-05	0.3364E-10	0.3364E-10	1.0000	10.4732
67	CuCl3 -				0.7255E-07	0.7422E-07	0.4425E-12	0.2969E-12	0.6710	12.5273
68	CuCl4 --				0.4869E-09	0.4981E-09	0.2457E-14	0.5111E-15	0.2080	15.2915
69	CuOH +				0.3094E-03	0.3165E-03	0.3981E-08	0.2671E-08	0.6710	8.5733
70	CuSO4				0.8766E-04	0.8967E-04	0.5692E-09	0.5692E-09	1.0000	9.2447
71	FeCl +				0.7697E-10	0.7874E-10	0.8737E-15	0.5862E-15	0.6710	15.2319
72	FeCl2				0.5145E-18	0.5263E-18	0.4207E-23	0.4207E-23	1.0000	23.3761
73	FeHPO4				0.8141E-13	0.8329E-13	0.5557E-18	0.5557E-18	1.0000	18.2551
74	H3PO4				0.2034E-09	0.2081E-09	0.2151E-14	0.2151E-14	1.0000	14.6673
75	FeOH +				0.2892E-10	0.2959E-10	0.4115E-15	0.2910E-15	0.7071	15.5362
76	Fe(OH)2				0.3115E-13	0.3187E-13	0.3593E-18	0.3593E-18	1.0000	18.4446
77	FeOOH -				0.2686E-13	0.2748E-13	0.3133E-18	0.2215E-18	0.7071	18.6546
78	FeSO4				0.4994E-09	0.5109E-09	0.3407E-14	0.3407E-14	1.0000	14.4676
79	FeCl ++				0.6863E-12	0.7021E-12	0.7791E-17	0.1621E-17	0.2080	17.7903
80	FeCl2 +				0.4400E-12	0.4501E-12	0.3598E-17	0.2544E-17	0.7071	17.5945
81	FeCl3				0.1368E-13	0.1399E-13	0.8738E-19	0.8738E-19	1.0000	19.0586
82	FeCl4 -				0.1026E-15	0.1049E-15	0.5377E-21	0.3608E-21	0.6710	21.4427
83	FeSO4 +				0.1001E-11	0.1024E-11	0.6831E-17	0.4831E-17	0.7071	17.3160
84	FeSO4)2-				0.1038E-23	0.1062E-23	0.4340E-29	0.2912E-29	0.6710	29.5358
85	FeOH ++				0.6227E-07	0.6370E-07	0.8858E-12	0.1843E-12	0.2080	12.7346
86	Fe(OH)2+				0.3697E-04	0.3782E-04	0.4264E-09	0.3069E-09	0.7198	9.5130
87	Fe(OH)3				0.2099E-02	0.2147E-02	0.2035E-07	0.2035E-07	1.0000	7.6913
88	Fe(OH)4-				0.1952E-02	0.1997E-02	0.1633E-07	0.1176E-07	0.7198	7.9297
89	B(OH)4 -				0.4342E+01	0.4442E+01	0.5708E-04	0.3462E-04	0.6065	4.4607
90	H2SiO4--				0.2150E-03	0.2199E-03	0.2367E-08	0.5288E-09	0.2234	9.2767
91	H3SiO4 -				0.2287E+00	0.2340E+00	0.2492E-05	0.1672E-05	0.6710	5.7767

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
92	HAsO3 --				0.1173E-07	0.1200E-07	0.9358E-13	0.1947E-13	0.2080	13.7107
96	HF				0.5016E-05	0.5131E-05	0.2598E-09	0.2598E-09	1.0000	9.5853
97	H2CO3				0.8454E+00	0.8648E+00	0.1413E-04	0.1413E-04	1.0000	4.8500
98	CO3 --				0.1922E+01	0.1966E+01	0.3319E-04	0.7413E-05	0.2234	5.1300
99	HPO4 --				0.1074E-01	0.1099E-01	0.1160E-06	0.2414E-07	0.2080	7.6173
100	H2PO4 -				0.3138E-03	0.3210E-03	0.3353E-08	0.2414E-08	0.7198	8.6173
103	HSO4 -				0.1671E-03	0.1709E-03	0.1784E-08	0.1231E-08	0.6899	8.9098
104	HNO3				0.4331E-10	0.4431E-10	0.7124E-15	0.7124E-15	1.0000	15.1473
105	HgCl +				0.1665E-12	0.1704E-12	0.7311E-18	0.4906E-18	0.6710	18.3093
106	HgCl2				0.4517E-06	0.4621E-06	0.1724E-11	0.1724E-11	1.0000	11.7634
107	HgCl3 -				0.3216E-04	0.3290E-04	0.1086E-09	0.7285E-10	0.6710	10.1376
108	HgCl4 --				0.1476E-04	0.1510E-04	0.4469E-10	0.9296E-11	0.2080	11.0317
109	HgSO4				0.1264E-19	0.1293E-19	0.4416E-25	0.4416E-25	1.0000	25.3550
113	KCl				0.2070E+02	0.2118E+02	0.2878E-03	0.2878E-03	1.0000	3.5409
114	KCO3 -				0.7987E-01	0.8171E-01	0.8352E-06	0.5536E-06	0.6629	6.2568
115	KHSO4				0.7277E-05	0.7445E-05	0.5539E-10	0.5539E-10	1.0000	10.2566
116	KSO4 -				0.1957E+02	0.2002E+02	0.1500E-03	0.1080E-03	0.7198	3.9666
117	KHPO4 -				0.5417E-04	0.5541E-04	0.4156E-09	0.2991E-09	0.7198	9.5241
118	LiOH				0.1098E-05	0.1123E-05	0.4751E-10	0.4751E-10	1.0000	10.3232
119	LiSO4 -				0.2650E-01	0.2711E-01	0.2666E-06	0.1885E-06	0.7071	6.7246
120	MgCO3				0.7265E+01	0.7432E+01	0.8930E-04	0.8930E-04	1.0000	4.0492
121	MgHCO3 +				0.1818E+02	0.1860E+02	0.2209E-03	0.1482E-03	0.6710	3.8292
122	MgF +				0.1373E+01	0.1405E+01	0.3286E-04	0.2267E-04	0.6899	4.6445
123	MgOH +				0.4244E+00	0.4341E+00	0.1064E-04	0.7988E-05	0.7505	5.0976
124	MgSO4				0.8054E+03	0.8240E+03	0.6934E-02	0.6934E-02	1.0000	2.1590
125	MgPO4 -				0.1041E-01	0.1065E-01	0.9042E-07	0.6509E-07	0.7198	7.1865
126	MgHPO4				0.4552E-01	0.4657E-01	0.3922E-06	0.3922E-06	1.0000	6.4065
127	MgH2PO4+				0.1363E-03	0.1395E-03	0.1165E-08	0.8385E-09	0.7198	9.0765
128	MnCl +				0.3839E-13	0.3927E-13	0.4401E-18	0.2953E-18	0.6710	18.5297
129	MnCl2				0.3094E-10	0.3165E-10	0.2548E-15	0.2548E-15	1.0000	15.5938
130	MnCl3 -				0.5098E-09	0.5215E-09	0.3276E-14	0.2198E-14	0.6710	14.6580
131	MnCl4 --				0.5472E-08	0.5598E-08	0.2882E-13	0.5996E-14	0.2080	14.2221
132	MnHCO3 +				0.8443E-08	0.8637E-08	0.7546E-13	0.5063E-13	0.6710	13.2956
133	MnSO4				0.1578E-06	0.1614E-06	0.1083E-11	0.1083E-11	1.0000	11.9654
134	MnHPO4				0.3633E-10	0.3717E-10	0.2495E-15	0.2495E-15	1.0000	15.6029
135	MnOH +				0.1233E-08	0.1261E-08	0.1776E-13	0.1191E-13	0.6710	13.9239
136	NO3 -	0.2900	0.2967	0.4847E-05	0.2900E+00	0.2967E+00	0.4847E-05	0.3039E-05	0.6269	5.5173
137	NaCl				0.8478E+03	0.8673E+03	0.1503E-01	0.1503E-01	1.0000	1.8229
138	NaCO3 -				0.4759E+01	0.4869E+01	0.5943E-04	0.4278E-04	0.7198	4.3688
139	NaHCO3				0.1413E+02	0.1445E+02	0.1743E-03	0.1743E-03	1.0000	3.7588
140	Na2CO3				0.1521E-01	0.1556E-01	0.1487E-06	0.1487E-06	1.0000	6.8276
141	Na2SO4				0.9321E+03	0.9536E+03	0.6801E-02	0.6801E-02	1.0000	2.1674
142	NaSO4 -				0.1838E+03	0.1880E+03	0.1600E-02	0.1152E-02	0.7198	2.9386
143	NaHPO4 -				0.2326E-02	0.2379E-02	0.2026E-07	0.1458E-07	0.7198	7.8361
144	NaF				0.4503E-01	0.4607E-01	0.1111E-05	0.1111E-05	1.0000	5.9541
146	NH4 +				0.3015E-01	0.3085E-01	0.1732E-05	0.1041E-05	0.6011	5.9824
147	NH4OH				0.3150E-02	0.3223E-02	0.9315E-07	0.9315E-07	1.0000	7.0308
148	PbCl +				0.2894E-05	0.2961E-05	0.1236E-10	0.8295E-11	0.6710	11.0812
149	PbCl2				0.2776E-05	0.2840E-05	0.1034E-10	0.1034E-10	1.0000	10.9853
150	PbCl3 -				0.7845E-06	0.8026E-06	0.2593E-11	0.1740E-11	0.6710	11.7594
151	PbCl4 --				0.6104E-06	0.6244E-06	0.1813E-11	0.3771E-12	0.2080	12.4236
152	PbSO4				0.3384E-06	0.3462E-06	0.1157E-11	0.1157E-11	1.0000	11.9368
153	MnCl ++				0.8401E-21	0.8595E-21	0.9633E-26	0.2004E-26	0.2080	26.6981

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
154	SrOH -				0.2067E-04	0.2114E-04	0.2047E-09	0.1448E-09	0.7071	9.8394
155	SrCO3				0.1296E-01	0.1326E-01	0.9100E-07	0.9100E-07	1.0000	7.0410
156	SrHCO3 +				0.6151E-01	0.6292E-01	0.4289E-06	0.2878E-06	0.6710	6.5410
157	SrSO4				0.1142E+01	0.1169E+01	0.6445E-05	0.6445E-05	1.0000	5.1908
158	ZnCl +				0.1473E-02	0.1507E-02	0.1514E-07	0.1016E-07	0.6710	7.9932
159	ZnCl2				0.7271E-03	0.7438E-03	0.5529E-08	0.5529E-08	1.0000	8.2573
160	ZnCl3 -				0.2461E-03	0.2518E-03	0.1485E-08	0.9966E-09	0.6710	9.0015
161	ZnCl4 --				0.2276E-03	0.2328E-03	0.1138E-08	0.2368E-09	0.2080	9.6256
162	ZnSO4				0.6217E-03	0.6360E-03	0.3991E-08	0.3991E-08	1.0000	8.3989
163	AlF5 --				0.2976E-13	0.3044E-13	0.2528E-18	0.5260E-19	0.2080	19.2791
164	AlF6 -3				0.1492E-16	0.1526E-16	0.1097E-21	0.4322E-23	0.0394	23.3644
165	HgOH +				0.1153E-13	0.1180E-13	0.5492E-19	0.3685E-19	0.6710	19.4335
166	Hg(OH)2				0.3411E-08	0.3490E-08	0.1507E-13	0.1507E-13	1.0000	13.8219
228	CH3COOH				0.1841E-04	0.1883E-04	0.3177E-09	0.3177E-09	1.0000	9.4980
229	AlAce ++				0.3920E-14	0.4010E-14	0.4722E-19	0.8901E-20	0.1885	20.0506
230	BaAce +				0.9235E-07	0.9447E-07	0.4874E-12	0.3362E-12	0.6899	12.4734
231	CaAce +				0.3723E-02	0.3809E-02	0.3892E-07	0.2685E-07	0.6899	7.5710
232	CuAce +				0.2733E-13	0.2796E-13	0.2311E-18	0.1594E-18	0.6899	18.7974
233	FeAce +				0.1622E-12	0.1660E-12	0.1463E-17	0.1010E-17	0.6899	17.9958
234	Fe(Ace)2				0.9354E-20	0.9569E-20	0.5574E-25	0.5574E-25	1.0000	25.2539
235	KAce				0.2146E-03	0.2195E-03	0.2266E-08	0.2266E-08	1.0000	8.6448
236	MgAce +				0.2288E-01	0.2340E-01	0.2844E-06	0.1962E-06	0.6899	6.7072
237	NaAce				0.1264E-01	0.1293E-01	0.1596E-06	0.1596E-06	1.0000	6.7968
238	PbAce +				0.5570E-10	0.5699E-10	0.2168E-15	0.1496E-15	0.6899	15.8251
239	Pb(Ace)2				0.9855E-15	0.1008E-14	0.3140E-20	0.3140E-20	1.0000	20.5031
240	Pb(Ace)3				0.1775E-20	0.1816E-20	0.4787E-26	0.3303E-26	0.6899	26.4811
241	SrAce +				0.4820E-04	0.4930E-04	0.3406E-09	0.2350E-09	0.6899	9.6290
244	ZnAce +				0.1391E-03	0.1423E-03	0.1159E-08	0.7997E-09	0.6899	9.0971
245	Zn(Ace)2				0.3411E-13	0.3490E-13	0.1927E-18	0.1927E-18	1.0000	18.7151
246	C2O4 --	0.1000	0.1023	0.1177E-05	0.9439E-02	0.9656E-02	0.1111E-06	0.2482E-07	0.2234	7.6051
247	HC2O4 -				0.3468E-09	0.3548E-09	0.4037E-14	0.2785E-14	0.6899	14.5551
248	H2C2O4				0.3117E-13	0.3189E-13	0.3588E-18	0.3588E-18	1.0000	18.4451
249	AlOxy +				0.5607E-13	0.5736E-13	0.5053E-18	0.3486E-18	0.6899	18.4576
250	AlOxy)2-				0.2457E-15	0.2514E-15	0.1254E-20	0.8654E-21	0.6899	21.0628
251	BaOxy				0.5714E-08	0.5845E-08	0.2628E-13	0.2628E-13	1.0000	13.5804
252	CaOxy				0.5546E-02	0.5673E-02	0.4487E-07	0.4487E-07	1.0000	7.3481
253	FeOxy				0.5006E-12	0.5122E-12	0.3606E-17	0.3606E-17	1.0000	17.4429
254	FeOxy +				0.3028E-13	0.3097E-13	0.2181E-18	0.1505E-18	0.6899	18.8225
255	KOxy -				0.1406E-03	0.1438E-03	0.1146E-08	0.7908E-09	0.6899	9.1019
256	MgOxy				0.1002E+00	0.1025E+00	0.9241E-06	0.9241E-06	1.0000	6.0343
257	MnOxy				0.9311E-10	0.9525E-10	0.6750E-15	0.6750E-15	1.0000	15.1707
258	MnOxy)2				0.7180E-03	0.7345E-03	0.3760E-08	0.8398E-09	0.2234	9.0758
259	MnOxy)3				0.1550E-06	0.1585E-06	0.6353E-12	0.1315E-14	0.0021	14.8809
260	MnOxy				0.2764E-19	0.2828E-19	0.2004E-24	0.1382E-24	0.6899	24.8593
261	NaOxy -				0.9487E-02	0.9705E-02	0.8857E-07	0.6110E-07	0.6899	7.2139
262	PbOxy				0.3651E-09	0.3735E-09	0.1282E-14	0.1282E-14	1.0000	14.8922
263	SrOxy				0.2710E-04	0.2773E-04	0.1599E-09	0.1599E-09	1.0000	9.7961
264	ZnOxy				0.3282E-05	0.3357E-05	0.2217E-10	0.2217E-10	1.0000	10.6542
265	C4H4O4--	0.1000	0.1023	0.8929E-06	0.6405E-01	0.6553E-01	0.5719E-06	0.1277E-06	0.2234	6.8937
266	HC4H4O4-				0.2140E-05	0.2190E-05	0.1895E-10	0.1307E-10	0.6899	10.8837
267	H2C4H4O4				0.4102E-08	0.4197E-08	0.3600E-13	0.3600E-13	1.0000	13.4437
268	AlSuc +				0.7162E-13	0.7326E-13	0.5188E-18	0.3579E-18	0.6899	18.4462
269	AlSuc)2-				0.4585E-15	0.4690E-15	0.3322E-20	0.2292E-20	0.6899	20.6399

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
270	BaSuc				0.9318E-07	0.9532E-07	0.3811E-12	0.3811E-12	1.0000	12.4190
271	CaSuc				0.3479E-02	0.3559E-02	0.2309E-07	0.2309E-07	1.0000	7.6366
272	FeSuc				0.1942E-13	0.1987E-13	0.1171E-18	0.1171E-18	1.0000	18.9315
273	FeSuc +				0.4911E-13	0.5024E-13	0.2960E-18	0.2042E-18	0.6899	18.6898
274	KSuc -				0.3516E-03	0.3597E-03	0.2348E-08	0.1620E-08	0.6899	8.7904
275	MgSuc				0.2449E-01	0.2505E-01	0.1808E-06	0.1808E-06	1.0000	6.7428
276	MnSuc				0.8478E-11	0.8673E-11	0.5138E-16	0.5138E-16	1.0000	16.2892
277	NaSuc -				0.1536E-01	0.1571E-01	0.1145E-06	0.7898E-07	0.6899	7.1025
278	PbSuc				0.1184E-09	0.1211E-09	0.3796E-15	0.3796E-15	1.0000	15.4207
279	SrSuc				0.4665E-04	0.4772E-04	0.2373E-09	0.2373E-09	1.0000	9.6246
280	ZnSuc				0.7253E-07	0.7420E-07	0.4143E-12	0.4143E-12	1.0000	12.3827
281	CaCl +				0.1773E+03	0.1814E+03	0.2433E-02	0.1633E-02	0.6710	2.7871
282	CaCl2				0.3377E+01	0.3455E+01	0.3153E-04	0.3153E-04	1.0000	4.5012
283	FeF ++				0.1510E-11	0.1545E-11	0.2091E-16	0.4350E-17	0.2080	17.3615
284	SiF6 --				0.1180E-28	0.1207E-28	0.8609E-34	0.1791E-34	0.2080	34.7469
285	CH4 Gas	0.1000	0.1023	0.6460E-05	0.1000E+00	0.1023E+00	0.6460E-05	0.0000E+00	1.0000	0.0000
288	PbCO3				0.1796E-04	0.1837E-04	0.6966E-10	0.6966E-10	1.0000	10.1570
289	PbOH +				0.3184E-04	0.3257E-04	0.1472E-09	0.9876E-10	0.6710	10.0054
292	ZnHCO3 +				0.5376E-04	0.5499E-04	0.4408E-09	0.2958E-09	0.6710	9.5290
293	ZnOH +				0.2323E-03	0.2377E-03	0.2923E-08	0.1961E-08	0.6710	8.7074
294	Zn(OH)2				0.1037E-04	0.1061E-04	0.1082E-09	0.1082E-09	1.0000	9.9658

SAMPLE IDENT - Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C TEMPERATURE = 25.00

MOLE RATIOS (USING ANALYTICAL MOLALITY)

CL/CA	CL/MG	CL/NA	CL/K	CL/AL	CL/FE	CL/SO4	CL/HCO3	CA/MG	SQRT(CA)/NA
0.5306E+02	0.1027E+02	0.1165E+01	0.5347E+02	0.7363E+07	0.1524E+08	0.1933E+02	0.2699E+03	0.1936E+00	0.2127E+00

NH3/NA	LI/NA	K/NA	MG/CA	SR/CA	BA/CA	SO4/CL	HCO3/CL	F/CL	B/CL
0.3760E-05	0.5568E-04	0.2179E-01	0.5166E+01	0.9031E-02	0.1416E-04	0.5173E-01	0.3705E-02	0.1341E-03	0.7542E-03

LOG OF ACTIVITY RATIOS

CA/H2	MG/H2	NA/H	K/H	AL/H3	FE/H2	CA/MG	NA/K
0.1366E+02	0.1450E+02	0.7691E+01	0.6003E+01	0.7747E+01	0.2162E+01	-0.8438E+00	0.1688E+01

LOG(NA/K)+1/3(LOG(SQRT(CA)/NA)) = 0.144E+01
LOG(NA/K)+4/3(LOG(SQRT(CA)/NA)) = 0.765E+00

CHEMICAL GEOTHERMOMETER TEMPERATURES (IN DEGREES CENTIGRADE)
("999.0" INDICATES THAT A VALUE GREATER THAN 0.0 WAS NOT CALCULATED)

TEMPERATURE		TEMP. WITH PRESSURE AND/OR ACTIVITY CORRECTION
14.0	QUARTZ (CONDUCTIVE)	15.2
24.2	QUARTZ (ADIABATIC)	25.3
999.0	CHALCEDONY WITH SIO2	999.0
999.0	ALFA CRISTOBALITE WITH SIO2	999.0
999.0	Amorphous Silica With SiO2	999.0
144.5	LOG (NA/K)	
174.7	LOG (NA/K) + 1/3 LOG(SQRT(CA)/NA)	
274.9	LOG (NA/K) + 4/3 LOG(SQRT(CA)/NA)	
194.0	LOG (NA/K) + 4/3 LOG(SQRT(CA)/NA) + 1.36+0.253*LOG(PCO2)	
999.0	MG CORRECTED 1/3 (NA-K-CA)	
10.2	LOG (SQRT(MG)/LI)	
13.1	LOG (NA/LI)	

A. IF THE WATER IS BOILING OR STEAM IS LOST DURING THE SAMPLING OF GROUNDWATERS THEN USE THE QUARTZ ADIABATIC TEMPERATURE.
B. IF THERE IS NO STEAM LOSS THEN USE THE QUARTZ CONDUCTIVE TEMPERATURE.
C. The Amorphous Silica Temperature Should Be Considered When The Sample Is Saturated With Amorphous Silica (THE DELTA G OF MINERAL NO. 275 IS POSITIVE).
D. IF THE IN SITU TEMPERATURE EXCEEDS 150 DEGREES THEN THE NA/K TEMPERATURE MAY BE USED.
E. ALTHOUGH THE 4/3 LOG TEMPERATURE IS GENERALLY USED WHEN THE TEMPERATURE IS LESS THAN 100 DEGREES IT IS CONSIDERED LESS RELIABLE THAN THE 1/3 LOG TEMPERATURE.
F. THE ACTIVITIES OF H4SIO4 AND WATER WILL BE COMPUTED AT THE SURFACE TEMPERATURE ONLY IF THE HITEMP OPTION IS SELECTED.
G. THE ORDER OF RELIABILITY OF THE CATION GEOTHERMOMETERS: MG-LI>MG-CORRECTED NA-K-CA>NA-LI>OTHERS
H. DETAILS OF THE EQUATIONS AND PARAMETERS CAN BE FOUND IN KHARAKA AND MARINER,1988).

SAMPLE IDENT - Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
1	ADULARIA	1.344	1.260	0.084	0.115	82	NATRTHRM	-6.156	-0.010	-6.146	-8.385
2	AKERMANI	33.530	45.460	-11.930	-16.276	83	NATRON	-6.231	-0.880	-5.351	-7.301
3	ALBITE	3.032	2.500	0.532	0.726	84	NEPHALIN	11.292	13.520	-2.228	-3.040
4	ALBITE L	3.032	3.110	-0.078	-0.106	85	NESQUHON	-7.054	-5.350	-1.704	-2.325
5	ALBITE H	3.032	4.430	-1.398	-1.907	86	NONT, Na	1.506	-11.480	12.986	17.716
6	ALUNITE	-8.924	-2.790	-6.134	-8.369	87	NONT, K	0.949	-11.810	12.759	17.407
7	AMESI14A	40.308	38.630	1.678	2.289	88	NONT, H	-1.032	-12.500	11.468	15.645
8	ANALCIME	7.154	6.050	1.104	1.506	89	NONT, Ca	1.222	-11.540	12.762	17.410
9	ANDALUSI	11.340	16.570	-5.230	-7.135	90	NONT, Mg	1.222	-11.560	12.782	17.437
10	ANDESITE	10.163	12.730	-2.567	-3.502	92	OLIGOCLA	6.597	8.730	-2.133	-2.909
11	ANHYDRIT	-5.403	-4.330	-1.073	-1.464	93	PARAGONI	18.493	14.390	4.103	5.598
12	ANNITE	7.797	29.140	-21.343	-29.117	94	PARAGASI	91.371	100.790	-9.419	-12.850
13	ANORTHIT	20.859	25.830	-4.971	-6.782	95	PERICLAS	14.492	21.510	-7.018	-9.574
14	APATCHLR	-49.451	-66.150	16.699	22.781	96	PHILLIPS	2.180	3.300	-1.120	-1.528
15	APATFLUR	-53.552	-68.340	14.788	20.174	97	PHLOGPIT	44.813	37.220	7.593	10.359
16	APATHYDX	-54.785	-60.390	5.605	7.646	98	PHLOGPTF	19.299	16.730	2.569	3.505
17	ARAGONIT	-7.873	-8.340	0.467	0.637	99	PORTLAN	-14.340	-5.420	-8.920	-12.169
18	AUGITE	24.989	32.560	-7.571	-10.329	100	POTASSI	11.998	84.120	-72.122	-98.391
19	AZURITE	-48.361	-39.460	-8.901	-12.144	101	PREHNITE	30.369	32.020	-1.651	-2.253
20	BARITE	-10.205	-9.960	-0.245	-0.334	102	PYROPHYL	-1.058	-0.100	-0.958	-1.308
21	BOEHMITE	7.731	6.950	0.781	1.065	103	QUARTZ	-4.130	-3.930	-0.200	-0.273
22	BRUCITE	-13.496	-11.470	-2.026	-2.764	104	SANIDINE	1.344	1.180	0.164	0.224
23	BYTOWNIT	17.293	18.600	-1.307	-1.783	105	SAPO, Na	33.401	26.880	6.521	8.897
24	CALCITE	-7.873	-8.480	0.607	0.828	106	SAPO, K	32.844	26.550	6.294	8.587
25	CELESTIT	-7.391	-6.430	-0.961	-1.311	107	SAPO, H	30.863	25.850	5.013	6.839
26	CHALCEDO	-4.130	-3.730	-0.400	-0.546	108	SAPO, Ca	33.117	26.820	6.297	8.590
27	CHAM, 7A	15.631	29.030	-13.399	-18.280	109	SAPO, Mg	33.256	26.800	6.456	8.807
28	CHLOR, 7	75.509	71.940	3.569	4.868	110	SEPIOLIT	33.131	31.520	1.611	2.198
29	CHLOR, 1	75.509	68.570	6.939	9.466	111	SILICAAM	-4.130	-2.700	-1.430	-1.951
30	CRYSOTIL	35.201	32.030	3.171	4.326	112	SILICGEL	-4.130	-2.710	-1.420	-1.937
31	C-ENSTAT	10.362	11.290	-0.928	-1.265	113	SILLIMAN	11.340	15.730	-4.390	-5.989
32	C-PTIL,N	-10.523	-7.900	-2.623	-3.578	114	SMEC Ca	5.104	6.140	-1.036	-1.414
33	C-PTIL,K	-13.899	-15.000	1.101	1.502	115	SMEC K	4.837	5.860	-1.023	-1.396
34	C-PTIL,C	-12.248	-9.300	-2.948	-4.022	116	SMEC Mg	5.244	6.040	-0.796	-1.085
35	C-PTIL,M	-11.404	-5.000	-6.404	-8.737	117	SMEC Na	5.394	6.120	-0.726	-0.991
36	CORUNDUM	15.470	21.400	-5.930	-8.090	118	Na2O	15.374	67.430	-52.056	-71.017
37	CRISTOBA	-4.130	-3.540	-0.590	-0.805	119	SPINEL	29.962	36.460	-6.498	-8.864
38	CRISTOBB	-4.130	-2.940	-1.190	-1.623	120	STILBITE	0.150	1.410	-1.260	-1.719
39	DICKITE	7.193	6.170	1.023	1.396	121	STRENGIT	-30.570	-27.200	-3.370	-4.598
40	DIOPSIDE	19.881	19.630	0.251	0.343	122	SrCO3	-9.861	-9.270	-0.591	-0.806
41	DOLOMITE	-14.902	-18.060	3.158	4.308	123	SYLVITE	-2.661	0.910	-3.571	-4.872
42	DSORD	-14.902	-16.520	1.618	2.207	124	TALC	26.949	21.130	5.819	7.939
43	ENSTATIT	10.362	11.470	-1.108	-1.511	125	THENARDI	-3.677	-0.290	-3.387	-4.621
44	EPIDOTE	36.164	31.990	4.174	5.695	126	TREMOLIT	66.711	60.890	5.821	7.942
45	FAYALITE	0.178	19.430	-19.252	-26.265	127	TRONA	-9.673	-0.630	-9.043	-12.337
46	FLUORITE	-11.874	-10.960	-0.914	-1.246	128	VIVIANIT	-66.295	-36.000	-30.295	-41.330
47	FORSTERI	24.855	29.070	-4.215	-5.750	129	WAIRAKIT	12.582	17.330	-4.748	-6.478
48	GIBBS AM	-34.248	-34.420	0.172	0.235	130	WITHERIT	-12.675	-8.630	-4.045	-5.519
49	GIBBSITE	-34.248	-34.920	0.672	0.917	131	WOLLASTO	9.519	12.600	-3.081	-4.204
50	GREENALI	-1.815	22.580	-24.395	-33.281	132	ZOISITE	38.108	42.100	-3.992	-5.446
51	GYPSUM	-5.420	-4.600	-0.820	-1.118	133	[illegible]LVER	-9.663	-0.500	-9.163	-12.501

SAMPLE IDENT - Test Sample #1 for SOLMINEQ.88 - Modified Seawater at 25 C (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
52	HALITE	-0.973	1.590	-2.563	-3.496
53	HALLOYSI	7.193	8.910	-1.717	-2.342
54	HEULANDI	0.158	1.410	-1.252	-1.707
55	HUNTITE	-28.960	-30.620	1.660	2.264
56	HYDRMAGN	-36.508	-38.530	2.022	2.759
57	HYPHILIT	-3.671	11.800	-15.471	-21.106
58	ILLITE	10.550	10.340	0.210	0.286
59	KAOLINIT	7.193	6.230	0.963	1.314
60	KENYAITE	-37.785	-25.000	-12.785	-17.441
61	K-SPAR	1.344	-0.550	1.894	2.584
62	KYANITE	11.340	14.480	-3.140	-4.284
63	LABRADOR	15.368	16.250	-0.882	-1.203
64	LARNITE	23.167	38.880	-15.713	-21.436
65	LAUMONTI	12.565	14.170	-1.605	-2.189
66	LEUCITE	5.474	6.520	-1.046	-1.427
67	LIME	-19.151	32.660	-51.811	-70.683
68	MAGADITE	-21.260	-14.340	-6.920	-9.441
69	MgFe2O4	26.075	21.100	4.975	6.787
70	MAGNESIT	-7.029	-8.050	1.021	1.393
71	MgCl2	-2.827	22.150	-24.977	-34.075
72	MARIALIT	8.123	1.710	6.413	8.749
73	MERWINIT	47.179	68.170	-20.991	-28.637
74	MICROCLN	1.344	-0.550	1.894	2.584
75	MIEONITE	54.703	69.950	-15.247	-20.801
76	MIRABILT	-3.761	-1.090	-2.671	-3.644
77	MONTICEL	24.011	30.150	-6.139	-8.375
78	MORD, Na	-5.253	-3.900	-1.353	-1.846
79	MORD, K	-6.941	-7.600	0.659	0.899
80	MUSCOVIT	16.805	12.880	3.925	5.355
81	NACHOLIT	-3.509	-0.430	-3.079	-4.200

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
134	AgCl	-14.686	-9.730	-4.956	-6.761
136	COPPER	-10.071	4.250	-14.321	-19.537
137	MALACHIT	-34.397	-33.580	-0.817	-1.114
138	CuO	7.557	7.670	-0.113	-0.155
139	Cu2O	-12.867	-1.900	-10.967	-14.962
144	FeCl2	-15.166	7.900	-23.066	-31.468
145	FeCl3	-20.189	12.340	-32.529	-44.377
146	FeCO3	-19.368	-10.540	-8.828	-12.043
147	FeO	2.154	13.500	-11.346	-15.479
148	Fe2O3HEM	11.582	0.040	11.542	15.747
149	Fe2O3MGH	11.582	6.400	5.182	7.070
150	Fe3O4	13.736	10.750	2.986	4.074
151	Fe(OH)3	-36.191	-37.200	1.009	1.376
152	GOETHITE	5.787	0.480	5.307	7.240
157	Hg(L)	-14.978	-2.840	-12.138	-16.560
158	HgCl2(C)	-25.023	-14.110	-10.913	-14.888
160	HgO	-7.704	2.440	-10.144	-13.838
163	MnCl2	-12.494	8.790	-21.284	-29.036
164	MnCO3	-16.696	-10.540	-6.156	-8.398
165	MnO	4.826	17.700	-12.874	-17.563
166	MnO2	-13.339	-8.330	-5.009	-6.834
168	PbCl2	-12.955	-4.820	-8.135	-11.098
169	PbCO3	-17.157	-12.890	-4.267	-5.821
170	PbOLITHR	4.365	12.550	-8.185	-11.167
171	PbOMASIC	4.365	12.690	-8.325	-11.358
173	PbSO4	-14.687	-7.800	-6.887	-9.395
174	ZnCO3	-13.079	-9.870	-3.209	-4.378
175	ZnO	8.443	11.200	-2.757	-3.762
177	ZnSO4	-10.609	3.540	-14.149	-19.302

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****** INPUT DATA ECHO ******

TITLE : Test Sample #2 - Mix caustic flood with formation water
      TEMP       HITEMP        DENS       PRESS
0.2500E+02  0.0000E+00  0.1000E+01  0.0000E+00
        PH         EHM        EHMC      EMFZSC
0.1092E+02  0.9000E+01  0.9000E+01  0.9000E+01
CONCENTRATION UNITS :  MOL/L
  Na           K           Li          Ca          Mg          Fe          Al
0.4000E-01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  SiO2         Cl          SO4         H2S         HCO3        CO3         TIC
0.0000E+00  0.2000E-01  0.0000E+00  0.0000E+00  0.2000E-01  0.0000E+00  0.0000E+00
  F           PO4         NO3         NH3         B           Sr          Ba
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  Pb          Zn          Cu          Mn          Hg          Ag
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  As          U           V
0.0000E+00  0.0000E+00  0.0000E+00
  Acetate     Oxalate     Succinate   CH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
      ALK      ITIC
     2          0
    DCO2         DH2S        DNH3        DCH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   ICCSAT      IMCO3       FIXIT       FCCSAT
     0           0     0.00000E+00      0.0500
  TCO2M       TCH4M       TH2SM       WROIL       KCO2OL      KCH4OL      KH2SOL      DSEP
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
Adsorption/Exchange option (N=no) = N
      IBMIX      ITMIX
     2          0
Number of mixtures =   1 starting at fraction of solution one =       0.5000 using a step increment of:       0.0000
and reading the second water composition from
the data set following this one.
LOG KT TO BE CHANGED AT TEMP =  25.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
LOG KT TO BE CHANGED AT TEMP =   0.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
       ANS1       ANS2
     0          0
Number of Additional Minerals =            0
FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    1
FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS:  0
FLAGS FOR CALCULATING REDOX SPECIES:
Fe  Cu  Hg  Mn   U   V
 1   1   1   1   0   0
PRINTING OPTIONS:
   INFORM       RATIO       GEOTH       IPRIN1      IPRIN2
      0           0           0           0           0
TOLERANCE FACTORS:  CONV1 =   0.5000E-04  CONV2 =   0.5000E-04
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SAMPLE IDENT:- Test Sample #2 - Mix caustic flood with formation water

PH	EH	TEMP
10.92	9.0000	25.00

	CATIONS	ANIONS	DIFFERENCE (MEQ/L)
ANAL=	40.0000	40.0000	0.0000
CALC=	35.7888	54.8365	-19.0477

--- H - OH BALANCE (MOLES) -------

HTOT	OHTOT	DIFFERENCE
0.2010E-02	0.1057E-02	0.9526E-03

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER
1.0000	2840.91	0.05935	0.9987

PRESSURE

P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0000	0.3169E-01	0.1287E-05	0.0000E+00	0.0000E+00	0.0000E+00

	Total Alkalinity as HCO3-	Total Alkalinity as CO3=	Total Alkalinity as CaCO3
(MG/L)=	0.2383E+04	0.1172E+04	0.1954E+04
(PPM)=	0.2383E+04	0.1172E+04	0.1954E+04
(MOLALITY)=	0.3916E-01	0.1958E-01	0.1958E-01

	Dissolved Inorganic Carbon as TIC	HCO3- Alkalinity	H2CO3 species	Sum of HCO3-	Sum of CO3=
(MG/L)=	0.2402E+03	0.2282E+04	0.2690E-02	0.1223E+03	0.1080E+04
(PPM)=	0.2402E+03	0.2282E+04	0.2690E-02	0.1223E+03	0.1080E+04
(MOLALITY)=	0.2006E-01	0.3810E-01	0.4349E-07	0.2010E-02	0.1805E-01

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	CALCULATED ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
3	Na +	919.6000	919.6000	0.4011E-01	0.8228E+03	0.8228E+03	0.3589E-01	0.2905E-01	0.8094	1.5368
5	Cl -	709.0600	709.0600	0.2006E-01	0.7067E+03	0.7067E+03	0.1999E-01	0.1596E-01	0.7981	1.7971
7	HCO3 -	1220.3400	1220.3400	0.2006E-01	0.1207E+03	0.1207E+03	0.1983E-02	0.1616E-02	0.8146	2.7916
8	H +				0.1419E-07	0.1419E-07	0.1412E-10	0.1202E-10	0.8513	10.9200
9	OH -				0.1793E+02	0.1793E+02	0.1057E-02	0.8500E-03	0.8039	3.0706
97	H2CO3				0.2690E-02	0.2690E-02	0.4349E-07	0.4349E-07	1.0000	7.3616
98	CO3 --				0.8327E+03	0.8327E+03	0.1392E-01	0.6286E-02	0.4517	2.2016
137	NaCl				0.3816E+01	0.3816E+01	0.6548E-04	0.6548E-04	1.0000	4.1839
138	NaCO3 -				0.3418E+03	0.3418E+03	0.4130E-02	0.3400E-02	0.8233	2.4685
139	NaHCO3				0.2211E+01	0.2211E+01	0.2639E-04	0.2639E-04	1.0000	4.5785
140	Na2CO3				0.1171E+00	0.1171E+00	0.1108E-05	0.1108E-05	1.0000	5.9553

SAMPLE IDENT - Test Sample #2 - Mix caustic flood with formation water (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
52	HALITE	-3.334	1.590	-4.924	-6.717	83	NATRON	-5.281	-0.880	-4.401	-6.004
81	NACHOLIT	-4.328	-0.430	-3.898	-5.318	118	Na2O	18.766	67.430	-48.664	-66.390
82	NATRTHRM	-5.276	-0.010	-5.266	-7.184	127	TRONA	-9.605	-0.630	-8.975	-12.244

*****This solution is to be mixed with the next solution.....

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****** INPUT DATA ECHO ******

TITLE : McMurray Formation Water
      TEMP       HITEMP        DENS       PRESS
0.2500E+02  0.0000E+00  0.1000E+01  0.0000E+00
        PH         EHM        EHMC      EMFZSC
0.7100E+01  0.9000E+01  0.9000E+01  0.9000E+01
CONCENTRATION UNITS :  MG/L
  Na          K           Li          Ca          Mg          Fe          Al
0.1572E+05  0.0000E+00  0.0000E+00  0.8010E+03  0.4430E+03  0.0000E+00  0.0000E+00
  SiO2        Cl          SO4         H2S         HCO3        CO3         TIC
0.0000E+00  0.2670E+05  0.1200E+02  0.0000E+00  0.4000E+03  0.0000E+00  0.0000E+00
  F           PO4         NO3         NH3         B           Sr          Ba
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  Pb          Zn          Cu          Mn          Hg          Ag
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  As          U           V
0.0000E+00  0.0000E+00  0.0000E+00
  Acetate     Oxalate     Succinate   CH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
      ALK     ITIC
      2        0
    DCO2        DH2S        DNH3        DCH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   ICCSAT      IMCO3       FIXIT       FCCSAT
     0           0     0.00000E+00      0.0500
  TCO2M       TCH4M       TH2SM       WROIL       KCO2OL      KCH4OL      KH2SOL      DSEP
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
Adsorption/Exchange option (N=no) = N
      IBMIX      ITMIX
      2          0
Because the Mixing option was chosen in the previous data set,
the MIXING information will not be read from this data set.
 LOG KT TO BE CHANGED AT TEMP =  25.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
 LOG KT TO BE CHANGED AT TEMP =   0.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
       ANS1       ANS2
      0          0
 Number of Additional Minerals =            0
 FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    1
 FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS:  0
 FLAGS FOR CALCULATING REDOX SPECIES:
 Fe  Cu  Hg  Mn   U   V
  1   1   1   1   0   0
 PRINTING OPTIONS:
    INFORM        RATIO        GEOTH       IPRIN1       IPRIN2
       0            0            0            0            0
 TOLERANCE FACTORS:  CONV1 =   0.5000E-04  CONV2 =   0.5000E-04
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SAMPLE IDENT:- McMurray Formation Water

PH	EH	TEMP		CATIONS	ANIONS	DIFFERENCE (MEQ/L)
7.10	9.0000	25.00	ANAL=	760.1885	759.9151	0.2734
			CALC=	724.0943	723.2526	0.8417

--- H - OH BALANCE (MOLES) -------

HTOT	OHTOT	DIFFERENCE
0.7400E-02	0.5210E-06	0.7399E-02

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER	PRESSURE P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0000	44076.00	0.79028	0.9743	1.0000	0.3169E-01	0.2089E-01	0.0000E+00	0.0000E+00	0.0000E+00

	Total Alkalinity as HCO3-	CO3=	CaCO3	Dissolved Inorganic Carbon as TIC	HCO3- Alkalinity	H2CO3 species	Sum of HCO3-	Sum of CO3=
(MG/L)=	0.3684E+03	0.1812E+03	0.3021E+03	0.7874E+02	0.3683E+03	0.3525E+02	0.3623E+03	0.3019E+01
(PPM)=	0.3684E+03	0.1812E+03	0.3021E+03	0.7874E+02	0.3683E+03	0.3525E+02	0.3623E+03	0.3019E+01
(MOLALITY)=	0.6317E-02	0.3158E-02	0.3158E-02	0.6858E-02	0.6316E-02	0.5945E-03	0.6211E-02	0.5263E-04

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
1	Ca ++	801.0000	801.0000	0.2091E-01	0.5506E+03	0.5506E+03	0.1437E-01	0.3388E-02	0.2358	2.4700
2	Mg ++	443.0000	443.0000	0.1906E-01	0.4360E+03	0.4360E+03	0.1876E-01	0.4776E-02	0.2546	2.3210
3	Na +	15720.0000	15720.0000	0.7153E+00	0.1504E+05	0.1504E+05	0.6845E+00	0.4554E+00	0.6653	0.3416
5	Cl -	26700.0000	26700.0000	0.7878E+00	0.2547E+05	0.2547E+05	0.7516E+00	0.4638E+00	0.6171	0.3336
6	SO4 --	12.0000	12.0000	0.1307E-03	0.4775E+01	0.4775E+01	0.5200E-04	0.8143E-05	0.1566	5.0892
7	HCO3 -	400.0000	400.0000	0.6858E-02	0.2843E+03	0.2843E+03	0.4875E-02	0.3343E-02	0.6858	2.4759
8	H +				0.9476E-04	0.9476E-04	0.9834E-07	0.7943E-07	0.8077	7.1000
9	OH -				0.3176E-02	0.3176E-02	0.1954E-06	0.1255E-06	0.6425	6.9013
55	CaCO3				0.1059E+01	0.1059E+01	0.1107E-04	0.1107E-04	1.0000	4.9559
56	CaHCO3 +				0.1914E+02	0.1914E+02	0.1980E-03	0.1459E-03	0.7369	3.8359
57	CaOH +				0.4347E-03	0.4347E-03	0.7966E-08	0.5871E-08	0.7369	8.2313
61	CaSO4				0.7164E+00	0.7164E+00	0.5505E-05	0.5505E-05	1.0000	5.2592
97	H2CO3				0.3525E+02	0.3525E+02	0.5945E-03	0.5945E-03	1.0000	3.2259
98	CO3 --				0.5310E+00	0.5310E+00	0.9257E-05	0.1969E-05	0.2126	5.7059
103	HSO4 -				0.7800E-05	0.7800E-05	0.8406E-10	0.5765E-10	0.6858	10.2392
120	MgCO3				0.7237E+00	0.7237E+00	0.8978E-05	0.8978E-05	1.0000	5.0468
121	MgHCO3 +				0.2300E+02	0.2300E+02	0.2820E-03	0.1876E-03	0.6653	3.7268
123	MgOH +				0.1255E-01	0.1255E-01	0.3177E-06	0.2386E-06	0.7512	6.6223
124	MgSO4				0.1124E+01	0.1124E+01	0.9768E-05	0.9768E-05	1.0000	5.0102
137	NaCl				0.1667E+04	0.1667E+04	0.2984E-01	0.2984E-01	1.0000	1.5253
138	NaCO3 -				0.1844E+01	0.1844E+01	0.2324E-04	0.1669E-04	0.7182	4.7775
139	NaHCO3				0.6875E+02	0.6875E+02	0.8561E-03	0.8561E-03	1.0000	3.0675
140	Na2CO3				0.8641E-02	0.8641E-02	0.8529E-07	0.8529E-07	1.0000	7.0691
141	Na2SO4				0.7419E+01	0.7419E+01	0.5464E-04	0.5464E-04	1.0000	4.2625
142	NaSO4 -				0.9979E+00	0.9979E+00	0.8769E-05	0.6297E-05	0.7182	5.2009
281	CaCl +				0.4487E+03	0.4487E+03	0.6214E-02	0.4134E-02	0.6653	2.3836
282	CaCl2				0.1144E+02	0.1144E+02	0.1078E-03	0.1078E-03	1.0000	3.9673

SAMPLE IDENT - McMurray Formation Water (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
11	ANHYDRIT	-7.559	-4.330	-3.229	-4.405	70	MAGNESIT	-8.027	-8.050	0.023	0.032
17	ARAGONIT	-8.176	-8.340	0.164	0.224	71	MgCl2	-2.988	22.150	-25.138	-34.295
22	BRUCITE	-16.124	-11.470	-4.654	-6.349	76	MIRABILT	-5.886	-1.090	-4.796	-6.542
24	CALCITE	-8.176	-8.480	0.304	0.415	81	NACHOLIT	-2.817	-0.430	-2.387	-3.257
41	DOLOMITE	-16.203	-18.060	1.857	2.534	82	NATRTHRM	-6.400	-0.010	-6.390	-8.718
42	DSORD	-16.203	-16.520	0.317	0.433	83	NATRON	-6.502	-0.880	-5.622	-7.670
51	GYPSUM	-7.582	-4.600	-2.982	-4.068	85	NESQUHON	-8.061	-5.350	-2.711	-3.698
52	HALITE	-0.675	1.590	-2.265	-3.090	95	PERICLAS	11.868	21.510	-9.642	-13.154
55	HUNTITE	-32.256	-30.620	-1.636	-2.232	99	PORTLAN	-16.273	-5.420	-10.853	-14.806
56	HYDRMAGN	-42.559	-38.530	-4.029	-5.496	118	Na2O	13.505	67.430	-53.925	-73.566
57	HYPHILIT	-3.137	11.800	-14.937	-20.378	125	THENARDI	-5.772	-0.290	-5.482	-7.479
67	LIME	-16.681	32.660	-49.341	-67.313	127	TRONA	-9.229	-0.630	-8.599	-11.731

**** Mixing of the two previous solutions in the following proportions:
Initial fraction of solution 1 = 0.5000
Number of mixtures = 1
and the increment between solutions = 0.5000

SAMPLE IDENT:- MIXTURE OF Test Sample #2 - Mix caustic flo AND McMurray Formation Water
(PROPORTIONS: 1= 0.50 2= 0.50)

PH	EH	TEMP
9.67	9.0000	25.00

	CATIONS	ANIONS	DIFFERENCE (MEQ/L)
ANAL=	407.6953	407.5557	0.1396
CALC=	386.6610	395.5575	-8.8965

--- H - OH BALANCE (MOLES) -------

HTOT	OHTOT	DIFFERENCE
0.4307E-02	0.1313E-03	0.4176E-02

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER
1.0000	23897.61	0.41785	0.9865

PRESSURE

P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0000	0.3169E-01	0.4037E-04	0.0000E+00	0.0000E+00	0.0000E+00

	Total Alkalinity as HCO3-	Total Alkalinity as CO3=	Total Alkalinity as CaCO3	Dissolved Inorganic Carbon as TIC	DIC HCO3- Alkalinity	DIC H2CO3 species	DIC Sum of HCO3-	DIC Sum of CO3=
(MG/L)=	0.1354E+04	0.6659E+03	0.1111E+04	0.1578E+03	0.1328E+04	0.7566E-01	0.2564E+03	0.5360E+03
(PPM)=	0.1354E+04	0.6659E+03	0.1111E+04	0.1578E+03	0.1328E+04	0.7566E-01	0.2564E+03	0.5360E+03
(MOLALITY)=	0.2274E-01	0.1137E-01	0.1137E-01	0.1346E-01	0.2261E-01	0.1250E-05	0.4305E-02	0.9151E-02

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
1	Ca ++	408.9541	408.9541	0.1045E-01	0.2642E+03	0.2642E+03	0.6752E-02	0.1845E-02	0.2732	2.7341
2	Mg ++	226.1756	226.1756	0.9531E-02	0.1913E+03	0.1913E+03	0.8060E-02	0.2337E-02	0.2900	2.6313
3	Na +	8476.0056	8476.0056	0.3777E+00	0.8178E+04	0.8178E+04	0.3644E+00	0.2513E+00	0.6896	0.5998
5	Cl -	13978.8458	13978.8458	0.4039E+00	0.1360E+05	0.1360E+05	0.3930E+00	0.2569E+00	0.6538	0.5902
6	SO4 --	6.1267	6.1267	0.6534E-04	0.3562E+01	0.3562E+01	0.3799E-04	0.7633E-05	0.2009	5.1173
7	HCO3 -	801.5070	801.5070	0.1346E-01	0.2229E+03	0.2229E+03	0.3742E-02	0.2639E-02	0.7052	2.5785
8	H +				0.2598E-06	0.2598E-06	0.2640E-09	0.2115E-09	0.8012	9.6747
9	OH -				0.1178E+01	0.1178E+01	0.7096E-04	0.4772E-04	0.6726	4.3213
55	CaCO3				0.1745E+03	0.1745E+03	0.1787E-02	0.1787E-02	1.0000	2.7480
56	CaHCO3 +				0.8310E+01	0.8310E+01	0.8422E-04	0.6271E-04	0.7447	4.2027
57	CaOH +				0.9093E-01	0.9093E-01	0.1632E-05	0.1215E-05	0.7447	5.9154
61	CaSO4				0.3733E+00	0.3733E+00	0.2809E-05	0.2809E-05	1.0000	5.5514
97	H2CO3				0.7566E-01	0.7566E-01	0.1250E-05	0.1250E-05	1.0000	5.9032
98	CO3 --				0.1355E+03	0.1355E+03	0.2313E-02	0.5836E-03	0.2523	3.2339
103	HSO4 -				0.1933E-07	0.1933E-07	0.2040E-12	0.1439E-12	0.7052	12.8420
120	MgCO3				0.1072E+03	0.1072E+03	0.1303E-02	0.1303E-02	1.0000	2.8852
121	MgHCO3 +				0.8752E+01	0.8752E+01	0.1051E-03	0.7246E-04	0.6896	4.1399
123	MgOH +				0.2369E+01	0.2369E+01	0.5874E-04	0.4440E-04	0.7558	4.3526
124	MgSO4				0.5265E+00	0.5265E+00	0.4481E-05	0.4481E-05	1.0000	5.3487
137	NaCl				0.5203E+03	0.5203E+03	0.9121E-02	0.9121E-02	1.0000	2.0399
138	NaCO3 -				0.3031E+03	0.3031E+03	0.3741E-02	0.2731E-02	0.7300	2.5636
139	NaHCO3				0.3059E+02	0.3059E+02	0.3730E-03	0.3730E-03	1.0000	3.4283
140	Na2CO3				0.7968E+00	0.7968E+00	0.7702E-05	0.7702E-05	1.0000	5.1134
141	Na2SO4				0.2163E+01	0.2163E+01	0.1560E-04	0.1560E-04	1.0000	4.8069
142	NaSO4 -				0.5186E+00	0.5186E+00	0.4462E-05	0.3258E-05	0.7300	5.4871
281	CaCl +				0.1333E+03	0.1333E+03	0.1808E-02	0.1247E-02	0.6896	2.9043
282	CaCl2				0.1951E+01	0.1951E+01	0.1801E-04	0.1801E-04	1.0000	4.7445

SAMPLE IDENT - MIXTURE OF Test Sample #2 - Mix caustic flo AND McMurray Formation Water (TEMPERATURE = 25.00)
(PROPORTIONS: 1= 0.50 2= 0.50)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
11	ANHYDRIT	-7.851	-4.330	-3.521	-4.804	70	MAGNESIT	-5.865	-8.050	2.185	2.981
17	ARAGONIT	-5.968	-8.340	2.372	3.236	71	MgCl2	-3.812	22.150	-25.962	-35.418
22	BRUCITE	-11.274	-11.470	0.196	0.268	76	MIRABILT	-6.376	-1.090	-5.286	-7.211
24	CALCITE	-5.968	-8.480	2.512	3.427	81	NACHOLIT	-3.178	-0.430	-2.748	-3.749
41	DOLOMITE	-11.833	-18.060	6.227	8.495	82	NATRTHRM	-4.439	-0.010	-4.429	-6.043
42	DSORD	-11.833	-16.520	4.687	6.394	83	NATRON	-4.493	-0.880	-3.613	-4.928
51	GYPSUM	-7.863	-4.600	-3.263	-4.452	85	NESQUHON	-5.883	-5.350	-0.533	-0.727
52	HALITE	-1.190	1.590	-2.780	-3.793	95	PERICLAS	16.712	21.510	-4.798	-6.546
55	HUNTITE	-23.564	-30.620	7.056	9.627	99	PORTLAN	-11.377	-5.420	-5.957	-8.126
56	HYDRMAGN	-31.519	-38.530	7.011	9.565	118	Na2O	18.144	67.430	-49.286	-67.238
57	HYPHILIT	-3.914	11.800	-15.714	-21.438	125	THENARDI	-6.317	-0.290	-6.027	-8.222
67	LIME	-22.089	32.660	-54.749	-74.691	127	TRONA	-7.624	-0.630	-6.994	-9.541

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****** INPUT DATA ECHO ******

TITLE : Test Sample #3 - Dissolve Anorthite to saturate with Gibbsite in seawater
      TEMP       HITEMP        DENS       PRESS
0.2500E+02  0.0000E+00  0.1023E+01  0.0000E+00
        PH         EHM        EHMC      EMFZSC
0.8200E+01  0.5000E+00  0.9000E+01  0.9000E+01
CONCENTRATION UNITS :  PPM
  Na          K           Li          Ca          Mg          Fe          Al
0.1077E+05  0.3991E+03  0.1810E+00  0.4123E+03  0.1292E+04  0.2000E-02  0.2000E-02
  SiO2        Cl          SO4         H2S         HCO3        CO3         TIC
0.4280E+01  0.1935E+05  0.2712E+04  0.0000E+00  0.1234E+03  0.0000E+00  0.0000E+00
  F           PO4         NO3         NH3         B           Sr          Ba
0.1390E+01  0.6000E-01  0.2900E+00  0.3000E-01  0.4450E+01  0.8140E+01  0.2000E-01
  Pb          Zn          Cu          Mn          Hg          Ag
0.5000E-04  0.4900E-02  0.7000E-03  0.2000E-03  0.3000E-04  0.4000E-04
  As          U           V
0.4000E-02  0.0000E+00  0.0000E+00
  Acetate     Oxalate     Succinate   CH4
0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00
     ALK      ITIC
     2         0
    DCO2        DH2S        DNH3        DCH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   ICCSAT      IMCO3       FIXIT       FCCSAT
     0           0     0.00000E+00      0.0500
  TCO2M       TCH4M       TH2SM       WROIL       KCO2OL      KCH4OL      KH2SOL      DSEP
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
Adsorption/Exchange option (N=no) = N
      IBMIX      ITMIX
      1          0
MINERAL TO BE DISSOLVED/PRECIPITATED TO SATURATION: GIBBSITE      Index number:  49
MINERAL TO BE DISSOLVED/PRECIPITATED:                ANORTHIT     Index number:  13
LOG KT TO BE CHANGED AT TEMP =  25.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
LOG KT TO BE CHANGED AT TEMP =   0.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
       ANS1        ANS2
      0           0
Number of Additional Minerals =           0
FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    1
FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS:  0
FLAGS FOR CALCULATING REDOX SPECIES:
Fe  Cu  Hg  Mn   U   V
 1   1   1   1   0   0
PRINTING OPTIONS:
    INFORM       RATIO       GEOTH       IPRIN1      IPRIN2
       0           0           0           0           0
TOLERANCE FACTORS:  CONV1 =   0.5000E-04  CONV2 =   0.5000E-04
                    .
                    .                                          (See pages 2-10 of Test Sample #1)
                    .
Total moles of ANORTHIT PPT/DISS         to achieve saturation: -.3076E-07
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SAMPLE IDENT:- Test Sample #3 - Dissolve Anorthite to saturate with Gibbsite in seawater
ANORTHIT PPT/DISS

PH	EH	TEMP		CATIONS	ANIONS	DIFFERENCE (MEQ/L)
8.20	9.0000	25.00	ANAL=	619.6745	618.2648	1.4097
			CALC=	577.6363	569.7726	7.8638

--- H - OH BALANCE (MOLES) -------

HTOT	OHTOT	DIFFERENCE
0.2198E-02	0.1350E-02	0.8477E-03

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER	PRESSURE P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0230	35906.27	0.64945	0.9809	1.0000	0.3169E-01	0.4780E-03	0.0000E+00	0.5252E-02	0.1644E-08

Total Alkalinity as

	HCO3-	CO3=	CaCO3
(MG/L)=	0.1423E+03	0.6998E+02	0.1167E+03
(PPM)=	0.1391E+03	0.6841E+02	0.1141E+03
(MOLALITY)=	0.2363E-02	0.1181E-02	0.1181E-02

Dissolved Inorganic Carbon

	as TIC	HCO3- Alkalinity	H2CO3 species	Sum of HCO3-	Sum of CO3=
(MG/L)=	0.2485E+02	0.1374E+03	0.8644E+00	0.1130E+03	0.1216E+02
(PPM)=	0.2429E+02	0.1343E+03	0.8450E+00	0.1105E+03	0.1189E+02
(MOLALITY)=	0.2096E-02	0.2287E-02	0.1412E-04	0.1877E-02	0.2053E-03

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
1	Ca ++	412.2988	421.7817	0.1066E-01	0.2844E+03	0.2909E+03	0.7353E-02	0.1807E-02	0.2458	2.7429
2	Mg ++	1292.0001	1321.7160	0.5508E-01	0.1121E+04	0.1147E+04	0.4779E-01	0.1261E-01	0.2640	1.8992
3	Na +	10770.0007	11017.7102	0.4855E+00	0.1024E+05	0.1048E+05	0.4618E+00	0.3099E+00	0.6710	0.5088
4	K +	399.1000	408.2793	0.1058E-01	0.3825E+03	0.3913E+03	0.1014E-01	0.6357E-02	0.6269	2.1968
5	Cl -	19350.0013	19795.0504	0.5656E+00	0.1874E+05	0.1917E+05	0.5478E+00	0.3434E+00	0.6269	0.4641
6	SO4 --	2712.0002	2774.3761	0.2926E-01	0.1203E+04	0.1231E+04	0.1298E-01	0.2189E-02	0.1687	2.6598
7	HCO3 -	123.4007	126.2389	0.2096E-02	0.8534E+02	0.8730E+02	0.1449E-02	0.1000E-02	0.6899	3.0000
8	H +				0.7635E-05	0.7810E-05	0.7850E-08	0.6307E-08	0.8034	8.2002
9	OH -				0.4017E-01	0.4110E-01	0.2448E-05	0.1592E-05	0.6501	5.7982
11	H4SiO4				0.6610E+01	0.6762E+01	0.7127E-04	0.7127E-04	1.0000	4.1471
12	SiO2	4.2764	4.3748	0.7376E-04						
13	Ag +	0.0000	0.0000	0.3843E-09	0.1039E-08	0.1063E-08	0.9982E-14	0.6000E-14	0.6011	14.2219
14	Al +3	0.0004	0.0004	0.1529E-07	0.8504E-12	0.8699E-12	0.3266E-16	0.2790E-17	0.0854	17.5544
15	Ba ++	0.0200	0.0205	0.1509E-06	0.1815E-01	0.1857E-01	0.1370E-06	0.2849E-07	0.2080	7.5453
16	Cu +	0.0007	0.0007	0.1142E-07	0.2749E-07	0.2812E-07	0.4483E-12	0.2695E-12	0.6011	12.5695
18	Fe ++	0.0020	0.0020	0.3711E-07	0.1667E-02	0.1705E-02	0.3094E-07	0.7604E-08	0.2458	8.1189
21	Hg ++	0.0000	0.0000	0.1550E-09	0.7474E-18	0.7646E-18	0.3861E-23	0.8033E-24	0.2080	24.0951
22	Li +	0.1810	0.1852	0.2703E-04	0.1792E+00	0.1833E+00	0.2677E-04	0.1973E-04	0.7373	4.7048
23	Mn ++	0.0002	0.0002	0.3773E-08	0.5864E-06	0.5999E-06	0.1106E-10	0.2719E-11	0.2458	11.5656
25	Pb ++	0.0001	0.0001	0.2501E-09	0.9962E-06	0.1019E-05	0.4983E-11	0.9393E-12	0.1885	12.0272
26	Sr ++	8.1400	8.3272	0.9628E-04	0.7551E+01	0.7725E+01	0.8931E-04	0.1858E-04	0.2080	4.7310
27	Zn ++	0.0049	0.0050	0.7768E-07	0.2885E-02	0.2952E-02	0.4575E-07	0.1124E-07	0.2458	7.9491
28	H2AsO3-	0.0067	0.0068	0.5281E-07	0.7212E-03	0.7378E-03	0.5708E-08	0.3830E-08	0.6710	8.4168
29	PO4 -3	0.0600	0.0614	0.6548E-06	0.5921E-05	0.6058E-05	0.6462E-10	0.1749E-11	0.0271	11.7572
30	F -	1.3900	1.4220	0.7583E-04	0.7672E+00	0.7848E+00	0.4185E-04	0.2721E-04	0.6501	4.5653
31	B(OH)3	25.4540	26.0394	0.4266E-03	0.2205E+02	0.2255E+02	0.3695E-03	0.3695E-03	1.0000	3.4323
32	NH3	0.0300	0.0307	0.1826E-05						
34	AlF ++				0.1407E-09	0.1440E-09	0.3172E-14	0.7085E-15	0.2234	15.1497
35	AlF2 +				0.6684E-09	0.6838E-09	0.1066E-13	0.7674E-14	0.7198	14.1150
36	AlF3				0.2034E-09	0.2081E-09	0.2510E-14	0.2510E-14	1.0000	14.6003
37	AlF4 -				0.2415E-11	0.2470E-11	0.2430E-16	0.1677E-16	0.6899	16.7756
38	Al(OH)++				0.9253E-09	0.9466E-09	0.2180E-13	0.4869E-14	0.2234	14.3125
39	Al(OH)2+				0.6635E-06	0.6787E-06	0.1127E-10	0.8115E-11	0.7198	11.0907
40	Al(OH)4-				0.1401E-02	0.1433E-02	0.1528E-07	0.1054E-07	0.6899	7.9771

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
41	AlSO4 +				0.1051E-11	0.1075E-11	0.8852E-17	0.6107E-17	0.6899	17.2142
42	AlSO4)2-				0.3179E-12	0.3252E-12	0.1504E-17	0.1038E-17	0.6899	17.9840
43	AgCl				0.5954E-06	0.6091E-06	0.4305E-11	0.4305E-11	1.0000	11.3660
44	AgCl2 -				0.3801E-04	0.3889E-04	0.2204E-09	0.1479E-09	0.6710	9.8301
45	AgCl3 --				0.3041E-04	0.3111E-04	0.1471E-09	0.3060E-10	0.2080	10.5143
46	AgCl4 -3				0.4054E-05	0.4148E-05	0.1683E-10	0.6631E-12	0.0394	12.1784
47	AgSO4 -				0.7863E-10	0.8044E-10	0.3996E-15	0.2681E-15	0.6710	15.5717
48	CH3COO -	0.1000	0.1023	0.1755E-05	0.7225E-01	0.7391E-01	0.1268E-05	0.8749E-06	0.6899	6.0580
49	H3AsO3				0.5724E-02	0.5856E-02	0.4710E-07	0.4710E-07	1.0000	7.3270
51	BaCO3				0.1272E-04	0.1302E-04	0.6681E-10	0.6681E-10	1.0000	10.1751
52	BaHCO3 +				0.2238E-03	0.2290E-03	0.1169E-08	0.7846E-09	0.6710	9.1053
53	BaOH +				0.3236E-07	0.3310E-07	0.2173E-12	0.1536E-12	0.7071	12.8135
54	BaSO4				0.2867E-02	0.2933E-02	0.1273E-07	0.1273E-07	1.0000	7.8951
55	CaCO3				0.2148E+01	0.2198E+01	0.2225E-04	0.2225E-04	1.0000	4.6528
56	CaHCO3 +				0.3081E+01	0.3152E+01	0.3158E-04	0.2328E-04	0.7373	4.6330
57	CaOH +				0.2967E-02	0.3035E-02	0.5386E-07	0.3971E-07	0.7373	7.4011
58	CaPO4 -				0.1689E-02	0.1728E-02	0.1296E-07	0.9330E-08	0.7198	8.0301
59	CaHPO4				0.2333E-02	0.2386E-02	0.1777E-07	0.1777E-07	1.0000	7.7503
60	CaH2PO4+				0.2206E-04	0.2257E-04	0.1668E-09	0.1201E-09	0.7198	9.9205
61	CaSO4				0.1037E+03	0.1061E+03	0.7893E-03	0.7893E-03	1.0000	3.1028
62	CuCl				0.4431E-05	0.4533E-05	0.4639E-10	0.4639E-10	1.0000	10.3336
63	CuCl2 -				0.5353E-03	0.5476E-03	0.4126E-08	0.2769E-08	0.6710	8.5577
64	CuCl3 --				0.1188E-02	0.1215E-02	0.7244E-08	0.1507E-08	0.2080	8.8219
71	FeCl +				0.1012E-03	0.1035E-03	0.1149E-08	0.7708E-09	0.6710	9.1131
72	FeCl2				0.6764E-12	0.6920E-12	0.5531E-17	0.5531E-17	1.0000	17.2572
73	FeHPO4				0.1070E-06	0.1095E-06	0.7306E-12	0.7306E-12	1.0000	12.1363
74	H3PO4				0.2032E-09	0.2079E-09	0.2149E-14	0.2149E-14	1.0000	14.6678
75	FeOH +				0.3805E-04	0.3892E-04	0.5412E-09	0.3827E-09	0.7071	9.4171
76	Fe(OH)2				0.4100E-07	0.4194E-07	0.4728E-12	0.4728E-12	1.0000	12.3253
77	FeOOH -				0.3536E-07	0.3618E-07	0.4125E-12	0.2917E-12	0.7071	12.5351
78	FeSO4				0.6566E-03	0.6717E-03	0.4480E-08	0.4480E-08	1.0000	8.3488
89	B(OH)4 -				0.4344E+01	0.4444E+01	0.5710E-04	0.3463E-04	0.6065	4.4605
90	H2SiO4--				0.2150E-03	0.2199E-03	0.2368E-08	0.5288E-09	0.2234	9.2767
91	H3SiO4 -				0.2286E+00	0.2339E+00	0.2491E-05	0.1671E-05	0.6710	5.7769
92	HAsO3 --				0.1174E-07	0.1201E-07	0.9366E-13	0.1948E-13	0.2080	13.7104
96	HF				0.5013E-05	0.5129E-05	0.2597E-09	0.2597E-09	1.0000	9.5855
97	H2CO3				0.8450E+00	0.8644E+00	0.1412E-04	0.1412E-04	1.0000	4.8502
98	CO3 --				0.1923E+01	0.1967E+01	0.3320E-04	0.7416E-05	0.2234	5.1298
99	HPO4 --				0.1074E-01	0.1099E-01	0.1160E-06	0.2413E-07	0.2080	7.6174
100	H2PO4 -				0.3136E-03	0.3208E-03	0.3351E-08	0.2412E-08	0.7198	8.6176
103	HSO4 -				0.1670E-03	0.1709E-03	0.1783E-08	0.1230E-08	0.6899	8.9100
104	HNO3				0.4329E-10	0.4429E-10	0.7120E-15	0.7120E-15	1.0000	15.1475
105	HgCl +				0.1665E-12	0.1704E-12	0.7311E-18	0.4906E-18	0.6710	18.3093
106	HgCl2				0.4517E-06	0.4621E-06	0.1724E-11	0.1724E-11	1.0000	11.7634
107	HgCl3 -				0.3216E-04	0.3290E-04	0.1086E-09	0.7285E-10	0.6710	10.1376
108	HgCl4 --				0.1476E-04	0.1510E-04	0.4469E-10	0.9296E-11	0.2080	11.0317
109	HgSO4				0.1264E-19	0.1293E-19	0.4416E-25	0.4416E-25	1.0000	25.3550
113	KCl				0.2070E+02	0.2118E+02	0.2878E-03	0.2878E-03	1.0000	3.5409
114	KCO3 -				0.7990E-01	0.8174E-01	0.8355E-06	0.5539E-06	0.6629	6.2566
115	KHSO4				0.7274E-05	0.7441E-05	0.5536E-10	0.5536E-10	1.0000	10.2568
116	KSO4 -				0.1957E+02	0.2002E+02	0.1500E-03	0.1080E-03	0.7198	3.9666
117	KHPO4 -				0.5416E-04	0.5541E-04	0.4155E-09	0.2991E-09	0.7198	9.5242
118	LiOH				0.1098E-05	0.1124E-05	0.4754E-10	0.4754E-10	1.0000	10.3230

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
119	LiSO4 -				0.2650E-01	0.2711E-01	0.2666E-06	0.1885E-06	0.7071	6.7246
120	MgCO3				0.7268E+01	0.7436E+01	0.8933E-04	0.8933E-04	1.0000	4.0490
121	MgHCO3 +				0.1818E+02	0.1860E+02	0.2209E-03	0.1482E-03	0.6710	3.8292
122	MgF +				0.1373E+01	0.1405E+01	0.3286E-04	0.2267E-04	0.6899	4.6445
123	MgOH +				0.4245E+00	0.4343E+00	0.1065E-04	0.7992E-05	0.7505	5.0974
124	MgSO4				0.8054E+03	0.8240E+03	0.6934E-02	0.6934E-02	1.0000	2.1590
125	MgPO4 -				0.1041E-01	0.1065E-01	0.9045E-07	0.6511E-07	0.7198	7.1864
126	MgHPO4				0.4552E-01	0.4656E-01	0.3922E-06	0.3922E-06	1.0000	6.4065
127	MgH2PO4+				0.1363E-03	0.1394E-03	0.1164E-08	0.8380E-09	0.7198	9.0767
128	MnCl +				0.3839E-13	0.3927E-13	0.4401E-18	0.2953E-18	0.6710	18.5297
129	MnCl2				0.3094E-10	0.3165E-10	0.2548E-15	0.2548E-15	1.0000	15.5938
130	MnCl3 -				0.5098E-09	0.5215E-09	0.3276E-14	0.2198E-14	0.6710	14.6580
131	MnCl4 --				0.5472E-08	0.5598E-08	0.2882E-13	0.5996E-14	0.2080	14.2221
132	MnHCO3 +				0.8443E-08	0.8637E-08	0.7546E-13	0.5063E-13	0.6710	13.2956
133	MnSO4				0.1578E-06	0.1614E-06	0.1083E-11	0.1083E-11	1.0000	11.9654
134	MnHPO4				0.3633E-10	0.3717E-10	0.2495E-15	0.2495E-15	1.0000	15.6029
135	MnOH +				0.1233E-08	0.1262E-08	0.1776E-13	0.1192E-13	0.6710	13.9237
136	NO3 -	0.2900	0.2967	0.4847E-05	0.2900E+00	0.2967E+00	0.4847E-05	0.3039E-05	0.6269	5.5173
137	NaCl				0.8478E+03	0.8673E+03	0.1503E-01	0.1503E-01	1.0000	1.8229
138	NaCO3 -				0.4761E+01	0.4871E+01	0.5945E-04	0.4279E-04	0.7198	4.3686
139	NaHCO3				0.1413E+02	0.1445E+02	0.1743E-03	0.1743E-03	1.0000	3.7588
140	Na2CO3				0.1522E-01	0.1557E-01	0.1488E-06	0.1488E-06	1.0000	6.8274
141	Na2SO4				0.9321E+03	0.9536E+03	0.6801E-02	0.6801E-02	1.0000	2.1674
142	NaSO4 -				0.1838E+03	0.1880E+03	0.1600E-02	0.1152E-02	0.7198	2.9386
143	NaHPO4 -				0.2326E-02	0.2379E-02	0.2026E-07	0.1458E-07	0.7198	7.8362
144	NaF				0.4503E-01	0.4607E-01	0.1111E-05	0.1111E-05	1.0000	5.9541
146	NH4 +				0.3015E-01	0.3085E-01	0.1732E-05	0.1041E-05	0.6011	5.9824
147	NH4OH				0.3151E-02	0.3224E-02	0.9319E-07	0.9319E-07	1.0000	7.0306
148	PbCl +				0.2893E-05	0.2960E-05	0.1236E-10	0.8292E-11	0.6710	11.0813
149	PbCl2				0.2775E-05	0.2838E-05	0.1034E-10	0.1034E-10	1.0000	10.9855
150	PbCl3 -				0.7843E-06	0.8023E-06	0.2592E-11	0.1739E-11	0.6710	11.7596
151	PbCl4 --				0.6102E-06	0.6242E-06	0.1812E-11	0.3769E-12	0.2080	12.4238
152	PbSO4				0.3383E-06	0.3461E-06	0.1156E-11	0.1156E-11	1.0000	11.9370
154	SrOH -				0.2068E-04	0.2115E-04	0.2048E-09	0.1448E-09	0.7071	9.8392
155	SrCO3				0.1297E-01	0.1327E-01	0.9104E-07	0.9104E-07	1.0000	7.0408
156	SrHCO3 +				0.6151E-01	0.6292E-01	0.4289E-06	0.2878E-06	0.6710	6.5410
157	SrSO4				0.1142E+01	0.1169E+01	0.6445E-05	0.6445E-05	1.0000	5.1908
158	ZnCl +				0.1473E-02	0.1507E-02	0.1514E-07	0.1016E-07	0.6710	7.9932
159	ZnCl2				0.7271E-03	0.7438E-03	0.5529E-08	0.5529E-08	1.0000	8.2573
160	ZnCl3 -				0.2461E-03	0.2518E-03	0.1485E-08	0.9966E-09	0.6710	9.0015
161	ZnCl4 --				0.2276E-03	0.2328E-03	0.1138E-08	0.2368E-09	0.2080	9.6256
162	ZnSO4				0.6217E-03	0.6360E-03	0.3991E-08	0.3991E-08	1.0000	8.3989
163	AlF5 --				0.5912E-14	0.6048E-14	0.5023E-19	0.1045E-19	0.2080	19.9809
164	AlF6 -3				0.2964E-17	0.3032E-17	0.2179E-22	0.8586E-24	0.0394	24.0662
165	HgOH +				0.1154E-13	0.1180E-13	0.5495E-19	0.3687E-19	0.6710	19.4333
166	Hg(OH)2				0.3414E-08	0.3493E-08	0.1508E-13	0.1508E-13	1.0000	13.8215
228	CH3COOH				0.1840E-04	0.1882E-04	0.3175E-09	0.3175E-09	1.0000	9.4982
229	AlAce ++				0.7788E-15	0.7967E-15	0.9382E-20	0.1769E-20	0.1885	20.7524
230	BaAce +				0.9235E-07	0.9447E-07	0.4874E-12	0.3362E-12	0.6899	12.4734
231	CaAce +				0.3723E-02	0.3809E-02	0.3892E-07	0.2685E-07	0.6899	7.5710
232	CuAce +				0.3138E-11	0.3210E-11	0.2653E-16	0.1830E-16	0.6899	16.7375
233	FeAce +				0.2133E-06	0.2182E-06	0.1924E-11	0.1327E-11	0.6899	11.8770
234	Fe(Ace)2				0.1230E-13	0.1258E-13	0.7328E-19	0.7328E-19	1.0000	19.1350

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
235	KAce				0.2146E-03	0.2195E-03	0.2266E-08	0.2266E-08	1.0000	8.6448
236	MgAce +				0.2288E-01	0.2340E-01	0.2844E-06	0.1962E-06	0.6899	6.7072
237	NaAce				0.1264E-01	0.1293E-01	0.1596E-06	0.1596E-06	1.0000	6.7968
238	PbAce +				0.5568E-10	0.5696E-10	0.2168E-15	0.1495E-15	0.6899	15.8252
239	Pb(Ace)2				0.9851E-15	0.1008E-14	0.3139E-20	0.3139E-20	1.0000	20.5033
240	Pb(Ace)3				0.1775E-20	0.1815E-20	0.4785E-26	0.3301E-26	0.6899	26.4813
241	SrAce +				0.4820E-04	0.4930E-04	0.3406E-09	0.2350E-09	0.6899	9.6290
244	ZnAce +				0.1391E-03	0.1423E-03	0.1159E-08	0.7997E-09	0.6899	9.0971
245	Zn(Ace)2				0.3411E-13	0.3490E-13	0.1927E-18	0.1927E-18	1.0000	18.7151
246	C2O4 --	0.1000	0.1023	0.1177E-05	0.9439E-02	0.9656E-02	0.1111E-06	0.2482E-07	0.2234	7.6051
247	HC2O4 -				0.3466E-09	0.3546E-09	0.4035E-14	0.2784E-14	0.6899	14.5553
248	H2C2O4				0.3114E-13	0.3186E-13	0.3585E-18	0.3585E-18	1.0000	18.4455
249	AlOxy +				0.1114E-13	0.1140E-13	0.1004E-18	0.6926E-19	0.6899	19.1595
250	AlOxy)2-				0.4882E-16	0.4994E-16	0.2492E-21	0.1719E-21	0.6899	21.7646
251	BaOxy				0.5714E-08	0.5845E-08	0.2628E-13	0.2628E-13	1.0000	13.5804
252	CaOxy				0.5546E-02	0.5673E-02	0.4487E-07	0.4487E-07	1.0000	7.3481
253	FeOxy				0.6582E-06	0.6734E-06	0.4742E-11	0.4742E-11	1.0000	11.3241
255	KOxy -				0.1406E-03	0.1438E-03	0.1146E-08	0.7908E-09	0.6899	9.1019
256	MgOxy				0.1002E+00	0.1025E+00	0.9241E-06	0.9241E-06	1.0000	6.0343
257	MnOxy				0.9311E-10	0.9525E-10	0.6750E-15	0.6750E-15	1.0000	15.1707
258	MnOxy)2				0.7180E-03	0.7345E-03	0.3760E-08	0.8398E-09	0.2234	9.0758
259	MnOxy)3				0.1550E-06	0.1585E-06	0.6353E-12	0.1315E-14	0.0021	14.8809
261	NaOxy -				0.9487E-02	0.9705E-02	0.8857E-07	0.6110E-07	0.6899	7.2139
262	PbOxy				0.3650E-09	0.3734E-09	0.1281E-14	0.1281E-14	1.0000	14.8923
263	SrOxy				0.2710E-04	0.2773E-04	0.1599E-09	0.1599E-09	1.0000	9.7961
264	ZnOxy				0.3282E-05	0.3357E-05	0.2217E-10	0.2217E-10	1.0000	10.6542
265	C4H4O4--	0.1000	0.1023	0.8929E-06	0.6405E-01	0.6553E-01	0.5719E-06	0.1277E-06	0.2234	6.8937
266	HC4H4O4-				0.2139E-05	0.2189E-05	0.1894E-10	0.1307E-10	0.6899	10.8839
267	H2C4H4O4				0.4099E-08	0.4193E-08	0.3597E-13	0.3597E-13	1.0000	13.4441
268	AlSuc +				0.1423E-13	0.1456E-13	0.1031E-18	0.7112E-19	0.6899	19.1480
269	AlSuc)2-				0.9109E-16	0.9319E-16	0.6599E-21	0.4553E-21	0.6899	21.3417
270	BaSuc				0.9318E-07	0.9532E-07	0.3811E-12	0.3811E-12	1.0000	12.4190
271	CaSuc				0.3479E-02	0.3559E-02	0.2309E-07	0.2309E-07	1.0000	7.6366
272	FeSuc				0.2554E-07	0.2613E-07	0.1540E-12	0.1540E-12	1.0000	12.8126
274	KSuc -				0.3516E-03	0.3597E-03	0.2348E-08	0.1620E-08	0.6899	8.7904
275	MgSuc				0.2449E-01	0.2505E-01	0.1808E-06	0.1808E-06	1.0000	6.7428
276	MnSuc				0.8478E-11	0.8673E-11	0.5138E-16	0.5138E-16	1.0000	16.2892
277	NaSuc -				0.1536E-01	0.1571E-01	0.1145E-06	0.7898E-07	0.6899	7.1025
278	PbSuc				0.1184E-09	0.1211E-09	0.3794E-15	0.3794E-15	1.0000	15.4209
279	SrSuc				0.4665E-04	0.4772E-04	0.2373E-09	0.2373E-09	1.0000	9.6246
280	ZnSuc				0.7253E-07	0.7419E-07	0.4143E-12	0.4143E-12	1.0000	12.3827
281	CaCl +				0.1773E+03	0.1814E+03	0.2433E-02	0.1633E-02	0.6710	2.7871
282	CaCl2				0.3377E+01	0.3455E+01	0.3153E-04	0.3153E-04	1.0000	4.5012
284	SiF6 --				0.1177E-28	0.1204E-28	0.8586E-34	0.1786E-34	0.2080	34.7481
285	CH4 Gas	0.1000	0.1023	0.6460E-05	0.1000E+00	0.1023E+00	0.6460E-05	0.0000E+00	1.0000	0.0000
288	PbCO3				0.1796E-04	0.1837E-04	0.6966E-10	0.6966E-10	1.0000	10.1570
289	PbOH +				0.3184E-04	0.3258E-04	0.1472E-09	0.9877E-10	0.6710	10.0054
292	ZnHCO3 +				0.5375E-04	0.5499E-04	0.4408E-09	0.2958E-09	0.6710	9.5291
293	ZnOH +				0.2324E-03	0.2378E-03	0.2924E-08	0.1962E-08	0.6710	8.7072
294	Zn(OH)2				0.1038E-04	0.1062E-04	0.1083E-09	0.1083E-09	1.0000	9.9654

SAMPLE IDENT - Test Sample #3 - Dissolve Anorthite to saturate with Gibbsite in seawater (TEMPERATURE = 25.00)
ANORTHIT PPT/DISS

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
1	ADULARIA	0.642	1.260	-0.618	-0.843	74	MICROCLN	0.642	-0.550	1.192	1.626
2	AKERMANI	33.530	45.460	-11.930	-16.275	75	MIEONITE	50.494	69.950	-19.456	-26.542
3	ALBITE	2.330	2.500	-0.170	-0.232	76	MIRABILT	-3.761	-1.090	-2.671	-3.644
4	ALBITE L	2.330	3.110	-0.780	-1.064	77	MONTICEL	24.012	30.150	-6.138	-8.374
5	ALBITE H	2.330	4.430	-2.100	-2.865	78	MORD, Na	-5.956	-3.900	-2.056	-2.805
6	ALUNITE	-11.029	-2.790	-8.239	-11.239	79	MORD, K	-7.644	-7.600	-0.044	-0.060
7	AMESI14A	38.906	38.630	0.276	0.376	80	MUSCOVIT	14.701	12.880	1.821	2.484
8	ANALCIME	6.452	6.050	0.402	0.548	81	NACHOLIT	-3.509	-0.430	-3.079	-4.200
9	ANDALUSI	9.937	16.570	-6.633	-9.049	82	NATRTHRM	-6.156	-0.010	-6.146	-8.384
10	ANDESITE	9.180	12.730	-3.550	-4.843	83	NATRON	-6.231	-0.880	-5.351	-7.300
11	ANHYDRIT	-5.403	-4.330	-1.073	-1.464	84	NEPHALIN	10.591	13.520	-2.929	-3.996
12	ANNITE	25.453	29.140	-3.687	-5.030	85	NESQUHON	-7.054	-5.350	-1.704	-2.325
13	ANORTHIT	19.456	25.830	-6.374	-8.696	92	OLIGOCLA	5.755	8.730	-2.975	-4.059
14	APATCHLR	-49.450	-66.150	16.700	22.782	93	PARAGONI	16.389	14.390	1.999	2.727
15	APATFLUR	-53.552	-68.340	14.788	20.175	94	PARAGASI	89.267	100.790	-11.523	-15.720
16	APATHYDX	-54.784	-60.390	5.606	7.647	95	PERICLAS	14.493	21.510	-7.017	-9.573
17	ARAGONIT	-7.873	-8.340	0.467	0.637	96	PHILLIPS	1.477	3.300	-1.823	-2.486
18	AUGITE	23.586	32.560	-8.974	-12.243	97	PHLOGPIT	44.112	37.220	6.892	9.402
20	BARITE	-10.205	-9.960	-0.245	-0.334	98	PHLOGPTF	18.598	16.730	1.868	2.548
21	BOEHMITE	7.029	6.950	0.079	0.108	99	PORTLAN	-14.339	-5.420	-8.919	-12.168
22	BRUCITE	-13.496	-11.470	-2.026	-2.763	100	POTASSI	11.998	84.120	-72.122	-98.391
23	BYTOWNIT	16.031	18.600	-2.569	-3.505	101	PREHNITE	28.966	32.020	-3.054	-4.166
24	CALCITE	-7.873	-8.480	0.607	0.828	102	PYROPHYL	-2.462	-0.100	-2.362	-3.223
25	CELESTIT	-7.391	-6.430	-0.961	-1.311	103	QUARTZ	-4.130	-3.930	-0.200	-0.273
26	CHALCEDO	-4.130	-3.730	-0.400	-0.546	104	SANIDINE	0.642	1.180	-0.538	-0.734
27	CHAM, 7A	26.466	29.030	-2.564	-3.497	105	SAPO, Na	33.170	26.880	6.290	8.581
28	CHLOR, 7	74.107	71.940	2.167	2.956	106	SAPO, K	32.613	26.550	6.063	8.271
29	CHLOR, 1	74.107	68.570	5.537	7.554	107	SAPO, H	30.632	25.850	4.782	6.523
30	CRYSOTIL	35.201	32.030	3.171	4.326	108	SAPO, Ca	32.885	26.820	6.065	8.274
31	C-ENSTAT	10.363	11.290	-0.927	-1.265	109	SAPO, Mg	33.024	26.800	6.224	8.491
32	C-PTIL,N	-11.929	-7.900	-4.029	-5.496	110	SEPIOLIT	33.131	31.520	1.611	2.197
33	C-PTIL,K	-15.305	-15.000	-0.305	-0.416	111	SILICAAM	-4.130	-2.700	-1.430	-1.951
34	C-PTIL,C	-13.654	-9.300	-4.354	-5.940	112	SILICGEL	-4.130	-2.710	-1.420	-1.938
35	C-PTIL,M	-12.810	-5.000	-7.810	-10.655	113	SILLIMAN	9.937	15.730	-5.793	-7.903
36	CORUNDUM	14.067	21.400	-7.333	-10.004	114	SMEC Ca	3.468	6.140	-2.672	-3.645
37	CRISTOBA	-4.130	-3.540	-0.590	-0.805	115	SMEC K	3.201	5.860	-2.659	-3.627
38	CRISTOBB	-4.130	-2.940	-1.190	-1.624	116	SMEC Mg	3.609	6.040	-2.431	-3.316
39	DICKITE	5.790	6.170	-0.380	-0.519	117	SMEC Na	3.758	6.120	-2.362	-3.222
40	DIOPSIDE	19.881	19.630	0.251	0.343	118	Na2O	15.374	67.430	-52.056	-71.016
41	DOLOMITE	-14.902	-18.060	3.158	4.309	119	SPINEL	28.560	36.460	-7.900	-10.777
42	DSORD	-14.902	-16.520	1.618	2.208	120	STILBITE	-1.255	1.410	-2.665	-3.635
43	ENSTATIT	10.363	11.470	-1.107	-1.511	122	SrCO3	-9.861	-9.270	-0.591	-0.806
45	FAYALITE	12.416	19.430	-7.014	-9.569	123	SYLVITE	-2.661	0.910	-3.571	-4.872
46	FLUORITE	-11.874	-10.960	-0.914	-1.246	124	TALC	26.949	21.130	5.819	7.938
47	FORSTERI	24.855	29.070	-4.215	-5.750	125	THENARDI	-3.677	-0.290	-3.387	-4.621
48	GIBBS AM	-34.949	-34.420	-0.529	-0.722	126	TREMOLIT	66.711	60.890	5.821	7.942
49	GIBBSITE	-34.949	-34.920	-0.029	-0.039	127	TRONA	-9.673	-0.630	-9.043	-12.337
50	GREENALI	16.542	22.580	-6.038	-8.238	128	VIVIANIT	-47.938	-36.000	-11.938	-16.287
51	GYPSUM	-5.420	-4.600	-0.820	-1.118	129	WAIRAKIT	11.178	17.330	-6.152	-8.392
52	HALITE	-0.973	1.590	-2.563	-3.496	130	WITHERIT	-12.675	-8.630	-4.045	-5.519
53	HALLOYSI	5.790	8.910	-3.120	-4.257	131	WOLLASTO	9.519	12.600	-3.081	-4.204

SAMPLE IDENT - Test Sample #3 - Dissolve Anorthite to saturate with Gibbsite in seawater (TEMPERATURE = 25.00)
ANORTHIT PPT/DISS

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
54	HEULANDI	-1.246	1.410	-2.656	-3.624	132	ZOISITE	36.004	42.100	-6.096	-8.317
55	HUNTITE	-28.960	-30.620	1.660	2.265	134	AgCl	-14.686	-9.730	-4.956	-6.761
56	HYDRMAGN	-36.507	-38.530	2.023	2.760	139	Cu2O	-8.747	-1.900	-6.847	-9.341
57	HYPHILIT	-3.671	11.800	-15.471	-21.106	144	FeCl2	-9.047	7.900	-16.947	-23.120
58	ILLITE	8.936	10.340	-1.404	-1.916	146	FeCO3	-13.249	-10.540	-2.709	-3.695
59	KAOLINIT	5.790	6.230	-0.440	-0.600	147	FeO	8.273	13.500	-5.227	-7.131
60	KENYAITE	-37.788	-25.000	-12.788	-17.446	158	HgCl2(C)	-25.023	-14.110	-10.913	-14.888
61	K-SPAR	0.642	-0.550	1.192	1.626	160	HgO	-7.703	2.440	-10.143	-13.838
62	KYANITE	9.937	14.480	-4.543	-6.198	163	MnCl2	-12.494	8.790	-21.284	-29.036
63	LABRADOR	14.245	16.250	-2.005	-2.735	164	MnCO3	-16.695	-10.540	-6.155	-8.397
64	LARNITE	23.168	38.880	-15.712	-21.435	165	MnO	4.826	17.700	-12.874	-17.563
65	LAUMONTI	11.162	14.170	-3.008	-4.104	168	PbCl2	-12.955	-4.820	-8.135	-11.099
66	LEUCITE	4.772	6.520	-1.748	-2.384	169	PbCO3	-17.157	-12.890	-4.267	-5.821
67	LIME	-19.152	32.660	-51.812	-70.683	170	PbOLITHR	4.365	12.550	-8.185	-11.167
68	MAGADITE	-21.263	-14.340	-6.923	-9.444	171	PbOMASIC	4.365	12.690	-8.325	-11.358
70	MAGNESIT	-7.029	-8.050	1.021	1.393	173	PbSO4	-14.687	-7.800	-6.887	-9.396
71	MgCl2	-2.827	22.150	-24.977	-34.075	174	ZnCO3	-13.079	-9.870	-3.209	-4.378
72	MARIALIT	6.017	1.710	4.307	5.875	175	ZnO	8.443	11.200	-2.757	-3.761
73	MERWINIT	47.179	68.170	-20.991	-28.636	177	ZnSO4	-10.609	3.540	-14.149	-19.302

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****** INPUT DATA ECHO ******

TITLE : Test Sample #4 - Ca/Mg exchange in seawater
      TEMP       HITEMP        DENS       PRESS
0.2500E+02  0.0000E+00  0.1023E+01  0.0000E+00
        PH         EHM        EHMC      EMFZSC
0.8200E+01  0.5000E+00  0.9000E+01  0.9000E+01
CONCENTRATION UNITS :  PPM
  Na          K           Li          Ca          Mg          Fe          Al
0.1077E+05  0.3991E+03  0.1810E+00  0.4123E+03  0.1292E+04  0.2000E-02  0.0000E+00
  SiO2        Cl          SO4         H2S         HCO3        CO3         TIC
0.4280E+01  0.1935E+05  0.2712E+04  0.1000E+02  0.1234E+03  0.0000E+00  0.0000E+00
  F           PO4         NO3         NH3         B           Sr          Ba
0.1390E+01  0.6000E-01  0.2900E+00  0.0000E+00  0.4450E+01  0.8140E+01  0.2000E-01
  Pb          Zn          Cu          Mn          Hg          Ag
0.5000E-04  0.4900E-02  0.7000E-03  0.2000E-03  0.3000E-04  0.4000E-04
  As          U           V
0.4000E-02  0.0000E+00  0.0000E+00
  Acetate     Oxalate     Succinate   CH4
0.1000E+00  0.1000E+00  0.1000E+00  0.1000E+00
      ALK       ITIC
     2          0
    DCO2        DH2S        DNH3        DCH4
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   ICCSAT      IMCO3       FIXIT       FCCSAT
     0          0     0.00000E+00       0.0000
  TCO2M       TCH4M       TH2SM       WROIL      KCO2OL      KCH4OL      KH2SOL      DSEP
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
Adsorption/Exchange option (N=no) = E
Surface Chemistry input for Ion Exchange:
    CEC         TAREA       SAREA         INSP
0.1000E+03  0.0000E+00  0.0000E+00        2
   NAME      CHARGE    Fract. Surf. Sites
CaX2              0     0.5000E+00
MgX2              0     0.5000E+00
        K  =   1. *              * Coef  *  ID    +   ....
      1.0000   CaX2           -0.10000E+01    1     -0.20000E+01    0
      1.0000   MgX2           -0.10000E+01    2     -0.20000E+01    0
      IBMIX      ITMIX
     0          0
LOG KT TO BE CHANGED AT TEMP =  25.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
LOG KT TO BE CHANGED AT TEMP =   0.00
    0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00          0 0.0000E+00
       ANS1       ANS2
     0          0
Number of Additional Minerals =            0
FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    1
FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS:  0
FLAGS FOR CALCULATING REDOX SPECIES:
Fe  Cu  Hg  Mn   U   V
 1   1   1   1   0   0
PRINTING OPTIONS:
   INFORM        RATIO        GEOTH       IPRIN1       IPRIN2
      0            0            0            0            0
TOLERANCE FACTORS:  CONV1 =   0.5000E-04  CONV2 =   0.5000E-04
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SAMPLE IDENT:- Test Sample #4 - Ca/Mg exchange in seawater

PH	EH	TEMP		CATIONS	ANIONS	DIFFERENCE (MEQ/L)	--- H - OH BALANCE (MOLES) -------		
							HTOT	OHTOT	DIFFERENCE
8.20	0.5000	25.00	ANAL=	619.6745	618.2648	1.4097			
			CALC=	577.6281	570.0555	7.5726	0.2514E-02	0.1350E-02	0.1163E-02

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER	PRESSURE P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0230	35916.54	0.64960	0.9809	1.0000	0.3169E-01	0.4782E-03	0.1449E-03	0.5252E-02	0.0000E+00

	Total Alkalinity as			Dissolved Inorganic Carbon as TIC	HCO3- Alkalinity	H2CO3 species	Sum of HCO3-	Sum of CO3=
	HCO3-	CO3=	CaCO3					
(MG/L)=	0.1594E+03	0.7840E+02	0.1308E+03	0.2485E+02	0.1373E+03	0.8648E+00	0.1130E+03	0.1216E+02
(PPM)=	0.1559E+03	0.7664E+02	0.1278E+03	0.2429E+02	0.1343E+03	0.8454E+00	0.1105E+03	0.1188E+02
(MOLALITY)=	0.2647E-02	0.1324E-02	0.1324E-02	0.2096E-02	0.2287E-02	0.1413E-04	0.1877E-02	0.2052E-03

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
1	Ca ++	412.3000	421.7829	0.1066E-01	0.2844E+03	0.2909E+03	0.7353E-02	0.1807E-02	0.2458	2.7430
2	Mg ++	1292.0000	1321.7160	0.5508E-01	0.1121E+04	0.1147E+04	0.4779E-01	0.1261E-01	0.2639	1.8992
3	Na +	10770.0000	11017.7100	0.4855E+00	0.1024E+05	0.1048E+05	0.4618E+00	0.3099E+00	0.6710	0.5088
4	K +	399.1000	408.2793	0.1058E-01	0.3825E+03	0.3913E+03	0.1014E-01	0.6356E-02	0.6269	2.1968
5	Cl -	19350.0000	19795.0500	0.5657E+00	0.1874E+05	0.1917E+05	0.5478E+00	0.3434E+00	0.6269	0.4641
6	SO4 --	2712.0000	2774.3760	0.2926E-01	0.1203E+04	0.1231E+04	0.1298E-01	0.2189E-02	0.1686	2.6598
7	HCO3 -	123.4000	126.2382	0.2096E-02	0.8534E+02	0.8730E+02	0.1449E-02	0.1000E-02	0.6899	3.0000
8	H +				0.7638E-05	0.7814E-05	0.7853E-08	0.6310E-08	0.8034	8.2000
9	OH -				0.4016E-01	0.4108E-01	0.2447E-05	0.1591E-05	0.6501	5.7984
11	H4SiO4				0.6615E+01	0.6767E+01	0.7133E-04	0.7133E-04	1.0000	4.1467
12	SiO2	4.2800	4.3784	0.7382E-04						
13	Ag +	0.0000	0.0000	0.3843E-09	0.1039E-08	0.1063E-08	0.9982E-14	0.6000E-14	0.6011	14.2219
15	Ba ++	0.0200	0.0205	0.1509E-06	0.1815E-01	0.1857E-01	0.1370E-06	0.2849E-07	0.2080	7.5453
16	Cu +	0.0007	0.0007	0.1142E-07	0.2394E-09	0.2450E-09	0.3906E-14	0.2348E-14	0.6011	14.6294
17	Cu ++				0.3648E-03	0.3732E-03	0.5950E-08	0.1462E-08	0.2458	8.8349
18	Fe ++	0.0020	0.0020	0.3712E-07	0.1268E-08	0.1297E-08	0.2353E-13	0.5784E-14	0.2458	14.2378
19	Fe +3				0.1009E-12	0.1032E-12	0.1872E-17	0.1599E-18	0.0854	18.7962
21	Hg ++	0.0000	0.0000	0.1550E-09	0.7470E-18	0.7642E-18	0.3860E-23	0.8029E-24	0.2080	24.0954
22	Li +	0.1810	0.1852	0.2703E-04	0.1792E+00	0.1833E+00	0.2677E-04	0.1973E-04	0.7373	4.7048
23	Mn ++	0.0002	0.0002	0.3773E-08	0.5864E-06	0.5998E-06	0.1106E-10	0.2719E-11	0.2458	11.5656
24	Mn +3				0.8886E-23	0.9091E-23	0.1676E-27	0.1432E-28	0.0854	28.8441
25	Pb ++	0.0001	0.0001	0.2501E-09	0.9758E-12	0.9983E-12	0.4881E-17	0.9200E-18	0.1885	18.0362
26	Sr ++	8.1400	8.3272	0.9628E-04	0.7551E+01	0.7725E+01	0.8932E-04	0.1858E-04	0.2080	4.7310
27	Zn ++	0.0049	0.0050	0.7769E-07	0.2691E-10	0.2753E-10	0.4267E-15	0.1049E-15	0.2458	15.9794
28	H2AsO3-	0.0067	0.0068	0.5281E-07	0.7209E-03	0.7375E-03	0.5706E-08	0.3829E-08	0.6710	8.4169
29	PO4 -3	0.0600	0.0614	0.6548E-06	0.5920E-05	0.6056E-05	0.6461E-10	0.1748E-11	0.0271	11.7573
30	F -	1.3900	1.4220	0.7583E-04	0.7672E+00	0.7848E+00	0.4185E-04	0.2721E-04	0.6501	4.5653
31	B(OH)3	25.4540	26.0394	0.4266E-03	0.2205E+02	0.2256E+02	0.3696E-03	0.3696E-03	1.0000	3.4323
33	H2S	10.0000	10.2300	0.3041E-03	0.3685E+00	0.3770E+00	0.1121E-04	0.1166E-04	1.0407	4.9332
43	AgCl				0.5954E-06	0.6091E-06	0.4305E-11	0.4305E-11	1.0000	11.3660
44	AgCl2 -				0.3801E-04	0.3889E-04	0.2204E-09	0.1479E-09	0.6710	9.8301
45	AgCl3 --				0.3041E-04	0.3111E-04	0.1471E-09	0.3060E-10	0.2080	10.5143
46	AgCl4 -3				0.4055E-05	0.4148E-05	0.1683E-10	0.6631E-12	0.0394	12.1784
47	AgSO4 -				0.7863E-10	0.8043E-10	0.3996E-15	0.2681E-15	0.6710	15.5717

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
48	CH3COO -	0.1000	0.1023	0.1755E-05	0.7230E-01	0.7396E-01	0.1269E-05	0.8755E-06	0.6899	6.0577
49	H3AsO3				0.5724E-02	0.5856E-02	0.4710E-07	0.4710E-07	1.0000	7.3269
51	BaCO3				0.1272E-04	0.1301E-04	0.6678E-10	0.6678E-10	1.0000	10.1753
52	BaHCO3 +				0.2238E-03	0.2290E-03	0.1169E-08	0.7846E-09	0.6710	9.1053
53	BaOH +				0.3234E-07	0.3308E-07	0.2172E-12	0.1536E-12	0.7071	12.8137
54	BaSO4				0.2867E-02	0.2933E-02	0.1273E-07	0.1273E-07	1.0000	7.8952
55	CaCO3				0.2147E+01	0.2197E+01	0.2224E-04	0.2224E-04	1.0000	4.6529
56	CaHCO3 +				0.3081E+01	0.3152E+01	0.3158E-04	0.2328E-04	0.7373	4.6329
57	CaOH +				0.2965E-02	0.3033E-02	0.5383E-07	0.3969E-07	0.7373	7.4013
58	CaPO4 -				0.1688E-02	0.1727E-02	0.1296E-07	0.9326E-08	0.7198	8.0303
59	CaHPO4				0.2333E-02	0.2387E-02	0.1777E-07	0.1777E-07	1.0000	7.7503
60	CaH2PO4+				0.2207E-04	0.2258E-04	0.1669E-09	0.1201E-09	0.7198	9.9203
61	CaSO4				0.1037E+03	0.1061E+03	0.7892E-03	0.7892E-03	1.0000	3.1028
62	CuCl				0.3860E-07	0.3948E-07	0.4041E-12	0.4041E-12	1.0000	12.3935
63	CuCl2 -				0.4663E-05	0.4770E-05	0.3594E-10	0.2412E-10	0.6710	10.6177
64	CuCl3 --				0.1035E-04	0.1058E-04	0.6311E-10	0.1313E-10	0.2080	10.8818
65	CuCl +				0.7487E-04	0.7659E-04	0.7838E-09	0.5259E-09	0.6710	9.2791
66	CuCl2				0.4363E-05	0.4464E-05	0.3364E-10	0.3364E-10	1.0000	10.4732
67	CuCl3 -				0.7255E-07	0.7421E-07	0.4425E-12	0.2969E-12	0.6710	12.5273
68	CuCl4 --				0.4869E-09	0.4981E-09	0.2457E-14	0.5111E-15	0.2080	15.2915
69	CuOH +				0.3094E-03	0.3165E-03	0.3981E-08	0.2671E-08	0.6710	8.5733
70	CuSO4				0.8765E-04	0.8967E-04	0.5692E-09	0.5692E-09	1.0000	9.2447
71	FeCl +				0.7697E-10	0.7874E-10	0.8737E-15	0.5862E-15	0.6710	15.2319
72	FeCl2				0.5145E-18	0.5263E-18	0.4207E-23	0.4207E-23	1.0000	23.3761
73	FeHPO4				0.8142E-13	0.8329E-13	0.5558E-18	0.5558E-18	1.0000	18.2551
74	H3PO4				0.2034E-09	0.2081E-09	0.2151E-14	0.2151E-14	1.0000	14.6673
75	FeOH +				0.2893E-10	0.2959E-10	0.4115E-15	0.2910E-15	0.7071	15.5362
76	Fe(OH)2				0.3115E-13	0.3187E-13	0.3593E-18	0.3593E-18	1.0000	18.4446
77	FeOOH -				0.2686E-13	0.2748E-13	0.3133E-18	0.2215E-18	0.7071	18.6546
78	FeSO4				0.4994E-09	0.5109E-09	0.3407E-14	0.3407E-14	1.0000	14.4676
79	FeCl ++				0.6864E-12	0.7022E-12	0.7791E-17	0.1621E-17	0.2080	17.7903
80	FeCl2 +				0.4400E-12	0.4502E-12	0.3598E-17	0.2544E-17	0.7071	17.5945
81	FeCl3				0.1368E-13	0.1399E-13	0.8738E-19	0.8738E-19	1.0000	19.0586
82	FeCl4 -				0.1025E-15	0.1049E-15	0.5377E-21	0.3608E-21	0.6710	21.4427
83	FeSO4 +				0.1001E-11	0.1024E-11	0.6831E-17	0.4831E-17	0.7071	17.3160
84	FeSO4)2-				0.1038E-23	0.1062E-23	0.4340E-29	0.2912E-29	0.6710	29.5358
85	FeOH ++				0.6227E-07	0.6370E-07	0.8859E-12	0.1843E-12	0.2080	12.7346
86	Fe(OH)2+				0.3697E-04	0.3782E-04	0.4264E-09	0.3069E-09	0.7198	9.5129
87	Fe(OH)3				0.2099E-02	0.2147E-02	0.2035E-07	0.2035E-07	1.0000	7.6913
88	Fe(OH)4-				0.1952E-02	0.1997E-02	0.1633E-07	0.1176E-07	0.7198	7.9297
89	B(OH)4 -				0.4342E+01	0.4442E+01	0.5708E-04	0.3462E-04	0.6065	4.4607
90	H2SiO4--				0.2150E-03	0.2199E-03	0.2368E-08	0.5288E-09	0.2233	9.2767
91	H3SiO4 -				0.2287E+00	0.2340E+00	0.2492E-05	0.1672E-05	0.6710	5.7767
92	HAsO3 --				0.1173E-07	0.1200E-07	0.9357E-13	0.1946E-13	0.2080	13.7108
96	HF				0.5016E-05	0.5131E-05	0.2598E-09	0.2598E-09	1.0000	9.5853
97	H2CO3				0.8454E+00	0.8648E+00	0.1413E-04	0.1413E-04	1.0000	4.8500
98	CO3 --				0.1922E+01	0.1966E+01	0.3319E-04	0.7413E-05	0.2233	5.1300
99	HPO4 --				0.1075E-01	0.1099E-01	0.1160E-06	0.2414E-07	0.2080	7.6173
100	H2PO4 -				0.3138E-03	0.3210E-03	0.3353E-08	0.2414E-08	0.7198	8.6173
101	HS -				0.9074E+01	0.9282E+01	0.2843E-03	0.1849E-03	0.6501	3.7332
102	S --				0.4357E-07	0.4458E-07	0.1408E-11	0.2930E-12	0.2080	12.5332
103	HSO4 -				0.1671E-03	0.1709E-03	0.1784E-08	0.1231E-08	0.6899	8.9098
104	HNO3				0.4331E-10	0.4431E-10	0.7124E-15	0.7124E-15	1.0000	15.1473

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
105	HgCl +				0.1664E-12	0.1703E-12	0.7308E-18	0.4903E-18	0.6710	18.3095
106	HgCl2				0.4514E-06	0.4618E-06	0.1723E-11	0.1723E-11	1.0000	11.7637
107	HgCl3 -				0.3214E-04	0.3288E-04	0.1085E-09	0.7281E-10	0.6710	10.1378
108	HgCl4 --				0.1476E-04	0.1510E-04	0.4467E-10	0.9291E-11	0.2080	11.0319
109	HgSO4				0.1263E-19	0.1292E-19	0.4414E-25	0.4414E-25	1.0000	25.3552
111	Hg(HS)3-				0.2343E-07	0.2397E-07	0.8098E-13	0.5434E-13	0.6710	13.2649
113	KCl				0.2070E+02	0.2118E+02	0.2878E-03	0.2878E-03	1.0000	3.5409
114	KCO3 -				0.7987E-01	0.8171E-01	0.8352E-06	0.5536E-06	0.6629	6.2568
115	KHSO4				0.7277E-05	0.7444E-05	0.5538E-10	0.5538E-10	1.0000	10.2566
116	KSO4 -				0.1957E+02	0.2002E+02	0.1500E-03	0.1080E-03	0.7198	3.9666
117	KHPO4 -				0.5417E-04	0.5541E-04	0.4156E-09	0.2991E-09	0.7198	9.5241
118	LiOH				0.1098E-05	0.1123E-05	0.4751E-10	0.4751E-10	1.0000	10.3232
119	LiSO4 -				0.2650E-01	0.2711E-01	0.2666E-06	0.1885E-06	0.7071	6.7246
120	MgCO3				0.7265E+01	0.7432E+01	0.8930E-04	0.8930E-04	1.0000	4.0492
121	MgHCO3 +				0.1818E+02	0.1860E+02	0.2209E-03	0.1482E-03	0.6710	3.8292
122	MgF +				0.1373E+01	0.1405E+01	0.3286E-04	0.2267E-04	0.6899	4.6445
123	MgOH +				0.4243E+00	0.4341E+00	0.1064E-04	0.7988E-05	0.7505	5.0976
124	MgSO4				0.8054E+03	0.8239E+03	0.6934E-02	0.6934E-02	1.0000	2.1590
125	MgPO4 -				0.1041E-01	0.1065E-01	0.9042E-07	0.6508E-07	0.7198	7.1865
126	MgHPO4				0.4552E-01	0.4657E-01	0.3922E-06	0.3922E-06	1.0000	6.4065
127	MgH2PO4+				0.1363E-03	0.1395E-03	0.1165E-08	0.8385E-09	0.7198	9.0765
128	MnCl +				0.3838E-13	0.3926E-13	0.4401E-18	0.2953E-18	0.6710	18.5298
129	MnCl2				0.3093E-10	0.3164E-10	0.2547E-15	0.2547E-15	1.0000	15.5939
130	MnCl3 -				0.5097E-09	0.5215E-09	0.3275E-14	0.2198E-14	0.6710	14.6581
131	MnCl4 --				0.5472E-08	0.5597E-08	0.2882E-13	0.5995E-14	0.2080	14.2222
132	MnHCO3 +				0.8442E-08	0.8636E-08	0.7545E-13	0.5063E-13	0.6710	13.2956
133	MnSO4				0.1578E-06	0.1614E-06	0.1083E-11	0.1083E-11	1.0000	11.9654
134	MnHPO4				0.3633E-10	0.3716E-10	0.2495E-15	0.2495E-15	1.0000	15.6030
135	MnOH +				0.1232E-08	0.1261E-08	0.1775E-13	0.1191E-13	0.6710	13.9240
136	NO3 -	0.2900	0.2967	0.4847E-05	0.2900E+00	0.2967E+00	0.4847E-05	0.3039E-05	0.6269	5.5173
137	NaCl				0.8477E+03	0.8672E+03	0.1503E-01	0.1503E-01	1.0000	1.8229
138	NaCO3 -				0.4759E+01	0.4869E+01	0.5943E-04	0.4278E-04	0.7198	4.3688
139	NaHCO3				0.1413E+02	0.1445E+02	0.1743E-03	0.1743E-03	1.0000	3.7588
140	Na2CO3				0.1521E-01	0.1556E-01	0.1487E-06	0.1487E-06	1.0000	6.8276
141	Na2SO4				0.9321E+03	0.9535E+03	0.6801E-02	0.6801E-02	1.0000	2.1674
142	NaSO4 -				0.1838E+03	0.1880E+03	0.1600E-02	0.1152E-02	0.7198	2.9386
143	NaHPO4 -				0.2326E-02	0.2379E-02	0.2026E-07	0.1458E-07	0.7198	7.8361
144	NaF				0.4503E-01	0.4607E-01	0.1111E-05	0.1111E-05	1.0000	5.9541
145	NaHS				0.4583E+00	0.4689E+00	0.8473E-05	0.8473E-05	1.0000	5.0720
148	PbCl +				0.2834E-11	0.2899E-11	0.1210E-16	0.8122E-17	0.6710	17.0904
149	PbCl2				0.2718E-11	0.2780E-11	0.1013E-16	0.1013E-16	1.0000	16.9945
150	PbCl3 -				0.7681E-12	0.7858E-12	0.2539E-17	0.1704E-17	0.6710	17.7686
151	PbCl4 --				0.5976E-12	0.6114E-12	0.1775E-17	0.3692E-18	0.2080	18.4328
152	PbSO4				0.3313E-12	0.3389E-12	0.1132E-17	0.1132E-17	1.0000	17.9460
153	MnCl ++				0.8400E-21	0.8594E-21	0.9632E-26	0.2003E-26	0.2080	26.6982
154	SrOH -				0.2067E-04	0.2114E-04	0.2047E-09	0.1448E-09	0.7071	9.8394
155	SrCO3				0.1296E-01	0.1326E-01	0.9100E-07	0.9100E-07	1.0000	7.0410
156	SrHCO3 +				0.6151E-01	0.6292E-01	0.4289E-06	0.2878E-06	0.6710	6.5410
157	SrSO4				0.1142E+01	0.1168E+01	0.6444E-05	0.6444E-05	1.0000	5.1908
158	ZnCl +				0.1374E-10	0.1405E-10	0.1412E-15	0.9473E-16	0.6710	16.0235
159	ZnCl2				0.6780E-11	0.6936E-11	0.5157E-16	0.5157E-16	1.0000	16.2876
160	ZnCl3 -				0.2295E-11	0.2348E-11	0.1385E-16	0.9294E-17	0.6710	17.0318
161	ZnCl4 --				0.2122E-11	0.2171E-11	0.1062E-16	0.2208E-17	0.2080	17.6559

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
162	ZnSO4				0.5798E-11	0.5931E-11	0.3722E-16	0.3722E-16	1.0000	16.4292
165	HgOH +				0.1153E-13	0.1179E-13	0.5490E-19	0.3683E-19	0.6710	19.4337
166	Hg(OH)2				0.3409E-08	0.3488E-08	0.1506E-13	0.1506E-13	1.0000	13.8221
228	CH3COOH				0.1842E-04	0.1884E-04	0.3179E-09	0.3179E-09	1.0000	9.4977
230	BaAce +				0.9241E-07	0.9453E-07	0.4877E-12	0.3364E-12	0.6899	12.4731
231	CaAce +				0.3725E-02	0.3811E-02	0.3895E-07	0.2687E-07	0.6899	7.5707
232	CuAce +				0.2735E-13	0.2798E-13	0.2312E-18	0.1595E-18	0.6899	18.7971
233	FeAce +				0.1624E-12	0.1661E-12	0.1464E-17	0.1010E-17	0.6899	17.9955
234	Fe(Ace)2				0.9367E-20	0.9582E-20	0.5581E-25	0.5581E-25	1.0000	25.2533
235	KAce				0.2147E-03	0.2196E-03	0.2267E-08	0.2267E-08	1.0000	8.6445
236	MgAce +				0.2289E-01	0.2342E-01	0.2846E-06	0.1964E-06	0.6899	6.7069
237	NaAce				0.1265E-01	0.1294E-01	0.1598E-06	0.1598E-06	1.0000	6.7965
238	PbAce +				0.5458E-16	0.5583E-16	0.2124E-21	0.1466E-21	0.6899	21.8340
239	Pb(Ace)2				0.9661E-21	0.9884E-21	0.3078E-26	0.3078E-26	1.0000	26.5117
240	Pb(Ace)3				0.1742E-26	0.1782E-26	0.4696E-32	0.3240E-32	0.6899	32.4894
241	SrAce +				0.4823E-04	0.4933E-04	0.3408E-09	0.2351E-09	0.6899	9.6287
244	ZnAce +				0.1299E-11	0.1328E-11	0.1082E-16	0.7463E-17	0.6899	17.1271
245	Zn(Ace)2				0.3185E-21	0.3259E-21	0.1800E-26	0.1800E-26	1.0000	26.7448
246	C2O4 --	0.1000	0.1023	0.1177E-05	0.9440E-02	0.9657E-02	0.1112E-06	0.2483E-07	0.2233	7.6051
247	HC2O4 -				0.3468E-09	0.3548E-09	0.4037E-14	0.2785E-14	0.6899	14.5551
248	H2C2O4				0.3117E-13	0.3189E-13	0.3588E-18	0.3588E-18	1.0000	18.4451
251	BaOxy				0.5714E-08	0.5845E-08	0.2628E-13	0.2628E-13	1.0000	13.5804
252	CaOxy				0.5546E-02	0.5673E-02	0.4487E-07	0.4487E-07	1.0000	7.3481
253	FeOxy				0.5007E-12	0.5122E-12	0.3607E-17	0.3607E-17	1.0000	17.4429
254	FeOxy +				0.3028E-13	0.3098E-13	0.2181E-18	0.1505E-18	0.6899	18.8225
255	KOxy -				0.1406E-03	0.1438E-03	0.1146E-08	0.7909E-09	0.6899	9.1019
256	MgOxy				0.1002E+00	0.1025E+00	0.9241E-06	0.9241E-06	1.0000	6.0343
257	MnOxy				0.9310E-10	0.9524E-10	0.6749E-15	0.6749E-15	1.0000	15.1707
258	MnOxy)2				0.7180E-03	0.7345E-03	0.3760E-08	0.8398E-09	0.2233	9.0758
259	MnOxy)3				0.1550E-06	0.1586E-06	0.6354E-12	0.1315E-14	0.0021	14.8809
260	MnOxy				0.2764E-19	0.2827E-19	0.2004E-24	0.1382E-24	0.6899	24.8594
261	NaOxy -				0.9487E-02	0.9705E-02	0.8857E-07	0.6111E-07	0.6899	7.2139
262	PbOxy				0.3575E-15	0.3657E-15	0.1255E-20	0.1255E-20	1.0000	20.9013
263	SrOxy				0.2710E-04	0.2773E-04	0.1599E-09	0.1599E-09	1.0000	9.7961
264	ZnOxy				0.3061E-13	0.3131E-13	0.2068E-18	0.2068E-18	1.0000	18.6845
265	C4H4O4--	0.1000	0.1023	0.8929E-06	0.6406E-01	0.6553E-01	0.5719E-06	0.1277E-06	0.2233	6.8937
266	HC4H4O4-				0.2140E-05	0.2190E-05	0.1895E-10	0.1307E-10	0.6899	10.8837
267	H2C4H4O4				0.4102E-08	0.4196E-08	0.3600E-13	0.3600E-13	1.0000	13.4437
270	BaSuc				0.9317E-07	0.9532E-07	0.3811E-12	0.3811E-12	1.0000	12.4190
271	CaSuc				0.3478E-02	0.3558E-02	0.2309E-07	0.2309E-07	1.0000	7.6366
272	FeSuc				0.1942E-13	0.1987E-13	0.1171E-18	0.1171E-18	1.0000	18.9315
273	FeSuc +				0.4911E-13	0.5024E-13	0.2960E-18	0.2042E-18	0.6899	18.6898
274	KSuc -				0.3516E-03	0.3597E-03	0.2348E-08	0.1620E-08	0.6899	8.7905
275	MgSuc				0.2449E-01	0.2505E-01	0.1808E-06	0.1808E-06	1.0000	6.7429
276	MnSuc				0.8476E-11	0.8671E-11	0.5137E-16	0.5137E-16	1.0000	16.2893
277	NaSuc -				0.1536E-01	0.1571E-01	0.1145E-06	0.7898E-07	0.6899	7.1025
278	PbSuc				0.1159E-15	0.1186E-15	0.3716E-21	0.3716E-21	1.0000	21.4299
279	SrSuc				0.4664E-04	0.4772E-04	0.2373E-09	0.2373E-09	1.0000	9.6247
280	ZnSuc				0.6764E-15	0.6919E-15	0.3863E-20	0.3863E-20	1.0000	20.4130
281	CaCl +				0.1773E+03	0.1814E+03	0.2433E-02	0.1633E-02	0.6710	2.7871
282	CaCl2				0.3377E+01	0.3454E+01	0.3153E-04	0.3153E-04	1.0000	4.5012
283	FeF ++				0.1510E-11	0.1545E-11	0.2091E-16	0.4350E-17	0.2080	17.3615
284	SiF6 --				0.1180E-28	0.1207E-28	0.8610E-34	0.1791E-34	0.2080	34.7469

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
285	CH4 Gas	0.1000	0.1023	0.6460E-05	0.1000E+00	0.1023E+00	0.6460E-05	0.0000E+00	1.0000	0.0000
286	Pb(HS)2				0.6586E-04	0.6737E-04	0.2497E-09	0.2497E-09	1.0000	9.6026
287	Pb(HS)3-				0.1170E-06	0.1197E-06	0.3959E-12	0.2656E-12	0.6710	12.5757
288	PbCO3				0.1758E-10	0.1799E-10	0.6820E-16	0.6820E-16	1.0000	16.1662
289	PbOH +				0.3117E-10	0.3189E-10	0.1441E-15	0.9670E-16	0.6710	16.0146
290	Zn(HS)2				0.2740E-04	0.2803E-04	0.2159E-09	0.2159E-09	1.0000	9.6657
291	Zn(HS)3-				0.1397E-05	0.1429E-05	0.8798E-11	0.5903E-11	0.6710	11.2289
292	ZnHCO3 +				0.5013E-12	0.5129E-12	0.4111E-17	0.2758E-17	0.6710	17.5593
293	ZnOH +				0.2167E-11	0.2217E-11	0.2726E-16	0.1829E-16	0.6710	16.7377
294	Zn(OH)2				0.9675E-13	0.9898E-13	0.1009E-17	0.1009E-17	1.0000	17.9961
295	ZnHSOH				0.8629E-02	0.8827E-02	0.7746E-07	0.7746E-07	1.0000	7.1109

SAMPLE IDENT - Test Sample #4 - Ca/Mg exchange in seawater (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
2	AKERMANI	33.530	45.460	-11.930	-16.276
11	ANHYDRIT	-5.403	-4.330	-1.073	-1.464
14	APATCHLR	-49.451	-66.150	16.699	22.781
15	APATFLUR	-53.552	-68.340	14.788	20.174
16	APATHYDX	-54.785	-60.390	5.605	7.646
17	ARAGONIT	-7.873	-8.340	0.467	0.637
19	AZURITE	-48.361	-39.460	-8.901	-12.144
20	BARITE	-10.205	-9.960	-0.245	-0.334
22	BRUCITE	-13.496	-11.470	-2.026	-2.764
24	CALCITE	-7.873	-8.480	0.607	0.828
25	CELESTIT	-7.391	-6.430	-0.961	-1.311
26	CHALCEDO	-4.130	-3.730	-0.400	-0.546
30	CRYSOTIL	35.201	32.030	3.171	4.325
31	C-ENSTAT	10.362	11.290	-0.928	-1.265
37	CRISTOBA	-4.130	-3.540	-0.590	-0.805
38	CRISTOBB	-4.130	-2.940	-1.190	-1.623
40	DIOPSIDE	19.881	19.630	0.251	0.343
41	DOLOMITE	-14.902	-18.060	3.158	4.308
42	DSORD	-14.902	-16.520	1.618	2.207
43	ENSTATIT	10.362	11.470	-1.108	-1.511
45	FAYALITE	0.178	19.430	-19.252	-26.265
46	FLUORITE	-11.874	-10.960	-0.914	-1.246
47	FORSTERI	24.855	29.070	-4.215	-5.750
50	GREENALI	-1.815	22.580	-24.395	-33.281
51	GYPSUM	-5.420	-4.600	-0.820	-1.118
52	HALITE	-0.973	1.590	-2.563	-3.496
55	HUNTITE	-28.960	-30.620	1.660	2.264
56	HYDRMAGN	-36.508	-38.530	2.022	2.759
57	HYPHILIT	-3.671	11.800	-15.471	-21.106
60	KENYAITE	-37.784	-25.000	-12.784	-17.441
64	LARNITE	23.167	38.880	-15.713	-21.436
67	LIME	-19.151	32.660	-51.811	-70.683
68	MAGADITE	-21.260	-14.340	-6.920	-9.441
69	MgFe2O4	26.075	21.100	4.975	6.787
70	MAGNESIT	-7.029	-8.050	1.021	1.393
71	MgCl2	-2.827	22.150	-24.977	-34.075
73	MERWINIT	47.178	68.170	-20.992	-28.637
76	MIRABILT	-3.761	-1.090	-2.671	-3.644
77	MONTICEL	24.011	30.150	-6.139	-8.375
81	NACHOLIT	-3.509	-0.430	-3.079	-4.200
82	NATRTHRM	-6.156	-0.010	-6.146	-8.385
83	NATRON	-6.231	-0.880	-5.351	-7.301
85	NESQUHON	-7.054	-5.350	-1.704	-2.325
91	OLDHAMIT	1.724	11.900	-10.176	-13.883
95	PERICLAS	14.492	21.510	-7.018	-9.574
99	PORTLAN	-14.340	-5.420	-8.920	-12.169
100	POTASSI	11.998	84.120	-72.122	-98.391
103	QUARTZ	-4.130	-3.930	-0.200	-0.273
110	SEPIOLIT	33.131	31.520	1.611	2.198
111	SILICAAM	-4.130	-2.700	-1.430	-1.951
112	SILICGEL	-4.130	-2.710	-1.420	-1.937
122	SrCO3	-9.861	-9.270	-0.591	-0.806
123	SYLVITE	-2.661	0.910	-3.571	-4.872
124	TALC	26.949	21.130	5.819	7.939
125	THENARDI	-3.677	-0.290	-3.387	-4.621
126	TREMOLIT	66.711	60.890	5.821	7.942
127	TRONA	-9.673	-0.630	-9.043	-12.337
128	VIVIANIT	-66.295	-36.000	-30.295	-41.330
130	WITHERIT	-12.675	-8.630	-4.045	-5.519
131	WOLLASTO	9.519	12.600	-3.081	-4.204
133	SILVER	-9.663	-0.500	-9.163	-12.501
134	AgCl	-14.686	-9.730	-4.956	-6.761
135	Ag2S	-23.977	-36.260	12.283	16.757
136	COPPER	-10.071	4.250	-14.321	-19.537
137	MALACHIT	-34.397	-33.580	-0.817	-1.114
138	CuO	7.557	7.670	-0.113	-0.155
139	Cu2O	-12.867	-1.900	-10.967	-14.962
140	CuS	-4.368	-22.830	18.462	25.186
141	Cu2S	-24.792	-34.950	10.158	13.858
142	CuFeS2	-14.139	-34.070	19.931	27.191
143	BORNITE	-63.723	-102.510	38.787	52.915
144	FeCl2	-15.166	7.900	-23.066	-31.468
145	FeCl3	-20.189	12.340	-32.529	-44.377
146	FeCO3	-19.368	-10.540	-8.828	-12.043
147	FeO	2.154	13.500	-11.346	-15.479
148	Fe2O3HEM	11.583	0.040	11.543	15.747
149	Fe2O3MGH	11.583	6.400	5.183	7.070
150	Fe3O4	13.736	10.750	2.986	4.074
151	Fe(OH)3	-36.191	-37.200	1.009	1.376
152	GOETHITE	5.787	0.480	5.307	7.240
153	FeSPYRHO	-9.771	-3.760	-6.011	-8.200
154	FeSTROLT	-9.771	-3.870	-5.901	-8.050
155	FeS2PYR	-23.477	-24.710	1.233	1.682
156	GREIGITE	-33.963	-45.000	11.037	15.057
157	Hg(L)	-14.979	-2.840	-12.139	-16.560
158	HgCl2(C)	-25.024	-14.110	-10.914	-14.889
160	HgO	-7.704	2.440	-10.144	-13.838
161	CINNABAR	-19.629	-39.860	20.231	27.601
162	CINABMET	-19.629	-38.580	18.951	25.854
163	MnCl2	-12.494	8.790	-21.284	-29.036
164	MnCO3	-16.696	-10.540	-6.156	-8.398
165	MnO	4.826	17.700	-12.874	-17.563
166	MnO2	-13.339	-8.330	-5.009	-6.834
167	MnS	-7.099	-0.470	-6.629	-9.043
168	PbCl2	-18.964	-4.820	-14.144	-19.296
169	PbCO3	-23.166	-12.890	-10.276	-14.019
170	PbOLITHR	-1.645	12.550	-14.195	-19.365
171	PbOMASIC	-1.645	12.690	-14.335	-19.556
172	PbS GALN	-13.569	-14.780	1.211	1.652
173	PbSO4	-20.696	-7.800	-12.896	-17.593
174	ZnCO3	-21.109	-9.870	-11.239	-15.333
175	ZnO	0.412	11.200	-10.788	-14.717

SAMPLE IDENT - Test Sample #4 - Ca/Mg exchange in seawater (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
118	Na2O	15.374	67.430	-52.056	-71.017	176	ZnS	-11.513	-11.790	0.277	0.379
121	STRENGIT	-30.570	-27.200	-3.370	-4.598	177	ZnSO4	-18.639	3.540	-22.179	-30.258

Initial Surface Conditions .....

Surface Complex	Moles on Surface	Moles of Surface Site	Fraction of Surface Sites
CaX2	0.25000E-01	0.50000E-01	0.5000
MgX2	0.25000E-01	0.50000E-01	0.5000

K Surface Comp. Species and Coef. ....

```
0.10000E+01 =  CaX2       * (Ca ++   ** -1.00) * (X-      ** -2.00)
0.10000E+01 =  MgX2       * (Mg ++   ** -1.00) * (X-      ** -2.00)
```

Final Equilibrium Surface Conditions .....

Surface Complex	Moles on Surface	Moles of Surface Site	Fraction of Surface Sites
CaX2	0.14040E-01	0.28079E-01	0.2808
MgX2	0.35960E-01	0.71921E-01	0.7192

CEC = 0.10000E+03 milli-equivalents
0.10000E+00 moles exchange capacity for monovalent cations and anions

SAMPLE IDENT:- Test Sample #4 - Ca/Mg exchange in seawater

PH	EH	TEMP		CATIONS	ANIONS	DIFFERENCE (MEQ/L)	--- H - OH BALANCE (MOLES) -------		
							HTOT	OHTOT	DIFFERENCE
8.19	0.5000	25.00	ANAL=	619.6745	618.2648	1.4097			
			CALC=	575.8476	568.1310	7.7167	0.2511E-02	0.1347E-02	0.1163E-02

DENSITY AT INPUT T	TOTAL DISSOLVED SOLIDS (MG/L)	IONIC STRENGTH	ACTIVITY OF WATER	PRESSURE P TOTAL (BARS)	PH2O (BARS)	PCO2 (BARS)	PH2S (BARS)	PCH4 (BARS)	PNH3 (BARS)
1.0230	35916.54	0.64588	0.9809	1.0000	0.3169E-01	0.4865E-03	0.1467E-03	0.5252E-02	0.0000E+00

	Total Alkalinity as			Dissolved Inorganic Carbon as	HCO3-	H2CO3	Sum of	Sum of
	HCO3-	CO3=	CaCO3	TIC	Alkalinity	species	HCO3-	CO3=
(MG/L)=	0.1594E+03	0.7840E+02	0.1308E+03	0.2485E+02	0.1375E+03	0.8799E+00	0.1128E+03	0.1235E+02
(PPM)=	0.1559E+03	0.7664E+02	0.1278E+03	0.2429E+02	0.1344E+03	0.8601E+00	0.1103E+03	0.1207E+02
(MOLALITY)=	0.2647E-02	0.1324E-02	0.1324E-02	0.2096E-02	0.2290E-02	0.1437E-04	0.1873E-02	0.2085E-03

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	CALCULATED ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
1	Ca ++	836.2569	855.4908	0.2162E-01	0.5762E+03	0.5895E+03	0.1490E-01	0.3667E-02	0.2461	2.4357
2	Mg ++	1034.8333	1058.6345	0.4411E-01	0.8953E+03	0.9159E+03	0.3817E-01	0.1008E-01	0.2642	1.9963
3	Na +	10770.0000	11017.7100	0.4855E+00	0.1024E+05	0.1048E+05	0.4617E+00	0.3099E+00	0.6712	0.5088
4	K +	399.1000	408.2793	0.1058E-01	0.3825E+03	0.3913E+03	0.1014E-01	0.6358E-02	0.6272	2.1967
5	Cl -	19350.0000	19795.0500	0.5657E+00	0.1866E+05	0.1908E+05	0.5454E+00	0.3421E+00	0.6272	0.4659
6	SO4 --	2712.0000	2774.3760	0.2926E-01	0.1226E+04	0.1254E+04	0.1322E-01	0.2235E-02	0.1690	2.6507
7	HCO3 -	123.4007	126.2389	0.2096E-02	0.8572E+02	0.8769E+02	0.1456E-02	0.1005E-02	0.6901	2.9980
8	H +				0.7736E-05	0.7914E-05	0.7954E-08	0.6390E-08	0.8034	8.1945
9	OH -				0.3964E-01	0.4055E-01	0.2415E-05	0.1571E-05	0.6503	5.8039
11	H4SiO4				0.6618E+01	0.6770E+01	0.7136E-04	0.7136E-04	1.0000	4.1465
12	SiO2	4.2800	4.3784	0.7382E-04						
13	Ag +	0.0000	0.0000	0.3843E-09	0.1050E-08	0.1074E-08	0.1009E-13	0.6066E-14	0.6015	14.2171
15	Ba ++	0.0200	0.0205	0.1509E-06	0.1811E-01	0.1853E-01	0.1367E-06	0.2848E-07	0.2084	7.5455
16	Cu +	0.0007	0.0007	0.1142E-07	0.2405E-09	0.2460E-09	0.3923E-14	0.2359E-14	0.6015	14.6272
17	Cu ++				0.3660E-03	0.3744E-03	0.5969E-08	0.1469E-08	0.2461	8.8330
18	Fe ++	0.0020	0.0020	0.3712E-07	0.1323E-08	0.1353E-08	0.2454E-13	0.6040E-14	0.2461	14.2189
19	Fe +3				0.1052E-12	0.1076E-12	0.1951E-17	0.1670E-18	0.0856	18.7773
21	Hg ++	0.0000	0.0000	0.1550E-09	0.7563E-18	0.7737E-18	0.3907E-23	0.8141E-24	0.2084	24.0893
22	Li +	0.1810	0.1852	0.2703E-04	0.1792E+00	0.1833E+00	0.2676E-04	0.1973E-04	0.7373	4.7049
23	Mn ++	0.0002	0.0002	0.3773E-08	0.4556E-06	0.4660E-06	0.8594E-11	0.2115E-11	0.2461	11.6747
24	Mn +3				0.6904E-23	0.7063E-23	0.1302E-27	0.1114E-28	0.0856	28.9529
25	Pb ++	0.0001	0.0001	0.2501E-09	0.9742E-12	0.9966E-12	0.4873E-17	0.9202E-18	0.1888	18.0361
26	Sr ++	8.1400	8.3272	0.9628E-04	0.7539E+01	0.7713E+01	0.8918E-04	0.1858E-04	0.2084	4.7309
27	Zn ++	0.0049	0.0050	0.7769E-07	0.2722E-10	0.2785E-10	0.4316E-15	0.1062E-15	0.2461	15.9738
28	H2AsO3-	0.0067	0.0068	0.5281E-07	0.7126E-03	0.7290E-03	0.5640E-08	0.3786E-08	0.6712	8.4218
29	PO4 -3	0.0600	0.0614	0.6548E-06	0.6480E-05	0.6629E-05	0.7071E-10	0.1922E-11	0.0272	11.7163
30	F -	1.3900	1.4220	0.7583E-04	0.8401E+00	0.8594E+00	0.4583E-04	0.2981E-04	0.6503	4.5257
31	B(OH)3	25.4540	26.0394	0.4266E-03	0.2209E+02	0.2260E+02	0.3702E-03	0.3702E-03	1.0000	3.4316
33	H2S	10.0000	10.2300	0.3041E-03	0.3732E+00	0.3818E+00	0.1135E-04	0.1181E-04	1.0407	4.9277
43	AgCl				0.5995E-06	0.6133E-06	0.4335E-11	0.4335E-11	1.0000	11.3630
44	AgCl2 -				0.3811E-04	0.3899E-04	0.2209E-09	0.1483E-09	0.6712	9.8289
45	AgCl3 --				0.3032E-04	0.3102E-04	0.1467E-09	0.3056E-10	0.2084	10.5148
46	AgCl4 -3				0.4020E-05	0.4113E-05	0.1669E-10	0.6596E-12	0.0395	12.1807
47	AgSO4 -				0.8115E-10	0.8301E-10	0.4124E-15	0.2768E-15	0.6712	15.5578

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
48	CH3COO -	0.1000	0.1023	0.1755E-05	0.7300E-01	0.7468E-01	0.1281E-05	0.8842E-06	0.6901	6.0534
49	H3AsO3				0.5732E-02	0.5864E-02	0.4717E-07	0.4717E-07	1.0000	7.3263
51	BaCO3				0.1261E-04	0.1290E-04	0.6623E-10	0.6623E-10	1.0000	10.1790
52	BaHCO3 +				0.2247E-03	0.2299E-03	0.1174E-08	0.7880E-09	0.6712	9.1035
53	BaOH +				0.3192E-07	0.3265E-07	0.2143E-12	0.1516E-12	0.7072	12.8194
54	BaSO4				0.2927E-02	0.2994E-02	0.1300E-07	0.1300E-07	1.0000	7.8862
55	CaCO3				0.4322E+01	0.4421E+01	0.4475E-04	0.4475E-04	1.0000	4.3492
56	CaHCO3 +				0.6279E+01	0.6424E+01	0.6437E-04	0.4746E-04	0.7373	4.3237
57	CaOH +				0.5940E-02	0.6077E-02	0.1078E-06	0.7951E-07	0.7373	7.0996
58	CaPO4 -				0.3765E-02	0.3851E-02	0.2889E-07	0.2080E-07	0.7199	7.6820
59	CaHPO4				0.5269E-02	0.5390E-02	0.4013E-07	0.4013E-07	1.0000	7.3965
60	CaH2PO4+				0.5049E-04	0.5165E-04	0.3817E-09	0.2748E-09	0.7199	9.5610
61	CaSO4				0.2148E+03	0.2197E+03	0.1635E-02	0.1635E-02	1.0000	2.7864
62	CuCl				0.3863E-07	0.3952E-07	0.4045E-12	0.4045E-12	1.0000	12.3931
63	CuCl2 -				0.4647E-05	0.4754E-05	0.3582E-10	0.2404E-10	0.6712	10.6190
64	CuCl3 --				0.1026E-04	0.1049E-04	0.6256E-10	0.1303E-10	0.2084	10.8849
65	CuCl +				0.7488E-04	0.7661E-04	0.7840E-09	0.5262E-09	0.6712	9.2789
66	CuCl2				0.4348E-05	0.4448E-05	0.3351E-10	0.3351E-10	1.0000	10.4748
67	CuCl3 -				0.7197E-07	0.7363E-07	0.4390E-12	0.2947E-12	0.6712	12.5307
68	CuCl4 --				0.4804E-09	0.4914E-09	0.2425E-14	0.5052E-15	0.2084	15.2966
69	CuOH +				0.3068E-03	0.3139E-03	0.3948E-08	0.2650E-08	0.6712	8.5768
70	CuSO4				0.8991E-04	0.9198E-04	0.5838E-09	0.5838E-09	1.0000	9.2337
71	FeCl +				0.8003E-10	0.8187E-10	0.9085E-15	0.6098E-15	0.6712	15.2148
72	FeCl2				0.5330E-18	0.5452E-18	0.4358E-23	0.4358E-23	1.0000	23.3607
73	FeHPO4				0.9464E-13	0.9682E-13	0.6461E-18	0.6461E-18	1.0000	18.1897
74	H3PO4				0.2322E-09	0.2376E-09	0.2456E-14	0.2456E-14	1.0000	14.6098
75	FeOH +				0.2982E-10	0.3051E-10	0.4243E-15	0.3000E-15	0.7072	15.5228
76	Fe(OH)2				0.3172E-13	0.3245E-13	0.3659E-18	0.3659E-18	1.0000	18.4367
77	FeOOH -				0.2700E-13	0.2762E-13	0.3149E-18	0.2227E-18	0.7072	18.6522
78	FeSO4				0.5326E-09	0.5448E-09	0.3633E-14	0.3633E-14	1.0000	14.4397
79	FeCl ++				0.7127E-12	0.7291E-12	0.8090E-17	0.1686E-17	0.2084	17.7732
80	FeCl2 +				0.4558E-12	0.4662E-12	0.3726E-17	0.2635E-17	0.7072	17.5791
81	FeCl3				0.1411E-13	0.1443E-13	0.9015E-19	0.9015E-19	1.0000	19.0450
82	FeCl4 -				0.1053E-15	0.1078E-15	0.5523E-21	0.3707E-21	0.6712	21.4309
83	FeSO4 +				0.1068E-11	0.1092E-11	0.7284E-17	0.5151E-17	0.7072	17.2881
84	FeSO4)2-				0.1130E-23	0.1156E-23	0.4724E-29	0.3171E-29	0.6712	29.4988
85	FeOH ++				0.6411E-07	0.6558E-07	0.9120E-12	0.1900E-12	0.2084	12.7212
86	Fe(OH)2+				0.3764E-04	0.3851E-04	0.4342E-09	0.3125E-09	0.7199	9.5051
87	Fe(OH)3				0.2110E-02	0.2159E-02	0.2047E-07	0.2047E-07	1.0000	7.6890
88	Fe(OH)4-				0.1938E-02	0.1983E-02	0.1621E-07	0.1167E-07	0.7199	7.9328
89	B(OH)4 -				0.4293E+01	0.4391E+01	0.5643E-04	0.3424E-04	0.6068	4.4654
90	H2SiO4--				0.2094E-03	0.2142E-03	0.2306E-08	0.5158E-09	0.2237	9.2876
91	H3SiO4 -				0.2258E+00	0.2310E+00	0.2461E-05	0.1652E-05	0.6712	5.7820
92	HAsO3 --				0.1147E-07	0.1174E-07	0.9151E-13	0.1907E-13	0.2084	13.7197
96	HF				0.5565E-05	0.5693E-05	0.2883E-09	0.2883E-09	1.0000	9.5402
97	H2CO3				0.8601E+00	0.8799E+00	0.1437E-04	0.1437E-04	1.0000	4.8425
98	CO3 --				0.1904E+01	0.1947E+01	0.3288E-04	0.7354E-05	0.2237	5.1335
99	HPO4 --				0.1194E-01	0.1222E-01	0.1289E-06	0.2687E-07	0.2084	7.5708
100	H2PO4 -				0.3537E-03	0.3618E-03	0.3780E-08	0.2721E-08	0.7199	8.5653
101	HS -				0.9069E+01	0.9278E+01	0.2842E-03	0.1848E-03	0.6503	3.7332
102	S --				0.4295E-07	0.4394E-07	0.1388E-11	0.2892E-12	0.2084	12.5387
103	HSO4 -				0.1728E-03	0.1767E-03	0.1844E-08	0.1273E-08	0.6901	8.8952
104	HNO3				0.4389E-10	0.4490E-10	0.7218E-15	0.7218E-15	1.0000	15.1416

	SPECIES	ANALYZED PPM	ANALYZED MG/L	ANALYZED MOLALITY	CALCULATED PPM	CALCULATED MG/L	CALCULATED MOLALITY	ACTIVITY	ACTIVITY COEFF.	-LOG10 ACTIVITY
105	HgCl +				0.1680E-12	0.1719E-12	0.7378E-18	0.4952E-18	0.6712	18.3052
106	HgCl2				0.4541E-06	0.4645E-06	0.1733E-11	0.1733E-11	1.0000	11.7611
107	HgCl3 -				0.3219E-04	0.3293E-04	0.1087E-09	0.7294E-10	0.6712	10.1370
108	HgCl4 --				0.1470E-04	0.1504E-04	0.4449E-10	0.9270E-11	0.2084	11.0329
109	HgSO4				0.1308E-19	0.1338E-19	0.4570E-25	0.4570E-25	1.0000	25.3400
111	Hg(HS)3-				0.2374E-07	0.2429E-07	0.8207E-13	0.5508E-13	0.6712	13.2590
113	KCl				0.2062E+02	0.2110E+02	0.2867E-03	0.2867E-03	1.0000	3.5426
114	KCO3 -				0.7923E-01	0.8105E-01	0.8285E-06	0.5494E-06	0.6631	6.2601
115	KHSO4				0.7528E-05	0.7701E-05	0.5729E-10	0.5729E-10	1.0000	10.2419
116	KSO4 -				0.1998E+02	0.2044E+02	0.1532E-03	0.1103E-03	0.7199	3.9574
117	KHPO4 -				0.6030E-04	0.6169E-04	0.4627E-09	0.3331E-09	0.7199	9.4775
118	LiOH				0.1084E-05	0.1109E-05	0.4691E-10	0.4691E-10	1.0000	10.3287
119	LiSO4 -				0.2705E-01	0.2767E-01	0.2722E-06	0.1925E-06	0.7072	6.7156
120	MgCO3				0.5762E+01	0.5895E+01	0.7082E-04	0.7082E-04	1.0000	4.1498
121	MgHCO3 +				0.1460E+02	0.1494E+02	0.1774E-03	0.1190E-03	0.6712	3.9243
122	MgF +				0.1203E+01	0.1230E+01	0.2878E-04	0.1986E-04	0.6901	4.7020
123	MgOH +				0.3350E+00	0.3427E+00	0.8403E-05	0.6307E-05	0.7505	5.2002
124	MgSO4				0.6576E+03	0.6727E+03	0.5661E-02	0.5661E-02	1.0000	2.2471
125	MgPO4 -				0.9144E-02	0.9355E-02	0.7945E-07	0.5720E-07	0.7199	7.2426
126	MgHPO4				0.4051E-01	0.4144E-01	0.3490E-06	0.3490E-06	1.0000	6.4571
127	MgH2PO4+				0.1229E-03	0.1257E-03	0.1050E-08	0.7558E-09	0.7199	9.1216
128	MnCl +				0.2973E-13	0.3041E-13	0.3408E-18	0.2288E-18	0.6712	18.6406
129	MnCl2				0.2387E-10	0.2442E-10	0.1966E-15	0.1966E-15	1.0000	15.7065
130	MnCl3 -				0.3916E-09	0.4006E-09	0.2516E-14	0.1689E-14	0.6712	14.7724
131	MnCl4 --				0.4181E-08	0.4277E-08	0.2202E-13	0.4589E-14	0.2084	14.3383
132	MnHCO3 +				0.6596E-08	0.6747E-08	0.5895E-13	0.3957E-13	0.6712	13.4027
133	MnSO4				0.1253E-06	0.1282E-06	0.8601E-12	0.8601E-12	1.0000	12.0654
134	MnHPO4				0.3146E-10	0.3218E-10	0.2160E-15	0.2160E-15	1.0000	15.6655
135	MnOH +				0.9464E-09	0.9682E-09	0.1363E-13	0.9150E-14	0.6712	14.0386
136	NO3 -	0.2900	0.2967	0.4847E-05	0.2900E+00	0.2967E+00	0.4847E-05	0.3040E-05	0.6272	5.5171
137	NaCl				0.8443E+03	0.8638E+03	0.1497E-01	0.1497E-01	1.0000	1.8247
138	NaCO3 -				0.4721E+01	0.4829E+01	0.5895E-04	0.4243E-04	0.7199	4.3723
139	NaHCO3				0.1419E+02	0.1452E+02	0.1751E-03	0.1751E-03	1.0000	3.7568
140	Na2CO3				0.1509E-01	0.1544E-01	0.1475E-06	0.1475E-06	1.0000	6.8311
141	Na2SO4				0.9519E+03	0.9737E+03	0.6945E-02	0.6945E-02	1.0000	2.1583
142	NaSO4 -				0.1877E+03	0.1920E+03	0.1634E-02	0.1176E-02	0.7199	2.9295
143	NaHPO4 -				0.2589E-02	0.2648E-02	0.2255E-07	0.1623E-07	0.7199	7.7896
144	NaF				0.4933E-01	0.5046E-01	0.1218E-05	0.1218E-05	1.0000	5.9145
145	NaHS				0.4583E+00	0.4688E+00	0.8472E-05	0.8472E-05	1.0000	5.0720
148	PbCl +				0.2822E-11	0.2887E-11	0.1205E-16	0.8091E-17	0.6712	17.0920
149	PbCl2				0.2696E-11	0.2758E-11	0.1005E-16	0.1005E-16	1.0000	16.9979
150	PbCl3 -				0.7588E-12	0.7762E-12	0.2508E-17	0.1683E-17	0.6712	17.7738
151	PbCl4 --				0.5872E-12	0.6007E-12	0.1744E-17	0.3633E-18	0.2084	18.4397
152	PbSO4				0.3384E-12	0.3462E-12	0.1157E-17	0.1157E-17	1.0000	17.9369
153	MnCl ++				0.6501E-21	0.6650E-21	0.7454E-26	0.1553E-26	0.2084	26.8088
154	SrOH -				0.2041E-04	0.2087E-04	0.2021E-09	0.1429E-09	0.7072	9.8448
155	SrCO3				0.1286E-01	0.1316E-01	0.9028E-07	0.9028E-07	1.0000	7.0444
156	SrHCO3 +				0.6178E-01	0.6320E-01	0.4308E-06	0.2891E-06	0.6712	6.5389
157	SrSO4				0.1166E+01	0.1193E+01	0.6581E-05	0.6581E-05	1.0000	5.1817
158	ZnCl +				0.1385E-10	0.1417E-10	0.1424E-15	0.9556E-16	0.6712	16.0197
159	ZnCl2				0.6812E-11	0.6968E-11	0.5180E-16	0.5180E-16	1.0000	16.2856
160	ZnCl3 -				0.2296E-11	0.2349E-11	0.1386E-16	0.9299E-17	0.6712	17.0315
161	ZnCl4 --				0.2111E-11	0.2160E-11	0.1056E-16	0.2201E-17	0.2084	17.6574

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
162	ZnSO4				0.5996E-11	0.6134E-11	0.3850E-16	0.3850E-16	1.0000	16.4146
165	HgOH +				0.1154E-13	0.1180E-13	0.5495E-19	0.3688E-19	0.6712	19.4332
166	Hg(OH)2				0.3371E-08	0.3449E-08	0.1489E-13	0.1489E-13	1.0000	13.8271
228	CH3COOH				0.1884E-04	0.1927E-04	0.3251E-09	0.3251E-09	1.0000	9.4879
230	BaAce +				0.9328E-07	0.9542E-07	0.4923E-12	0.3397E-12	0.6901	12.4689
231	CaAce +				0.7632E-02	0.7808E-02	0.7980E-07	0.5506E-07	0.6901	7.2591
232	CuAce +				0.2776E-13	0.2840E-13	0.2347E-18	0.1619E-18	0.6901	18.7906
233	FeAce +				0.1712E-12	0.1751E-12	0.1544E-17	0.1066E-17	0.6901	17.9724
234	Fe(Ace)2				0.9978E-20	0.1021E-19	0.5945E-25	0.5945E-25	1.0000	25.2258
235	KAce				0.2169E-03	0.2219E-03	0.2290E-08	0.2290E-08	1.0000	8.6401
236	MgAce +				0.1848E-01	0.1891E-01	0.2298E-06	0.1586E-06	0.6901	6.7998
237	NaAce				0.1277E-01	0.1307E-01	0.1613E-06	0.1613E-06	1.0000	6.7922
238	PbAce +				0.5512E-16	0.5639E-16	0.2146E-21	0.1481E-21	0.6901	21.8296
239	Pb(Ace)2				0.9857E-21	0.1008E-20	0.3141E-26	0.3141E-26	1.0000	26.5030
240	Pb(Ace)3				0.1794E-26	0.1835E-26	0.4838E-32	0.3339E-32	0.6901	32.4764
241	SrAce +				0.4870E-04	0.4982E-04	0.3441E-09	0.2375E-09	0.6901	9.6244
244	ZnAce +				0.1328E-11	0.1359E-11	0.1106E-16	0.7634E-17	0.6901	17.1173
245	Zn(Ace)2				0.3291E-21	0.3366E-21	0.1859E-26	0.1859E-26	1.0000	26.7307
246	C2O4 --	0.1000	0.1023	0.1177E-05	0.1070E-01	0.1094E-01	0.1260E-06	0.2818E-07	0.2237	7.5501
247	HC2O4 -				0.3986E-09	0.4078E-09	0.4640E-14	0.3202E-14	0.6901	14.4946
248	H2C2O4				0.3629E-13	0.3713E-13	0.4178E-18	0.4178E-18	1.0000	18.3791
251	BaOxy				0.6483E-08	0.6632E-08	0.2981E-13	0.2981E-13	1.0000	13.5256
252	CaOxy				0.1277E-01	0.1307E-01	0.1033E-06	0.1033E-06	1.0000	6.9858
253	FeOxy				0.5935E-12	0.6071E-12	0.4275E-17	0.4275E-17	1.0000	17.3690
254	FeOxy +				0.3589E-13	0.3672E-13	0.2586E-18	0.1784E-18	0.6901	18.7485
255	KOxy -				0.1596E-03	0.1633E-03	0.1301E-08	0.8979E-09	0.6901	9.0468
256	MgOxy				0.9090E-01	0.9299E-01	0.8386E-06	0.8386E-06	1.0000	6.0764
257	MnOxy				0.8220E-10	0.8409E-10	0.5959E-15	0.5959E-15	1.0000	15.2248
258	MnOxy)2				0.7185E-03	0.7350E-03	0.3763E-08	0.8416E-09	0.2237	9.0749
259	MnOxy)3				0.1751E-06	0.1791E-06	0.7178E-12	0.1496E-14	0.0021	14.8250
260	MnOxy				0.2438E-19	0.2494E-19	0.1768E-24	0.1220E-24	0.6901	24.9138
261	NaOxy -				0.1077E-01	0.1101E-01	0.1005E-06	0.6936E-07	0.6901	7.1589
262	PbOxy				0.4059E-15	0.4152E-15	0.1425E-20	0.1425E-20	1.0000	20.8462
263	SrOxy				0.3077E-04	0.3147E-04	0.1815E-09	0.1815E-09	1.0000	9.7410
264	ZnOxy				0.3518E-13	0.3599E-13	0.2377E-18	0.2377E-18	1.0000	18.6239
265	C4H4O4--	0.1000	0.1023	0.8929E-06	0.6493E-01	0.6642E-01	0.5798E-06	0.1297E-06	0.2237	6.8871
266	HC4H4O4-				0.2200E-05	0.2251E-05	0.1948E-10	0.1344E-10	0.6901	10.8716
267	H2C4H4O4				0.4271E-08	0.4370E-08	0.3749E-13	0.3749E-13	1.0000	13.4261
270	BaSuc				0.9456E-07	0.9673E-07	0.3867E-12	0.3867E-12	1.0000	12.4126
271	CaSuc				0.7165E-02	0.7329E-02	0.4755E-07	0.4755E-07	1.0000	7.3228
272	FeSuc				0.2059E-13	0.2107E-13	0.1241E-18	0.1241E-18	1.0000	18.9061
273	FeSuc +				0.5205E-13	0.5325E-13	0.3138E-18	0.2165E-18	0.6901	18.6645
274	KSuc -				0.3570E-03	0.3652E-03	0.2384E-08	0.1645E-08	0.6901	8.7838
275	MgSuc				0.1988E-01	0.2033E-01	0.1467E-06	0.1467E-06	1.0000	6.8335
276	MnSuc				0.6694E-11	0.6848E-11	0.4057E-16	0.4057E-16	1.0000	16.3918
277	NaSuc -				0.1559E-01	0.1595E-01	0.1162E-06	0.8018E-07	0.6901	7.0959
278	PbSuc				0.1177E-15	0.1204E-15	0.3774E-21	0.3774E-21	1.0000	21.4232
279	SrSuc				0.4736E-04	0.4845E-04	0.2409E-09	0.2409E-09	1.0000	9.6181
280	ZnSuc				0.6954E-15	0.7114E-15	0.3972E-20	0.3972E-20	1.0000	20.4010
281	CaCl +				0.3582E+03	0.3665E+03	0.4915E-02	0.3299E-02	0.6712	2.4816
282	CaCl2				0.6796E+01	0.6952E+01	0.6346E-04	0.6346E-04	1.0000	4.1975
283	FeF ++				0.1725E-11	0.1765E-11	0.2389E-16	0.4977E-17	0.2084	17.3030
284	SiF6 --				0.2147E-28	0.2196E-28	0.1566E-33	0.3262E-34	0.2084	34.4865

		ANALYZED			CALCULATED				ACTIVITY	-LOG10
	SPECIES	PPM	MG/L	MOLALITY	PPM	MG/L	MOLALITY	ACTIVITY	COEFF.	ACTIVITY
285	CH4 Gas	0.1000	0.1023	0.6460E-05	0.1000E+00	0.1023E+00	0.6460E-05	0.0000E+00	1.0000	0.0000
286	Pb(HS)2				0.6586E-04	0.6737E-04	0.2497E-09	0.2497E-09	1.0000	9.6026
287	Pb(HS)3-				0.1170E-06	0.1197E-06	0.3957E-12	0.2656E-12	0.6712	12.5758
288	PbCO3				0.1745E-10	0.1785E-10	0.6767E-16	0.6767E-16	1.0000	16.1696
289	PbOH +				0.3078E-10	0.3149E-10	0.1423E-15	0.9550E-16	0.6712	16.0200
290	Zn(HS)2				0.2774E-04	0.2838E-04	0.2186E-09	0.2186E-09	1.0000	9.6603
291	Zn(HS)3-				0.1414E-05	0.1447E-05	0.8905E-11	0.5977E-11	0.6712	11.2235
292	ZnHCO3 +				0.5100E-12	0.5217E-12	0.4182E-17	0.2807E-17	0.6712	17.5518
293	ZnOH +				0.2166E-11	0.2216E-11	0.2726E-16	0.1829E-16	0.6712	16.7377
294	Zn(OH)2				0.9555E-13	0.9774E-13	0.9964E-18	0.9964E-18	1.0000	18.0016
295	ZnHSOH				0.8628E-02	0.8827E-02	0.7746E-07	0.7746E-07	1.0000	7.1109

SAMPLE IDENT - Test Sample #4 - Ca/Mg exchange in seawater (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
2	AKERMANI	34.015	45.460	-11.445	-15.614	122	SrCO3	-9.864	-9.270	-0.594	-0.811
11	ANHYDRIT	-5.086	-4.330	-0.756	-1.032	123	SYLVITE	-2.663	0.910	-3.573	-4.874
14	APATCHLR	-47.793	-66.150	18.357	25.043	124	TALC	26.625	21.130	5.495	7.497
15	APATFLUR	-51.853	-68.340	16.487	22.492	125	THENARDI	-3.668	-0.290	-3.378	-4.609
16	APATHYDX	-53.131	-60.390	7.259	9.903	126	TREMOLIT	66.764	60.890	5.874	8.014
17	ARAGONIT	-7.569	-8.340	0.771	1.052	127	TRONA	-9.675	-0.630	-9.045	-12.339
19	AZURITE	-48.374	-39.460	-8.914	-12.160	128	VIVIANIT	-66.156	-36.000	-30.156	-41.140
20	BARITE	-10.196	-9.960	-0.236	-0.322	130	WITHERIT	-12.679	-8.630	-4.049	-5.524
22	BRUCITE	-13.604	-11.470	-2.134	-2.911	131	WOLLASTO	9.815	12.600	-2.785	-3.799
24	CALCITE	-7.569	-8.480	0.911	1.243	133	SILVER	-9.659	-0.500	-9.159	-12.495
25	CELESTIT	-7.382	-6.430	-0.952	-1.298	134	AgCl	-14.683	-9.730	-4.953	-6.757
26	CHALCEDO	-4.130	-3.730	-0.400	-0.545	135	Ag2S	-23.973	-36.260	12.287	16.762
30	CRYSOTIL	34.877	32.030	2.847	3.883	136	COPPER	-10.069	4.250	-14.319	-19.534
31	C-ENSTAT	10.254	11.290	-1.036	-1.413	137	MALACHIT	-34.407	-33.580	-0.827	-1.128
37	CRISTOBA	-4.130	-3.540	-0.590	-0.805	138	CuO	7.548	7.670	-0.122	-0.167
38	CRISTOBB	-4.130	-2.940	-1.190	-1.623	139	Cu2O	-12.874	-1.900	-10.974	-14.971
40	DIOPSIDE	20.070	19.630	0.440	0.600	140	CuS	-4.372	-22.830	18.458	25.182
41	DOLOMITE	-14.699	-18.060	3.361	4.585	141	Cu2S	-24.793	-34.950	10.157	13.856
42	DSORD	-14.699	-16.520	1.821	2.484	142	CuFeS2	-14.129	-34.070	19.941	27.204
43	ENSTATIT	10.254	11.470	-1.216	-1.658	143	BORNITE	-63.716	-102.510	38.794	52.925
45	FAYALITE	0.194	19.430	-19.236	-26.243	144	FeCl2	-15.151	7.900	-23.051	-31.447
46	FLUORITE	-11.487	-10.960	-0.527	-0.719	145	FeCl3	-20.175	12.340	-32.515	-44.358
47	FORSTERI	24.639	29.070	-4.431	-6.045	146	FeCO3	-19.352	-10.540	-8.812	-12.022
50	GREENALI	-1.791	22.580	-24.371	-33.248	147	FeO	2.162	13.500	-11.338	-15.468
51	GYPSUM	-5.103	-4.600	-0.503	-0.686	148	Fe2O3HEM	11.587	0.040	11.547	15.753
52	HALITE	-0.975	1.590	-2.565	-3.499	149	Fe2O3MGH	11.587	6.400	5.187	7.077
55	HUNTITE	-28.959	-30.620	1.661	2.266	150	Fe3O4	13.749	10.750	2.999	4.091
56	HYDRMAGN	-37.015	-38.530	1.515	2.067	151	Fe(OH)3	-36.189	-37.200	1.011	1.379
57	HYPHILIT	-3.367	11.800	-15.167	-20.692	152	GOETHITE	5.789	0.480	5.309	7.243
60	KENYAITE	-37.788	-25.000	-12.788	-17.446	153	FeSPYRHO	-9.758	-3.760	-5.998	-8.182
64	LARNITE	23.760	38.880	-15.120	-20.627	154	FeSTROLT	-9.758	-3.870	-5.888	-8.032
67	LIME	-18.833	32.660	-51.493	-70.249	155	FeS2PYR	-23.455	-24.710	1.255	1.712
68	MAGADITE	-21.265	-14.340	-6.925	-9.447	156	GREIGITE	-33.929	-45.000	11.071	15.104
69	MgFe2O4	25.971	21.100	4.871	6.646	157	Hg(L)	-14.973	-2.840	-12.133	-16.552
70	MAGNESIT	-7.130	-8.050	0.920	1.255	158	HgCl2(C)	-25.021	-14.110	-10.911	-14.885
71	MgCl2	-2.928	22.150	-25.078	-34.213	160	HgO	-7.709	2.440	-10.149	-13.845
73	MERWINIT	47.959	68.170	-20.211	-27.572	161	CINNABAR	-19.628	-39.860	20.232	27.601
76	MIRABILT	-3.752	-1.090	-2.662	-3.632	162	CINABMET	-19.628	-38.580	18.952	25.855
77	MONTICEL	24.199	30.150	-5.951	-8.118	163	MnCl2	-12.607	8.790	-21.397	-29.190
81	NACHOLIT	-3.507	-0.430	-3.077	-4.197	164	MnCO3	-16.808	-10.540	-6.268	-8.551
82	NATRTHRM	-6.159	-0.010	-6.149	-8.389	165	MnO	4.706	17.700	-12.994	-17.727
83	NATRON	-6.235	-0.880	-5.355	-7.305	166	MnO2	-13.470	-8.330	-5.140	-7.012
85	NESQUHON	-7.155	-5.350	-1.805	-2.462	167	MnS	-7.213	-0.470	-6.743	-9.200
91	OLDHAMIT	2.026	11.900	-9.874	-13.471	168	PbCl2	-18.968	-4.820	-14.148	-19.301
95	PERICLAS	14.384	21.510	-7.126	-9.721	169	PbCO3	-23.170	-12.890	-10.280	-14.024
99	PORTLAN	-14.043	-5.420	-8.623	-11.764	170	PbOLITHR	-1.655	12.550	-14.205	-19.380
100	POTASSI	11.987	84.120	-72.133	-98.406	171	PbOMASIC	-1.655	12.690	-14.345	-19.571
103	QUARTZ	-4.130	-3.930	-0.200	-0.273	172	PbS GALN	-13.575	-14.780	1.205	1.644
110	SEPIOLIT	32.700	31.520	1.180	1.609	173	PbSO4	-20.687	-7.800	-12.887	-17.581
111	SILICAAM	-4.130	-2.700	-1.430	-1.951	174	ZnCO3	-21.107	-9.870	-11.237	-15.330
112	SILICGEL	-4.130	-2.710	-1.420	-1.937	175	ZnO	0.407	11.200	-10.793	-14.725

SAMPLE IDENT - Test Sample #4 - Ca/Mg exchange in seawater (TEMPERATURE = 25.00)

	PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG		PHASE	LOG (AP)	LOG (KT)	LOG (AP/KT)	DELG
118	Na2O	15.363	67.430	-52.067	-71.032	176	ZnS	-11.513	-11.790	0.277	0.378
121	STRENGIT	-30.510	-27.200	-3.310	-4.516	177	ZnSO4	-18.625	3.540	-22.165	-30.238

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Pg 207 follows

APPENDIX IV. Listing of SOLMINEQ.88

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      PROGRAM SOLMIN                                                        SOL 0010
C =====================================================================|SOL 0020
C     Program SOLMINEQ.88 : SOLution-MINeral EQuilibrium  1/11/89 JDD  |SOL 0030
C                                                                       |SOL 0040
C     Written by:          P.K. Aggarwal (now at Battelle)              |SOL 0050
C                          J.D. DeBraal  (U.S. Geological Survey)       |SOL 0060
C                          W.D. Gunter   (Alberta Research Council)     |SOL 0070
C                          R.W. Hull     (U.S. Geological Survey)       |SOL 0080
C                          Y.K. Kharaka  (U.S. Geological Survey)       |SOL 0090
C                          E.H. Perkins  (Alberta Research Council)     |SOL 0100
C                          D.J. Specht   (U.S. Geological Survey)       |SOL 0110
C                                                                       |SOL 0120
C     SOLMINEQ.88 is based on SOLMNEQ (Kharaka and Barnes, 1973),       |SOL 0130
C     SOLMNEQF (Aggarwal and others, 1986), and many other unpublished  |SOL 0140
C     versions.                                                         |SOL 0150
C                                                                       |SOL 0160
C     This version has been extensively re-written and modified by      |SOL 0170
C     E.H. Perkins.  The input format was redesigned in conjunction     |SOL 0180
C     with W.D. Gunter and Y.K. Kharaka; these changes were             |SOL 0190
C     implemented by J.D. DeBraal.                                      |SOL 0200
C                                                                       |SOL 0210
C     Financial support for designing SOLMINEQ.88 was provided by       |SOL 0220
C     Brian Hitchon (Alberta Geological Survey) and by the Oil Sands    |SOL 0230
C     and Hydrocarbon Recovery department, Alberta Research Council.    |SOL 0240
C                                                                       |SOL 0250
C     Input/output units:                                               |SOL 0260
C          5: Sample input file                                         |SOL 0270
C          6: Output from solmineq.88                                   |SOL 0280
C          7: Data file for Pitzer's equations                          |SOL 0290
C         10: Main data file for solmineq.88                            |SOL 0300
C         12: Data file for dissolution reactions of the minerals       |SOL 0310
C                                                                       |SOL 0320
C     Routines and their purpose                                        |SOL 0330
C                                                                       |SOL 0340
C     ACTIVE :  Calculate and print activity products of minerals       |SOL 0350
C     ADSORB :  Routine for calculating surface adsorption              |SOL 0360
C                 and ion exchange                                      |SOL 0370
C     AITLIM :  Determines the maximum stepsize for convergence on the  |SOL 0380
C                 anions                                                |SOL 0390
C     CALCUL :  Calculate analyzed molality, cation-anion balance,      |SOL 0400
C               stoichiometric ionic strength, activity coefficients    |SOL 0410
C               of neutral species, temperature effects on debye-huckel |SOL 0420
C               constants, and bdot.                                    |SOL 0430
C     CO2OPT :  Routine for titrating co2 to a given criterion          |SOL 0440
C                 (pH, pco2, m(h2co3), or saturation with calcite,      |SOL 0450
C                 siderite, or dolomite)                                |SOL 0460
C     DISTRB :  Calculate the distribution of species                   |SOL 0470
C     DPVT   :  Calculate the vapor pressure and vapor density          |SOL 0480
C     GASES  :  Routine for partitioning of a gas phase (co2/ch4)       |SOL 0490
C               Between liquid, oil, and vapor                          |SOL 0500
C     GUESS  :  Routine for calculating the root of a function which    |SOL 0510
C                 is known to change sign in a given interval           |SOL 0520
C     INPUT  :  Read sample input file from unit 5                      |SOL 0530
C     INTIAL :  Initialize several variable to 0.0 or default values    |SOL 0540
C     LAGINT :  Calculate logk values for aqueous complexes and         |SOL 0550
C                 minerals at the desired temperature (t)               |SOL 0560
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C     MIXER  :  Routine for precipitation/dissolution, mixing, boiling |SOL 0570
C     NACALC :  Calculate the osmotic coefficient of NaCl (aq) and     |SOL 0580
C                 pure water                                           |SOL 0590
C     PAGE   :  Keeps track of output paging                           |SOL 0600
C     PCLOGK :  Calculate the effect of pressure on logk if pressure   |SOL 0610
C                 is greater than ph2o                                 |SOL 0620
C     PHCALC :  Routine for calculating pH at a higher temperature     |SOL 0630
C     PHOPT  :  Routine for the pH option (adjust pH to saturation     |SOL 0640
C                 with calcite or siderite or dolomite)                |SOL 0650
C     PITZER :  Calculate the activity of aqueous species and the      |SOL 0660
C                 osmotic coefficient based up the pitzer ion pairing  |SOL 0670
C                 model                                                |SOL 0680
C     POLY   :  Solves the cubic equation which describes the          |SOL 0690
C                 partitioning between gas, oil, and water.            |SOL 0700
C     PRATIO :  Print mole ratio, log of activity ratio, and           |SOL 0710
C                 calculated subsurface temperatures                   |SOL 0720
C     PRINTR :  Print calculated distribution of species               |SOL 0730
C     PRNTAB :  Print the calculated values of aqueous log k           |SOL 0740
C     PSAT   :  Calculate the vapor saturated pressure of water (ph2o) |SOL 0750
C                 at temperature t                                     |SOL 0760
C     PTZINT :  Calculate the parameters for the pitzer equation as a  |SOL 0770
C                 function of temperature                              |SOL 0780
C     SORTA  :  Sorts arrays                                           |SOL 0790
C     STORE  :  Creates the restart file                               |SOL 0800
C     TABLES :  Read main data file from unit 10                       |SOL 0810
C     WAPVT  :  Calculate the properties of pure water                 |SOL 0820
C     WDBP   :  Calculate the dielectric properties of water           |SOL 0830
C                                                                      |SOL 0840
C     Functions                                                        |SOL 0850
C                                                                      |SOL 0860
C     ATCPRD :  Calculates the activity product of a mineral           |SOL 0870
C     DEBYE  :  Determines the value of an unknown ion size parameter  |SOL 0880
C     GETUNT :  Return the unit number of a file                       |SOL 0890
C     KHCH4  :  Calculate the Henry's law constant for CH4             |SOL 0900
C     KHCO2  :  Calculate the Henry's law constant for CO2             |SOL 0910
C     KHH2S  :  Calculate the Henry's law constant for H2S             |SOL 0920
C     KHNH3  :  Calculate the Henry's law constant for NH3             |SOL 0930
C     LENGTH :  Determines the length of a character string            |SOL 0940
C     SEXP10 :  Substitute exponetial function                         |SOL 0950
C     SLOG10 :  Substitute common log function                         |SOL 0960
C -----------------------------------------------------------------------|SOL 0970
C     Declare constants                                                |SOL 0980
C ---------------------                                                |SOL 0990
C     CPUMAX    DBL   Largest positive real value program uses         |SOL 1000
C     CPUMIN    DBL   Smallest positive real value program uses        |SOL 1010
C     NMAX      INT   General array dimension to allow easy expansion  |SOL 1020
C     UNI       INT   File unit assigned for input file                |SOL 1030
C     UNO       INT   File unit assigned for output file               |SOL 1040
C -----------------------------------------------------------------------|SOL 1050
      INTEGER NMAX, UNI, UNO                                            SOL 1060
      DOUBLE PRECISION CPUMAX, CPUMIN                                   SOL 1070
      PARAMETER (NMAX = 340, UNI = 5, UNO = 6)                          SOL 1080
      PARAMETER (CPUMAX = 1.0D+35, CPUMIN = 1.0D-35)                    SOL 1090
                                                                        SOL 1100
C -----------------------------------------------------------------------|SOL 1110
C     Declare variables                                                |SOL 1120
C ---------------------                                                |SOL 1130
C     A         DBL   Molal Debye-Huckel coefficient                   |SOL 1140
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C     A1MIX     DBL   HTOT, OHTOT, and TIC for comp 1 of a mixture     |SOL 1150
C     ADENS     DBL   Density of solution A                            |SOL 1160
C     ADEX      INT   Flag for surface chemistry option                |SOL 1170
C     AHI       DBL   Pressure correction fit parameter                |SOL 1180
C     ALFA      DBL   Activity of aqueous species i                    |SOL 1190
C     ALK       INT   Flag for distribution of carbonate species       |SOL 1200
C     ALOW      DBL   Pressure correction fit parameter                |SOL 1210
C     AMOL      DBL   Molality of aqueous/mineral species added        |SOL 1220
C     ANALM     DBL   Analyzed molality of species i                   |SOL 1230
C     ANMMIX    DBL   Analyzed molality of species i in solution A     |SOL 1240
C     ANMTIC    DBL   Analysed TIC                                     |SOL 1250
C     ATEMP     DBL   Temperature of solution A                        |SOL 1260
C     B         DBL   Molal Debye-Huckel coefficient                   |SOL 1270
C     B2MIX     DBL   HTOT, OHTOT, and TIC for comp 1 of a mixture     |SOL 1280
C     BDAT      DBL   B-dot as a function of temperature               |SOL 1290
C     BDENS     DBL   Density of solution B                            |SOL 1300
C     BDOT      DBL   Activity coefficient deviation function          |SOL 1310
C     BHI       DBL   Pressure correction fit parameter                |SOL 1320
C     BLOW      DBL   Pressure correction fit parameter                |SOL 1330
C     BNMMIX    DBL   Analyzed molality of species i in solution B     |SOL 1340
C     BTEMP     DBL   Temperature of solution B                        |SOL 1350
C     BUFFER    CHA   Used for memory/memory writes                    |SOL 1360
C     CEC       DBL   Cation exchange capacity                         |SOL 1370
C     CHI       DBL   Pressure correction fit parameter                |SOL 1380
C     CLOW      DBL   Pressure correction fit parameter                |SOL 1390
C     CO2F      DBL   Sum of CO2 plus CO2 lost from solution           |SOL 1400
C     COEF      DBL   Stoichiometric coefficient and Id number         |SOL 1410
C     CONV1     DBL   Tolerance factor for convergence of anions       |SOL 1420
C     CONV2     DBL   Tolerance factor for hydronium mass-balance      |SOL 1430
C     CR        CHA   Inserts carriage returns in output               |SOL 1440
C     CUNITS    DBL   Analytical input concentration                   |SOL 1450
C     DCH4      DBL   Used to add/remove CH4 from water                |SOL 1460
C     DDCH4     DBL   Concentration of CH4 lost before pH measurement  |SOL 1470
C     DCO2      DBL   Used to add/remove CO2 from water                |SOL 1480
C     DDCO2     DBL   Concentration of CO2 lost before pH measurement  |SOL 1490
C     DH2S      DBL   Used to add/remove H2S from Water                |SOL 1500
C     DDH2S     DBL   Concentration of H2S lost before pH measurement  |SOL 1510
C     DNH3      DBL   Used to add/remove NH3 from water                |SOL 1520
C     DDNH3     DBL   Concentration of NH3 lost before pH measurement  |SOL 1530
C     DELVR     DBL   Change in volume at 25 degrees                   |SOL 1540
C     DENS      DBL   Density                                          |SOL 1550
C     DFRAC1    DBL   Smallest fraction of soln 1 mixed with soln 2    |SOL 1560
C     DHA       DBL   Ion size parameter                               |SOL 1570
C     DINC      DBL   Increment of solution 1 to be added              |SOL 1580
C     DNS       CHA   Determines if density should be calculated       |SOL 1590
C     DP        DBL   Dissolution/precipitation switch                 |SOL 1600
C     DSEP      DBL   Density of oil at 15 degree C                    |SOL 1610
C     EHM       DBL   Measured Eh in volts                             |SOL 1620
C     EHMC      DBL   Measured Eh using the Calomel electrode          |SOL 1630
C     EMFZSC    DBL   Measured Eh using the Zobell's solution          |SOL 1640
C     EXELT     DBL   Total moles of component.                        |SOL 1650
C     FBOIL     DBL   Fraction of solution boiled-off as steam         |SOL 1660
C     FCCSAT    DBL   Tolerance factor for pH and CO2 options          |SOL 1670
C     FILEIN    CHA   Name of input file                               |SOL 1680
C     FILEOT    CHA   Name of output file                              |SOL 1690
C     FIXIT     DBL   Fixing value in the CO2 option                   |SOL 1700
C     FLAGS     INT   Selection flags for calculation of redox equil.  |SOL 1710
C     FMIX      DBL   Stores fraction of mixing                        |SOL 1720
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C     GAMMA     DBL   Activity coefficient                                  |SOL 1730
C     GEOTH     INT   Flag to select geothermometer                         |SOL 1740
C     GFW       DBL   Gram formula weight of aqueous species                |SOL 1750
C     HITEMP    DBL   In-situ temperature                                   |SOL 1760
C     HTOT      DBL   Current sum of all H+ in solution                     |SOL 1770
C     HTOTI     DBL   Target sum of all H+ in solution                      |SOL 1780
C     I         INT   Loop variable/counter                                 |SOL 1790
C     IACT      INT   Switch for printing activity ratios                   |SOL 1800
C     IADJ      INT   Has HITEMP been calculated or not                     |SOL 1810
C     IBMIX     INT   Switch for mixing option                              |SOL 1820
C     ICALL     INT   Loop variable                                         |SOL 1830
C     ICCSAT    INT   Switch for pH option                                  |SOL 1840
C     ICO2      INT   Switch for CO2 option                                 |SOL 1850
C     IDDP      INT   Id number of the mineral to be dissolved/ppt          |SOL 1860
C     IDMIX     INT   Id number of the aqueous species to be added          |SOL 1870
C     IDN       INT   Id numbers of the ISCOMP components adsorption        |SOL 1880
C     IDSAT     INT   Id number of the mineral to be equilibrated           |SOL 1890
C     IEXCH     INT   Switch for adsorption/ion exchange                    |SOL 1900
C     IGAS      INT   Loop variable for gas option                          |SOL 1910
C     ILO       INT   Lower limit for index for low/high T log K's          |SOL 1920
C     IMAX      INT   Max number of iterations for various options          |SOL 1930
C     IMCO3     INT   Selects CO2 option                                    |SOL 1940
C     IMIX      INT   Switch used in MIXER routines                         |SOL 1950
C     INFORM    INT   Flag to print all the log K values in data base       |SOL 1960
C     INMIX     INT   Total number of mixtures of two solution mixed        |SOL 1970
C     INSP      INT   Total number of surface sites for adsorption          |SOL 1980
C     IOPT      INT   Switch for CO2 option                                 |SOL 1990
C     IPAGE     INT   Current page number of output file                    |SOL 2000
C     IPGLN     INT   Current line number of the output file                |SOL 2010
C     IPHASE    INT   Switch used for GAS options                           |SOL 2020
C     IPHNUM    INT   Counter used in PHCALC                                |SOL 2030
C     IPIT      INT   Flag to use pitzer activity coefficients              |SOL 2040
C     IPRIN1    INT   Flag for printing iteration of anions                 |SOL 2050
C     IPRIN2    INT   Flag for printing hydronium balance                   |SOL 2060
C     IRUN      INT   Keeps track of the number of runs completed           |SOL 2070
C     IRXDP     INT   Id number of the aqueous species to be added          |SOL 2080
C     ISALT     INT   Switch used in mixer to indicate option               |SOL 2090
C     ISAT      INT   Counter used in co2opt                                |SOL 2100
C     ISCHG     INT   Charge of each surface site for adsorption            |SOL 2110
C     ISCOMP    INT   Total number of components in dissociation            |SOL 2120
C     ITIC      INT   Hitemp distribution of carbonate species              |SOL 2130
C     ITMIX     INT   Switch for the mineral saturation option              |SOL 2140
C     ITWR      INT   Switch to control printing of some headings           |SOL 2150
C     J         INT   Loop counter                                          |SOL 2160
C     JCCST     INT   Switch indicating if phopt called 1st time            |SOL 2170
C     JCO3      INT   Switch to control printing of some headings           |SOL 2180
C     JMIXTR    INT   Counter for maximum number of mixtures                |SOL 2190
C     KCH4OL    DBL   Henry's law coefficient for CH4 in oil                |SOL 2200
C     KCO2OL    DBL   Henry's law coefficient for CO2 in oil                |SOL 2210
C     KH2SOL    DBL   Henry's law coefficient for H2S in oil                |SOL 2220
C     KRXN      DBL   K for dissociation reaction of surface species        |SOL 2230
C     KT1       DBL   Equilibrium constant of the aqueous reactions         |SOL 2240
C     LKT1      DBL   Log K for aqueous species with temperature            |SOL 2250
C     LKT2      DBL   Log K for minerals with temperature                   |SOL 2260
C     LOGKT1    DBL   Log K for aqueous species at specified temp.          |SOL 2270
C     LOGKT2    DBL   Log K for minerals at specified temperature           |SOL 2280
C     M         DBL   Calculated molality of aqueous species                |SOL 2290
C     MBASE     DBL   Equivalence Mole Fraction (initial) on surface        |SOL 2300
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C     MINCO     DBL   Stoichiometric coefficient for added minerals     |SOL 2310
C     MININD    INT   Index number of the added mineral                |SOL 2320
C     MINLOG    DBL   Log K values for added minerals                  |SOL 2330
C     MNACLD    DBL   Sum of Molality * charge / 2                     |SOL 2340
C     MU        DBL   Ionic strength of aqueous solution               |SOL 2350
C     MXAQK     INT   Total number of aqueous log k values             |SOL 2360
C     MXMNK     INT   Total number of mineral log k values             |SOL 2370
C     MXPC      INT   Total number of mineral pressure constants       |SOL 2380
C     MXSP      INT   Total number of aqueous species                  |SOL 2390
C     NDUM      INT   Id of mineral/aqueous complex with K(T) changed  |SOL 2400
C     NH2O      DBL   Number of water ionization reactions             |SOL 2410
C     NUFLAG    INT   Sets the activity coefficients of neutral species|SOL 2420
C     ODUM      CHA   Switch to indicate a mineral/aqueous complex     |SOL 2430
C     OHTOT     DBL   Current sum of all OH- in solution               |SOL 2440
C     OHTOTI    DBL   Target sum of all OH- in solution                |SOL 2450
C     OK        INT   Error flag for Lagrange interpolation routine    |SOL 2460
C     OUTIN     CHA   Name of restart file name                        |SOL 2470
C     PAGE1     CHA   Names of aqueous species                         |SOL 2480
C     PAGE2     CHA   Names of equilibrium constants                   |SOL 2490
C     PAGE3     CHA   Names of solubility constants                    |SOL 2500
C     PCO2      DBL   Partial pressure of CO2                          |SOL 2510
C     PH        DBL   Measured pH of the solution                      |SOL 2520
C     PH2O      DBL   Partial pressure of H2O                          |SOL 2530
C     PHHIT     INT   Hitemp switch, used to control phcalc            |SOL 2540
C     PPHHIT    INT   Switch to control calling phcalc                 |SOL 2550
C     PRESS     DBL   Total pressure                                   |SOL 2560
C     RATIO     INT   Flag for printing activity ratios of elements    |SOL 2570
C     RXDP      DBL   Molal amount of the aqueous species added        |SOL 2580
C     SAREA     DBL   Total surface area per kilogram of solvent       |SOL 2590
C     SCO2      DBL   Sum of CO2 species                               |SOL 2600
C     SPN       CHA   Name of each surface species adsorption          |SOL 2610
C     TAREA     DBL   Site density per unit area                       |SOL 2620
C     TCH4M     DBL   Moles CH4 distributed between oil, water, vapor  |SOL 2630
C     TCO2      DBL   Activity coefficients of CO2 with temperature    |SOL 2640
C     TCO2M     DBL   Moles CO2 distributed between oil, water, vapor  |SOL 2650
C     TDS       DBL   Total Dissolved Solids   (UNITS = KG/L)          |SOL 2660
C     TEMP      DBL   Temperature of the solution when pH was measured |SOL 2670
C     TH2SM     DBL   Moles H2S distributed between oil, water, vapor  |SOL 2680
C     TIC       DBL   Concentration of total inorganic carbon          |SOL 2690
C     TIT1      CHA   Name of solution A                               |SOL 2700
C     TIT2      CHA   Name of solution B                               |SOL 2710
C     TITLE     CHA   Name of the sample                               |SOL 2720
C     TITMIX    CHA   Title for mixtures                               |SOL 2730
C     TITR      DBL   Iteration array in DISTRB, used for guesses      |SOL 2740
C     TK        DBL   Temperature steps used by program                |SOL 2750
C     TOF       CHA   Places a form feed in output file                |SOL 2760
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                 |SOL 2770
C     UNITS     CHA   Units of concentration                           |SOL 2780
C     UNM       INT   File unit connected the external mixing file     |SOL 2790
C     WROIL     DBL   Oil to water weight ratio                        |SOL 2800
C     XD        DBL   Holds Log K's for additional anions & cations    |SOL 2810
C     XDUM      DBL   New log K(T) value                               |SOL 2820
C     Y28       INT   Set at hitemp to skip unneeded calculations      |SOL 2830
C     Z         INT   Charge of aqueous species                        |SOL 2840
C -------------------------------------------------------------------- |SOL 2850
      INTEGER ALK, ANS1, ANS2, FLAGS(6), GEOTH                          SOL 2860
      INTEGER I, IACT, IADJ, IBMIX, ICALL, ICCSAT, ICO2, IDDP           SOL 2870
      INTEGER IDMIX(50), IDN(10,10), IDONE, IDSAT                       SOL 2880
```

```
      INTEGER IEXCH, IGAS, ILO, IMAX, IMCO3, IMIX, INFORM, INMIX, INSP  SOL 2890
      INTEGER IOPT, IPAGE, IPGLN, IPHASE, IPHNUM, IPIT, IPRIN1, IPRIN2  SOL 2900
      INTEGER IRUN, IRXDP(10), ISALT, ISAT, ISCHG(10), ISCOMP(10)       SOL 2910
      INTEGER ITIC, ITMIX, ITT, ITWR, J, JCCST, JCO3, JMIXTR, LEN       SOL 2920
      INTEGER LENGTH, MININD(8,5), MIXFLG, MXAQK, MXMNK, MXPC, MXSP     SOL 2930
      INTEGER NDUM(12), NUFLAG, NUM, NUMCOM, NUMINS, OK, PHHIT, PPHHIT  SOL 2940
      INTEGER RATIO, UNM, Y28, Z(NMAX)                                  SOL 2950
                                                                        SOL 2960
      CHARACTER*1  ADEX, CR, DNS, ODUM(12), TOF                         SOL 2970
      CHARACTER*5  UNITS                                                SOL 2980
      CHARACTER*8  PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                SOL 2990
      CHARACTER*10 SPN(10)                                              SOL 3000
      CHARACTER*32 TIT1, TIT2                                           SOL 3010
      CHARACTER*40 TITMIX                                               SOL 3020
      CHARACTER*80 ANS, BUFFER, FILEIN, FILEOT, MIXFLE, OUTIN, TITLE    SOL 3030
                                                                        SOL 3040
      DOUBLE PRECISION A, A1MIX(5), ADENS, AHI(200), ALFA(NMAX)         SOL 3050
      DOUBLE PRECISION ALOW(200), AMOL(50), ANALM(NMAX), ANMMIX(NMAX)   SOL 3060
      DOUBLE PRECISION ANMTIC, ATEMP, B, B2MIX(5), BDAT(10), BDENS, BDOTSOL 3070
      DOUBLE PRECISION BHI(200), BLOW(200), BNMMIX(NMAX), BTEMP         SOL 3080
      DOUBLE PRECISION CEC, CHI(200), CLOW(200), CO2F                   SOL 3090
      DOUBLE PRECISION COEF(10,10), CONV1, CONV2                        SOL 3100
      DOUBLE PRECISION CUNITS(NMAX), DCH4, DCO2, DDCH4, DDCO2, DDH2S    SOL 3110
      DOUBLE PRECISION DDNH3, DELVR(NMAX), DENS, DFRAC1, DH2S           SOL 3120
      DOUBLE PRECISION DHA(NMAX), DINC, DNH3, DP                        SOL 3130
      DOUBLE PRECISION EHM, EHMC, EMFZSC, EXELT(35)                     SOL 3140
      DOUBLE PRECISION FBOIL, FCCSAT, FIXIT, FMIX(10)                   SOL 3150
      DOUBLE PRECISION GAMMA(NMAX), GFW(NMAX), HITEMP, HTOT, HTOTI      SOL 3160
      DOUBLE PRECISION KCH4OL, KCO2OL, KH2SOL, KRXN(10)                 SOL 3170
      DOUBLE PRECISION KT1(NMAX)                                        SOL 3180
      DOUBLE PRECISION LKT1(NMAX,11), LKT2(NMAX,11)                     SOL 3190
      DOUBLE PRECISION LOGKT1(NMAX), LOGKT2(NMAX), M(NMAX)              SOL 3200
      DOUBLE PRECISION MBASE(10), MINCO(9,5), MINLOG(2,5)               SOL 3210
      DOUBLE PRECISION MNACLD, MU, NH2O(NMAX), OHTOT, OHTOTI            SOL 3220
      DOUBLE PRECISION PCO2, PH, PH2O, PRESS, DSEP, RXDP(10)            SOL 3230
      DOUBLE PRECISION SAREA, SCO2                                      SOL 3240
      DOUBLE PRECISION TAREA, TCH4M, TCO2(10), TCO2M, TDS, TEMP         SOL 3250
      DOUBLE PRECISION TH2SM, TIC, TITR(11), TK(11), TOTEL(5)           SOL 3260
      DOUBLE PRECISION WROIL, XD(2,45), XDUM(12)                        SOL 3270
                                                                        SOL 3280
      EXTERNAL ACTIVE, ADSORB, CALCUL, CO2OPT, DISTRB, GASES, INPUT     SOL 3290
      EXTERNAL INTIAL, LENGTH, MIXER, PHCALC, PHOPT, PRATIO, PRINTR     SOL 3300
      EXTERNAL PRNTAB, PSAT, PCLOGK, STORE, TABLES, LAGINT, PAGE        SOL 3310
                                                                        SOL 3320
      INTRINSIC DABS, DLOG10, INDEX                                     SOL 3330
                                                                        SOL 3340
      COMMON /AL    / NDUM, XDUM                                        SOL 3350
      COMMON /ALOGK / LOGKT1, LOGKT2                                    SOL 3360
      COMMON /AMM   / IDMIX, AMOL, ITMIX, INMIX, DFRAC1, DINC, FBOIL    SOL 3370
      COMMON /BASIC / DENS, PRESS, EHM, EHMC, EMFZSC, TIC, FCCSAT, XD,  SOL 3380
     .                NUMCOM, NUMINS, MINLOG, MINCO, MININD, CONV1,     SOL 3390
     .                CONV2                                             SOL 3400
      COMMON /CH    / ODUM                                              SOL 3410
      COMMON /DIST  / TCO2M,  TCH4M, TH2SM, WROIL, KCH4OL, KCO2OL,      SOL 3420
     .                KH2SOL, IPHASE, DSEP                              SOL 3430
      COMMON /EXCHAN/ COEF, MBASE, KRXN, CEC, TAREA,                    SOL 3440
     .                SAREA, IDN, ISCHG, ISCOMP, INSP                   SOL 3450
      COMMON /EXTOT / EXELT, TOTEL, TITR                                SOL 3460
```

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      COMMON /FLAGCM/ ALK, ITIC, ICCSAT, IMCO3, ITT, ANS1, ANS2,          SOL 3470
     .                NUFLAG, IPIT, FLAGS, INFORM, RATIO, GEOTH,          SOL 3480
     .                IPRIN1, IPRIN2                                      SOL 3490
      COMMON /FMFD  / TOF, CR, TITMIX                                     SOL 3500
      COMMON /FORM  / IPAGE, IPGLN                                        SOL 3510
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,              SOL 3520
     .                DCH4, DDCH4, IOPT, FIXIT                            SOL 3530
      COMMON /IMM   / IBMIX, IMIX                                         SOL 3540
      COMMON /KK    / LKT1, LKT2                                          SOL 3550
      COMMON /MM    / ANMMIX, A1MIX, B2MIX, FMIX, BNMMIX, ADENS, BDENS,   SOL 3560
     .                ATEMP, BTEMP                                        SOL 3570
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                          SOL 3580
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                 SOL 3590
      COMMON /NAMES2/ SPN                                                 SOL 3600
      COMMON /NAMES3/ MIXFLE, OUTIN, TITLE, UNITS, ADEX                   SOL 3610
      COMMON /PTK   / DELVR, NH2O, ALOW, BLOW, CLOW, AHI, BHI, CHI        SOL 3620
      COMMON /SAT/    IDDP, IDSAT, DP, RXDP, IRXDP                        SOL 3630
      COMMON /TABCOM/ MXSP, MXMNK, GFW, Z, DHA                            SOL 3640
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                                 SOL 3650
      COMMON /TTK   / KT1                                                 SOL 3660
      COMMON /ZPH   / PHHIT, PPHHIT, JCO3, SCO2, HTOT, OHTOT              SOL 3670
                                                                          SOL 3680
C ========================================================================|SOL 3690
                                                                          SOL 3700
C ------------------------------------------------------------------------|SOL 3710
C     The following open statements have been commented out by            |SOL 3720
C     Ernie Perkins (ORSD, ARC) in order to allow a command               |SOL 3730
C     proceedure under VMS 4.5 on DEC VAX's to assign the files           |SOL 3740
C     external to the program.                                            |SOL 3750
                                                                          SOL 3760
      PRINT *, '  ENTER THE NAME OF THE SAMPLE INPUT FILE ?'              SOL 3770
      PRINT *, '  Default = [SOLMINEQ.IN]'                                SOL 3780
      READ  '(A)', FILEIN                                                 SOL 3790
      IF (FILEIN .EQ. ' ') FILEIN = 'SOLMINEQ.IN'                         SOL 3800
                                                                          SOL 3810
      NUM = INDEX (FILEIN, '.')                                           SOL 3820
                                                                          SOL 3830
      IF (NUM .EQ. 0) THEN                                                SOL 3840
        NUM = LENGTH(FILEIN)                                              SOL 3850
        FILEOT = FILEIN(1:NUM) // '.OUT'                                  SOL 3860
      ELSE                                                                SOL 3870
        FILEOT = FILEIN(1:NUM) // 'OUT'                                   SOL 3880
      END IF                                                              SOL 3890
                                                                          SOL 3900
      LEN = LENGTH(FILEOT)                                                SOL 3910
                                                                          SOL 3920
      PRINT *, '  ENTER THE NAME OF THE OUTPUT FILE ?'                     SOL 3930
      PRINT '(1X, A, A, A)', '  Default = [', FILEOT(1:LEN), ']'          SOL 3940
      READ  '(A)', ANS                                                    SOL 3950
      IF (ANS .NE. ' ') FILEOT = ANS                                      SOL 3960
                                                                          SOL 3970
      OPEN (UNIT=UNI, FILE = FILEIN, STATUS = 'OLD')                      SOL 3980
      OPEN (UNIT=UNO, FILE = FILEOT, STATUS = 'UNKNOWN')                  SOL 3990
C ------------------------------------------------------------------------|SOL 4000
                                                                          SOL 4010
      TOF = '1'                                                           SOL 4020
      CR  = '+'                                                           SOL 4030
                                                                          SOL 4040
```

```
      MIXFLG = 0                                                        SOL 4050
      IRUN   = 0                                                        SOL 4060
      IPGLN  = 0                                                        SOL 4070
      IPAGE  = 0                                                        SOL 4080
                                                                        SOL 4090
      DO 10 I = 1, NMAX                                                 SOL 4100
        PAGE1(I) = '          '                                         SOL 4110
        GFW(I) = 0.0                                                    SOL 4120
        DHA(I) = 0.0                                                    SOL 4130
        Z(I)   = 0                                                      SOL 4140
   10 CONTINUE                                                          SOL 4150
                                                                        SOL 4160
C -------------------------------------------------------------------|SOL 4170
C     Read the data base on unit 10                                   |SOL 4180
C -------------------------------------------------------------------|SOL 4190
                                                                        SOL 4200
      CALL TABLES (MXAQK, BDAT, TK, TCO2, MXPC)                         SOL 4210
                                                                        SOL 4220
C -------------------------------------------------------------------|SOL 4230
C     Initialize values for each new sample input                     |SOL 4240
C -------------------------------------------------------------------|SOL 4250
                                                                        SOL 4260
   20 CONTINUE                                                          SOL 4270
      ICALL  = 0                                                        SOL 4280
      ISALT  = 0                                                        SOL 4290
      IMIX   = 0                                                        SOL 4300
      IBMIX  = 0                                                        SOL 4310
      JMIXTR = 0                                                        SOL 4320
      INMIX  = 0                                                        SOL 4330
      TITMIX = '                                                        SOL 4340
                                                                        SOL 4350
      CALL INTIAL (OK, ALK, INFORM, RATIO, GAMMA, TEMP, HITEMP, PRESS,  SOL 4360
     .             HTOTI, OHTOTI, ICO2, IMCO3, IBMIX, FCCSAT, IEXCH,  SOL 4370
     .             ISAT, IPHNUM, JCCST)                               SOL 4380
                                                                        SOL 4390
C -------------------------------------------------------------------|SOL 4400
C     Read one data set from the input file on unit 5                 |SOL 4410
C -------------------------------------------------------------------|SOL 4420
                                                                        SOL 4430
      CALL INPUT (UNI, TEMP, HITEMP, DNS, PHHIT, IEXCH, ICO2, MIXFLG)   SOL 4440
                                                                        SOL 4450
      ILO = 1                                                           SOL 4460
                                                                        SOL 4470
C -------------------------------------------------------------------|SOL 4480
C     Compute aqueous LOGKT'S at the desired temperature              |SOL 4490
C -------------------------------------------------------------------|SOL 4500
                                                                        SOL 4510
   30 CONTINUE                                                          SOL 4520
      CALL LAGINT (TK, LKT1, TEMP, LOGKT1, MXAQK, NMAX, OK)             SOL 4530
                                                                        SOL 4540
C -------------------------------------------------------------------|SOL 4550
C     If the sample "TEMP" is within the range from 0-350 degrees     |SOL 4560
C     then continue, otherwise get the next data set or stop.         |SOL 4570
C -------------------------------------------------------------------|SOL 4580
                                                                        SOL 4590
      IF (OK .NE. 1) THEN                                               SOL 4600
        CALL STORE (TEMP, HITEMP)                                       SOL 4610
        GO TO 20                                                        SOL 4620
```

```
      END IF                                                              SOL 4630
                                                                          SOL 4640
C -----------------------------------------------------------------------|SOL 4650
C     Compute mineral LOGKT'S at the desired temperature.                 |SOL 4660
C -----------------------------------------------------------------------|SOL 4670
                                                                          SOL 4680
      CALL LAGINT (TK, LKT2, TEMP, LOGKT2, MXMNK, NMAX, OK)               SOL 4690
                                                                          SOL 4700
C -----------------------------------------------------------------------|SOL 4710
C     Calculate the saturation pressure of H2O                            |SOL 4720
C -----------------------------------------------------------------------|SOL 4730
                                                                          SOL 4740
      CALL PSAT (TEMP, PH2O)                                              SOL 4750
                                                                          SOL 4760
                                                                          SOL 4770
C -----------------------------------------------------------------------|SOL 4780
C     If input pressure is greater than PH2O, the logkt of                |SOL 4790
C     aqueous species are adjusted using the "density model" of mesmer.   |SOL 4800
C     If hitemp is > 0, adjustment of logkt is done only at hitemp.       |SOL 4810
C -----------------------------------------------------------------------|SOL 4820
                                                                          SOL 4830
      IADJ  = 0                                                           SOL 4840
      IF (PHHIT .EQ. 1) THEN                                              SOL 4850
        IF (DABS(HITEMP - TEMP) .LT. CPUMIN) THEN                         SOL 4860
          ILO =  7                                                        SOL 4870
        ELSE                                                              SOL 4880
          IADJ = 1                                                        SOL 4890
        END IF                                                            SOL 4900
      END IF                                                              SOL 4910
                                                                          SOL 4920
C -----------------------------------------------------------------------|SOL 4930
C     Replace some of the logkt's that were read in input                 |SOL 4940
C -----------------------------------------------------------------------|SOL 4950
                                                                          SOL 4960
      DO 40 I = ILO, (ILO + 5)                                            SOL 4970
        IF (NDUM(I) .GT. 0) THEN                                          SOL 4980
          IF (ODUM(I).EQ.'A') THEN                                        SOL 4990
            LOGKT1(NDUM(I)) = XDUM(I)                                     SOL 5000
          ELSE IF (ODUM(I).EQ.'M') THEN                                   SOL 5010
            LOGKT2(NDUM(I)) = XDUM(I)                                     SOL 5020
          END IF                                                          SOL 5030
        END IF                                                            SOL 5040
   40 CONTINUE                                                            SOL 5050
                                                                          SOL 5060
      DO 50 I = 2, 15                                                     SOL 5070
        IF (DABS(HITEMP - TEMP) .LT. CPUMIN) THEN                         SOL 5080
          LOGKT1(MXAQK+I- 1) = XD(2,I)                                    SOL 5090
          LOGKT1(MXAQK+I+13) = XD(2,I+15)                                 SOL 5100
          LOGKT1(MXAQK+I+27) = XD(2,I+30)                                 SOL 5110
        ELSE                                                              SOL 5120
          LOGKT1(MXAQK+I- 1) = XD(1,I)                                    SOL 5130
          LOGKT1(MXAQK+I+13) = XD(1,I+15)                                 SOL 5140
          LOGKT1(MXAQK+I+27) = XD(1,I+30)                                 SOL 5150
        END IF                                                            SOL 5160
   50 CONTINUE                                                            SOL 5170
                                                                          SOL 5180
      DO 60 I = 1, 5                                                      SOL 5190
        IF (DABS(HITEMP - TEMP) .LT. CPUMIN) THEN                         SOL 5200
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        LOGKT2(MXMNK+I) = MINLOG(2,I)                                    SOL 5210
      ELSE                                                               SOL 5220
        LOGKT2(MXMNK+I) = MINLOG(1,I)                                    SOL 5230
      END IF                                                             SOL 5240
   60 CONTINUE                                                           SOL 5250
                                                                         SOL 5260
C ---------------------------------------------------------------------|SOL 5270
C     Adjust aqueous logkts for the pressure difference (press - ph2o) |SOL 5280
C ---------------------------------------------------------------------|SOL 5290
                                                                         SOL 5300
      IF (IADJ .EQ. 0 .AND. PRESS .GT. PH2O .AND. PRESS .GT. 1.0D00)     SOL 5310
     .  CALL PCLOGK (TEMP, PH2O, PRESS, MXAQK, MXPC)                     SOL 5320
                                                                         SOL 5330
C ---------------------------------------------------------------------|SOL 5340
C     Reset aqueous logkt's so there will be no zero divide and        |SOL 5350
C     calculate kt from logkt                                          |SOL 5360
C ---------------------------------------------------------------------|SOL 5370
                                                                         SOL 5380
      DO 70 I = 1, NMAX                                                  SOL 5390
        IF (LOGKT1(I) .LT. DLOG10(CPUMIN)) LOGKT1(I) = DLOG10(CPUMIN)    SOL 5400
        IF (LOGKT1(I) .GT. DLOG10(CPUMAX)) LOGKT1(I) = DLOG10(CPUMAX)    SOL 5410
        KT1(I) = 10.0**(LOGKT1(I))                                       SOL 5420
   70 CONTINUE                                                           SOL 5430
                                                                         SOL 5440
C ---------------------------------------------------------------------|SOL 5450
C     Print log k values                                               |SOL 5460
C ---------------------------------------------------------------------|SOL 5470
                                                                         SOL 5480
      IF (INFORM .EQ. 1) CALL PRNTAB (TITLE, TEMP, MXAQK)                SOL 5490
      Y28 = 1                                                            SOL 5500
                                                                         SOL 5510
C ---------------------------------------------------------------------|SOL 5520
C     If "temp" is greater than 0 and equal to "hitemp" then go to     |SOL 5530
C     calculate.                                                       |SOL 5540
C ---------------------------------------------------------------------|SOL 5550
                                                                         SOL 5560
      IF (TEMP.GT.1.0D-10.AND.(DABS(HITEMP-TEMP)).LT.1.0D-10) GO TO 80   SOL 5570
      ALFA(8) = 10.0D00**(-PH)                                           SOL 5580
                                                                         SOL 5590
C ---------------------------------------------------------------------|SOL 5600
C     Calculate the molality of total inorganic carbon from            |SOL 5610
C     the given value of tic and assign first-guess values             |SOL 5620
C     to the concentration of hco3 and co3                             |SOL 5630
C ---------------------------------------------------------------------|SOL 5640
                                                                         SOL 5650
      IF (TIC .GT. CPUMIN) THEN                                          SOL 5660
        IF (UNITS .NE. 'MOL/L' .AND. UNITS .NE. 'MOL/K') THEN            SOL 5670
          ANMTIC = TIC / 12011.0                                         SOL 5680
          CUNITS(98) = (TIC / 12011.0) / (1.0D00 + (ALFA(8) / KT1(1))    SOL 5690
     .                          + (ALFA(8)**2.0 / (KT1(1) * KT1(72))))  SOL 5700
          CUNITS( 7) = CUNITS(98) * ALFA(8) / KT1(1)                     SOL 5710
          CUNITS(98) = CUNITS(98) * 1.0D3 * GFW(98)                      SOL 5720
          CUNITS( 7) = CUNITS( 7) * 1.0D3 * GFW( 7)                      SOL 5730
        ELSE                                                             SOL 5740
          ANMTIC     = TIC                                               SOL 5750
          CUNITS(98) = TIC / (1.0D00 + (ALFA(8) / KT1(1))                SOL 5760
     .                       + (ALFA(8)**2.0 / (KT1(1) * KT1(72))))     SOL 5770
          CUNITS( 7) = (CUNITS(98) * ALFA(8) / KT1(1))                   SOL 5780
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        END IF                                                          SOL 5790
        ALK = 2                                                         SOL 5800
      END IF                                                            SOL 5810
                                                                        SOL 5820
      Y28 = 0                                                           SOL 5830
                                                                        SOL 5840
C -----------------------------------------------------------------|SOL 5850
C     Calculation of eh, cation-anion balance, gamma of neutral species|SOL 5860
C     temperature effects on debye-huckel constants and assignment     |SOL 5870
C     of mass-balance criteria for speciation calculations             |SOL 5880
C -----------------------------------------------------------------|SOL 5890
                                                                        SOL 5900
   80 CONTINUE                                                          SOL 5910
      CALL CALCUL (A, B, TDS, Y28, DNS, TEMP, HITEMP, PRESS, DENS, EHM, SOL 5920
     .             EHMC, EMFZSC, GFW, Z, UNITS, MXSP, TIC, ANMTIC,     SOL 5930
     .             GAMMA, TCO2, BDAT, BDOT, MNACLD, NUFLAG)            SOL 5940
                                                                        SOL 5950
C -----------------------------------------------------------------|SOL 5960
C     ITWR is set equal to 1 in distrb to avoid the printing of        |SOL 5970
C     headings during ph calculations                                  |SOL 5980
C -----------------------------------------------------------------|SOL 5990
                                                                        SOL 6000
      ITWR = 0                                                          SOL 6010
                                                                        SOL 6020
   90 CONTINUE                                                          SOL 6030
      IACT = 0                                                          SOL 6040
                                                                        SOL 6050
C -----------------------------------------------------------------|SOL 6060
C     Distribution of species calculations                             |SOL 6070
C -----------------------------------------------------------------|SOL 6080
                                                                        SOL 6090
      CALL DISTRB (NUFLAG, FLAGS, GAMMA, Z, DHA, TEMP, HITEMP, EHM, ALK,SOL 6100
     .             TITLE, A, B, MXSP, MXAQK, MU, IPRIN1, IPIT, TK,     SOL 6110
     .             CONV1, ANMTIC, ITIC, HTOT, OHTOT, SCO2, JCO3, ITWR, SOL 6120
     .             BDOT)                                               SOL 6130
                                                                        SOL 6140
      IF (PHHIT .EQ. 1 .AND. DABS(HITEMP-TEMP) .LT. 1.0D-10) GO TO 110  SOL 6150
      IF (PHHIT .NE. 1 .AND. IOPT .GT. 0) GO TO 120                     SOL 6160
                                                                        SOL 6170
      IF (ICCSAT .EQ. 0) THEN                                           SOL 6180
        IACT = 1                                                        SOL 6190
        GO TO 100                                                       SOL 6200
      END IF                                                            SOL 6210
                                                                        SOL 6220
C -----------------------------------------------------------------|SOL 6230
C     Do the ph option, if asked for                                   |SOL 6240
C -----------------------------------------------------------------|SOL 6250
                                                                        SOL 6260
      IF (ICCSAT .GT. 0) CALL PHOPT (ICCSAT, FCCSAT, ITWR, JCCST, *90)  SOL 6270
      IF (PHHIT . EQ. 1) IACT = 1                                       SOL 6280
                                                                        SOL 6290
C -----------------------------------------------------------------|SOL 6300
C     Print the distribution of species calculations.                  |SOL 6310
C -----------------------------------------------------------------|SOL 6320
                                                                        SOL 6330
  100 CONTINUE                                                          SOL 6340
      CALL PRINTR (TITLE, EHM, UNITS, DENS, PRESS, GFW, TEMP, Z, GAMMA, SOL 6350
     .             PH2O, PCO2, TDS, MU, MNACLD, SCO2, HTOT, OHTOT, MXSP)SOL 6360
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                                                                      SOL 6370
      IF (IACT .EQ. 1) GO TO 210                                      SOL 6380
                                                                      SOL 6390
C -------------------------------------------------------------------|SOL 6400
C     Iteration routine for the calculation of a new ph              |SOL 6410
C -------------------------------------------------------------------|SOL 6420
                                                                      SOL 6430
  110 CONTINUE                                                        SOL 6440
      IF (PPHHIT .EQ. 0) CALL PHCALC (TEMP, HITEMP, CONV2, ITIC, ITWR,SOL 6450
     .                                ISALT, IPHNUM, IPRIN2, *30, *90,SOL 6460
     .                                *100, *220)                     SOL 6470
                                                                      SOL 6480
C -----------------------------------------------------------------------|SOL 6490
C     Do the co2 option                                                |SOL 6500
C -----------------------------------------------------------------------|SOL 6510
                                                                      SOL 6520
  120 CONTINUE                                                        SOL 6530
      IF (IOPT .GT. 0) THEN                                           SOL 6540
          CALL CO2OPT (TEMP, HITEMP, GAMMA, ICO2, IMCO3, FCCSAT, MNACLD,SOL 6550
     .                 ITIC, ISAT, IPRIN2, *100)                     SOL 6560
          GO TO 110                                                   SOL 6570
      END IF                                                          SOL 6580
                                                                      SOL 6590
C -------------------------------------------------------------------|SOL 6600
C     Gas distribution option.  Note a max. of twenty five tries     |SOL 6610
C -------------------------------------------------------------------|SOL 6620
                                                                      SOL 6630
      IF (IPHASE .GT. 0) THEN                                         SOL 6640
        IMAX = 25                                                     SOL 6650
        DO 150 IGAS = 1, IMAX                                         SOL 6660
          I = IGAS                                                    SOL 6670
          CALL GASES (TEMP, PRESS, MNACLD, PH2O, FCCSAT, I, IMAX,     SOL 6680
     .                IPRIN2)                                         SOL 6690
          IF (IPHASE .LE. 0) GO TO 160                                SOL 6700
          JCO3 = 0                                                    SOL 6710
          ITIC = 2                                                    SOL 6720
          IOPT   = 0                                                  SOL 6730
          PHHIT  = 1                                                  SOL 6740
          PPHHIT = 0                                                  SOL 6750
          IPHNUM = 0                                                  SOL 6760
          DO 140 J = 1, IMAX                                          SOL 6770
            CALL PHCALC (TEMP, HITEMP, CONV2, ITIC, ITWR, ISALT, IPHNUM,SOL 6780
     .                   IPRIN2, *150, *130, *150, *150)             SOL 6790
            GO TO 150                                                 SOL 6800
  130       CONTINUE                                                  SOL 6810
            CALL DISTRB (NUFLAG, FLAGS, GAMMA, Z, DHA, TEMP, HITEMP,  SOL 6820
     .                   EHM, ALK, TITLE, A, B, MXSP, MXAQK, MU, IPRIN1,SOL 6830
     .                   IPIT, TK, CONV1, ANMTIC, ITIC, HTOT, OHTOT,  SOL 6840
     .                   SCO2, JCO3, ITWR, BDOT)                      SOL 6850
  140     CONTINUE                                                    SOL 6860
  150   CONTINUE                                                      SOL 6870
  160   CONTINUE                                                      SOL 6880
        IACT = 0                                                      SOL 6890
        CALL PRINTR (TITLE, EHM, UNITS, DENS, PRESS, GFW, TEMP, Z,    SOL 6900
     .               GAMMA, PH2O, PCO2, TDS, MU, MNACLD, SCO2, HTOT,  SOL 6910
     .               OHTOT, MXSP)                                     SOL 6920
      END IF                                                          SOL 6930
                                                                      SOL 6940
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C -----------------------------------------------------------------|SOL 6950
C     Exchange and adsorption options                              |SOL 6960
C -----------------------------------------------------------------|SOL 6970
                                                                     SOL 6980
      IF (IEXCH .GT. 0) THEN                                         SOL 6990
        UNITS  = 'MOL/K'                                             SOL 7000
        IMAX = 100                                                   SOL 7010
        HITEMP = TEMP                                                SOL 7020
        DO 190 ICALL = 1, IMAX                                       SOL 7030
          I = ICALL                                                  SOL 7040
          CALL ADSORB (TEMP, Z, IDONE, I, IEXCH, MXSP, IPRIN2)       SOL 7050
          IF (IDONE .LE. 0) THEN                                     SOL 7060
            IEXCH = 0                                                SOL 7070
            GO TO 200                                                SOL 7080
          END IF                                                     SOL 7090
          JCO3 = 0                                                   SOL 7100
          ITIC = 2                                                   SOL 7110
          IOPT   = 0                                                 SOL 7120
          PHHIT  = 1                                                 SOL 7130
          PPHHIT = 0                                                 SOL 7140
          IPHNUM = 0                                                 SOL 7150
          CALL DISTRB (NUFLAG, FLAGS, GAMMA, Z, DHA, TEMP, HITEMP, EHM, SOL 7160
     .                 ALK, TITLE, A, B, MXSP, MXAQK, MU, IPRIN1,    SOL 7170
     .                 IPIT, TK, CONV1, ANMTIC, ITIC, HTOT, OHTOT,   SOL 7180
     .                 SCO2, JCO3, ITWR, BDOT)                       SOL 7190
          DO 180 J = 1, IMAX                                         SOL 7200
            CALL PHCALC (TEMP, HITEMP, CONV2, ITIC, ITWR, ISALT, IPHNUM,SOL 7210
     .                   IPRIN2, *190, *170, *190, *190)             SOL 7220
            GO TO 190                                                SOL 7230
  170       CONTINUE                                                 SOL 7240
            CALL DISTRB (NUFLAG, FLAGS, GAMMA, Z, DHA, TEMP, HITEMP, SOL 7250
     .                   EHM, ALK, TITLE, A, B, MXSP, MXAQK, MU,     SOL 7260
     .                   IPRIN1, IPIT, TK, CONV1, ANMTIC, ITIC, HTOT,SOL 7270
     .                   OHTOT, SCO2, JCO3, ITWR, BDOT)              SOL 7280
  180     CONTINUE                                                   SOL 7290
  190   CONTINUE                                                     SOL 7300
                                                                     SOL 7310
        IPGLN = IPGLN + 6                                            SOL 7320
        IF (IPGLN .GT. 58) CALL PAGE                                 SOL 7330
        WRITE (UNO, 910)                                             SOL 7340
                                                                     SOL 7350
  200   CONTINUE                                                     SOL 7360
        IACT = 0                                                     SOL 7370
        CALL PRINTR (TITLE, EHM, UNITS, DENS, PRESS, GFW, TEMP, Z,   SOL 7380
     .               GAMMA, PH2O, PCO2, TDS, MU, MNACLD, SCO2, HTOT, SOL 7390
     .               OHTOT, MXSP)                                    SOL 7400
      END IF                                                         SOL 7410
                                                                     SOL 7420
      IF (IACT .EQ. 1) GO TO 220                                     SOL 7430
                                                                     SOL 7440
C -----------------------------------------------------------------|SOL 7450
C     Print mole ratios, log of activity ratios, and temperatures  |SOL 7460
C     calculated by chemical geothermometers                       |SOL 7470
C -----------------------------------------------------------------|SOL 7480
                                                                     SOL 7490
  210 CONTINUE                                                       SOL 7500
      CALL PRATIO (TITLE, PRESS, TEMP, DENS, UNITS, PCO2, GEOTH, RATIO) SOL 7510
                                                                     SOL 7520
```

```
C -------------------------------------------------------------------|SOL 7530
C     Calculate and print activity products of phases                |SOL 7540
C -------------------------------------------------------------------|SOL 7550
                                                                      SOL 7560
      CALL ACTIVE (TITLE, ALFA, TEMP, MXMNK, LOGKT2, PAGE3, MINCO,    SOL 7570
     .             MININD)                                          SOL 7580
                                                                      SOL 7590
      IF (IACT .EQ. 1) GO TO 110                                      SOL 7600
                                                                      SOL 7610
C -------------------------------------------------------------------|SOL 7620
C     Process the mixing/boiling/mineral saturation option           |SOL 7630
C -------------------------------------------------------------------|SOL 7640
                                                                      SOL 7650
  220 CONTINUE                                                        SOL 7660
      IF (IBMIX .NE. 0) THEN                                          SOL 7670
        IF (IRUN .EQ. 0 .AND. ISALT .EQ. 0) THEN                      SOL 7680
          TIT1 = TITLE                                                SOL 7690
        END IF                                                        SOL 7700
        IF (IBMIX .EQ. 1) THEN                                        SOL 7710
          IF (ICALL .NE. 3) THEN                                      SOL 7720
            ICALL = 1                                                 SOL 7730
            ISALT = 1                                                 SOL 7740
            IMIX  = 1                                                 SOL 7750
            IF (ITMIX .EQ. 0) ISALT = 3                               SOL 7760
            IF (ISALT .EQ. 1) TITLE = 'MIXTURE OF '// TIT1 //        SOL 7770
     .                                ' WITH A SALT OR MINERAL'      SOL 7780
          END IF                                                      SOL 7790
          CALL MIXER (TEMP, MNACLD, PRESS, DENS, ICALL, ISALT, IRUN,  SOL 7800
     .                MXSP, FCCSAT, PH2O, IPRIN2, MXMNK)            SOL 7810
          IF (ICALL .EQ. 1) THEN                                      SOL 7820
            PHHIT  = 0                                                SOL 7830
            PPHHIT = 1                                                SOL 7840
            IMIX   = 0                                                SOL 7850
            IBMIX  = 0                                                SOL 7860
            GO TO 100                                                 SOL 7870
          ELSE                                                        SOL 7880
            IF (ISALT .EQ. 1) IBMIX = 0                               SOL 7890
            GO TO 230                                                 SOL 7900
          END IF                                                      SOL 7910
        ELSE IF (IBMIX .EQ. 2) THEN                                   SOL 7920
          ICALL = 1                                                   SOL 7930
          IF (IRUN .NE. 0) THEN                                       SOL 7940
            ICALL = 2                                                 SOL 7950
            IMIX = 1                                                  SOL 7960
            TIT2 = TITLE                                              SOL 7970
          END IF                                                      SOL 7980
          CALL MIXER (TEMP, MNACLD, PRESS, DENS, ICALL, ISALT, IRUN,  SOL 7990
     .                MXSP, FCCSAT, PH2O, IPRIN2, MXMNK)            SOL 8000
          IF (IMIX .EQ. 1) THEN                                       SOL 8010
            IBMIX = 0                                                 SOL 8020
            TITLE = 'MIXTURE OF '//TIT1//' AND ' // TIT2              SOL 8030
            GO TO 250                                                 SOL 8040
          END IF                                                      SOL 8050
          ICALL  = 0                                                  SOL 8060
          ISALT  = 0                                                  SOL 8070
          IMIX   = 0                                                  SOL 8080
          JMIXTR = 0                                                  SOL 8090
          TITMIX = '                                                  SOL 8100
```

```
                                                                      SOL 8110
      CALL INTIAL (OK, ALK, INFORM, RATIO, GAMMA, TEMP, HITEMP,       SOL 8120
     .             PRESS, HTOTI, OHTOTI, ICO2, IMCO3, IBMIX,         SOL 8130
     .             FCCSAT, IEXCH, ISAT, IPHNUM, JCCST)               SOL 8140
                                                                      SOL 8150
      IF (MIXFLE .EQ. ' ') THEN                                       SOL 8160
        CALL INPUT (UNI, TEMP, HITEMP, DNS, PHHIT, IEXCH, ICO2,       SOL 8170
     .              MIXFLG)                                          SOL 8180
      ELSE                                                            SOL 8190
        UNM   = 39                                                    SOL 8200
        OPEN (UNM, FILE = MIXFLE, STATUS = 'OLD')                     SOL 8210
        CALL INPUT (UNM, TEMP, HITEMP, DNS, PHHIT, IEXCH, ICO2,       SOL 8220
     .              MIXFLG)                                          SOL 8230
        CLOSE (UNM)                                                   SOL 8240
      END IF                                                          SOL 8250
      IBMIX = 2                                                       SOL 8260
      ILO   = 1                                                       SOL 8270
      GO TO 30                                                        SOL 8280
    ELSE                                                              SOL 8290
      IF (ISALT .NE. 2) THEN                                          SOL 8300
        ICALL = 1                                                     SOL 8310
        IMIX = 1                                                      SOL 8320
        ISALT = 2                                                     SOL 8330
        TITLE = 'SOLUTION AFTER BOILING OF .. ' // TIT1               SOL 8340
      END IF                                                          SOL 8350
      CALL MIXER (TEMP, MNACLD, PRESS, DENS, ICALL, ISALT, IRUN,      SOL 8360
     .            MXSP, FCCSAT, PH2O, IPRIN2, MXMNK)                SOL 8370
      IF (ICALL .EQ. 1) THEN                                          SOL 8380
        PHHIT  = 0                                                    SOL 8390
        PPHHIT = 1                                                    SOL 8400
        IMIX   = 0                                                    SOL 8410
        IBMIX  = 0                                                    SOL 8420
        GO TO 100                                                     SOL 8430
      ELSE                                                            SOL 8440
        GO TO 230                                                     SOL 8450
      END IF                                                          SOL 8460
    END IF                                                            SOL 8470
  END IF                                                              SOL 8480
                                                                      SOL 8490
  IMIX = 0                                                            SOL 8500
  IF (INMIX .EQ. 0) THEN                                              SOL 8510
    CALL STORE (TEMP, HITEMP)                                         SOL 8520
    GO TO 20                                                          SOL 8530
  END IF                                                              SOL 8540
                                                                      SOL 8550
C -------------------------------------------------------------------|SOL 8560
C     Change the solution parameters to those of the mixture          |SOL 8570
C -------------------------------------------------------------------|SOL 8580
                                                                      SOL 8590
  230 CONTINUE                                                        SOL 8600
      IF (IMIX .EQ. 1) THEN                                           SOL 8610
        CALL INTIAL (OK, ALK, INFORM, RATIO, GAMMA, TEMP, HITEMP, PRESS,SOL 8620
     .               HTOTI, OHTOTI, ICO2, IMCO3, IMIX, FCCSAT, IEXCH, SOL 8630
     .               ISAT, IPHNUM, JCCST)                             SOL 8640
                                                                      SOL 8650
        UNITS  = 'MOL/K'                                              SOL 8660
        ALK    = 2                                                    SOL 8670
        ITIC   = 0                                                    SOL 8680
```

```
        HITEMP = TEMP                                                    SOL 8690
        EHM    = 9.0D0                                                   SOL 8700
        EMFZSC = 9.0D0                                                   SOL 8710
        EHMC   = 9.0D0                                                   SOL 8720
        Y28    = 0                                                       SOL 8730
        PHHIT  = 1                                                       SOL 8740
        HTOTI  = TOTEL(1)                                                SOL 8750
        OHTOTI = TOTEL(2)                                                SOL 8760
        ANMTIC = TOTEL(3)                                                SOL 8770
        DO 240 I = 1, NMAX                                               SOL 8780
          IF (I .EQ. 8) ANALM(I) = 0.0D00                                SOL 8790
          IF (I .EQ. 9) ANALM(I) = 0.0D00                                SOL 8800
          CUNITS(I) = ANALM(I)                                           SOL 8810
          M(I) = ANALM(I)                                                SOL 8820
  240   CONTINUE                                                         SOL 8830
        GO TO 80                                                         SOL 8840
      END IF                                                             SOL 8850
                                                                         SOL 8860
C -------------------------------------------------------------------   |SOL 8870
C     Mix the two solution in a single or multiple mixtures case         |SOL 8880
C -------------------------------------------------------------------   |SOL 8890
                                                                         SOL 8900
  250 CONTINUE                                                           SOL 8910
      JMIXTR = JMIXTR + 1                                                SOL 8920
      CALL STORE (TEMP, HITEMP)                                          SOL 8930
      IF (INMIX .LT. JMIXTR) GO TO 20                                    SOL 8940
                                                                         SOL 8950
      WRITE (BUFFER, 900) FMIX(JMIXTR), (1.0D0 - FMIX(JMIXTR))          SOL 8960
      READ (BUFFER, '(A)') TITMIX                                        SOL 8970
                                                                         SOL 8980
      DO 260 I = 1, MXSP + 44                                            SOL 8990
        ANALM(I) = (ANMMIX(I) * FMIX(JMIXTR))                            SOL 9000
     .           + (BNMMIX(I) * (1.0D0 - FMIX(JMIXTR)))                  SOL 9010
  260 CONTINUE                                                           SOL 9020
                                                                         SOL 9030
      DO 270 I = 1, 5                                                    SOL 9040
        TOTEL(I) = (A1MIX(I) * FMIX(JMIXTR))                            SOL 9050
     .           + (B2MIX(I) * (1.0D0 - FMIX(JMIXTR)))                  SOL 9060
  270 CONTINUE                                                           SOL 9070
                                                                         SOL 9080
      IMIX = 1                                                           SOL 9090
      DNS  = 'Y'                                                         SOL 9100
      DENS = (ADENS * FMIX(JMIXTR)) + (BDENS * (1.0D0 - FMIX(JMIXTR)))   SOL 9110
      TEMP = (ATEMP * FMIX(JMIXTR)) + (BTEMP * (1.0D0 - FMIX(JMIXTR)))   SOL 9120
      HITEMP = 0.0D00                                                    SOL 9130
      GO TO 230                                                          SOL 9140
                                                                         SOL 9150
  900 FORMAT('(PROPORTIONS: 1= ',F4.2,' 2= ',F4.2,')')                   SOL 9160
  910 FORMAT(//, ' ***************WARNING*******************',           SOL 9170
     .           /, ' Convergence not reached in ADSORBPTION',           SOL 9180
     .           /, ' /ION EXCHANGE routine.  Following results',        SOL 9190
     .           /, ' may be in error . ',                               SOL 9200
     .           /)                                                      SOL 9210
      END                                                                SOL 9220
```

```
      SUBROUTINE ACTIVE (TITLE, ALFA, TEMP, MXMNK, LOGKT2, PAGE3,          ACT 0010
     .                   MINCO, MININD)                                    ACT 0020
C ==========================================================================|ACT 0030
C     This routine calculates and prints activity products of phases       |ACT 0040
C --------------------------------------------------------------------------|ACT 0050
C     Declare constants                                                    |ACT 0060
C ---------------------                                                    |ACT 0070
C     CPUMIN     DBL   Smallest positive real value program uses           |ACT 0080
C     NMAX       INT   General array dimension to allow easy expansion     |ACT 0090
C     UNO        INT   File unit assigned for output file                  |ACT 0100
C     UNR        INT   File unit assigned for reaction file                |ACT 0110
C --------------------------------------------------------------------------|ACT 0120
      INTEGER NMAX, UNO, UNR                                               ACT 0130
      DOUBLE PRECISION R, CPUMIN                                           ACT 0140
      PARAMETER (NMAX = 340, UNO = 6, UNR = 12)                            ACT 0150
      PARAMETER (R = 1.98719D-3, CPUMIN=1.0D-35)                           ACT 0160
                                                                           ACT 0170
C --------------------------------------------------------------------------|ACT 0180
C     ALFA       DBL   Activity of aqueous species i                       |ACT 0190
C     AP         DBL   Activity product of the reaction                    |ACT 0200
C     C2         DBL   Saturation index                                    |ACT 0210
C     COEF       DBL   Coefficient of species in reaction                  |ACT 0220
C     CR         CHA   Inserts carriage returns in output                  |ACT 0230
C     DUMM       DBL   Delta gibbs free energy difference                  |ACT 0240
C     I          INT   Loop counting variable                              |ACT 0250
C     IC         INT   Number of components in reaction                    |ACT 0260
C     IFIN       INT   Formats the output                                  |ACT 0270
C     INDEX      INT   Index values of the minerals to be printed out      |ACT 0280
C     INDX       INT   Index of the species in the reaction                |ACT 0290
C     IPAGE      INT   Current page number of output file                  |ACT 0300
C     IPGLN      INT   Current line number of the output file              |ACT 0310
C     J          INT   Loop counting variable                              |ACT 0320
C     K          INT   Index number of the right side of the output        |ACT 0330
C     L          INT   Index number of the left side of the output         |ACT 0340
C     LOGKT2     DBL   Log K for minerals at specified temperature         |ACT 0350
C     MCOEF      DBL   Coefficient of species read in from table           |ACT 0360
C     MINCO      DBL   Stoichiometric coefficient for added minerals       |ACT 0370
C     MINDX      DBL   Index number of the species read in form table      |ACT 0380
C     MININD     INT   Index number of the added mineral                   |ACT 0390
C     MXMNK      INT   Total number of mineral log k values                |ACT 0400
C     NUM        INT   Count of minerals to be printed out                 |ACT 0410
C     PAGE3      CHA   Names of solubility constants                       |ACT 0420
C     R          DBL   Gas constant                                        |ACT 0430
C     T          DBL   Current temperature in degrees kelvin               |ACT 0440
C     TEMP       DBL   Current temperature in degrees centigrade           |ACT 0450
C     TITLE      CHA   Name of the sample                                  |ACT 0460
C     TITMIX     CHA   Title used for mixing                               |ACT 0470
C     TOF        CHA   Places a form feed in output file                   |ACT 0480
C --------------------------------------------------------------------------|ACT 0490
                                                                           ACT 0500
      INTEGER I, IC, IFIN, INDEX(NMAX), INDX(10), IPGLN, IPAGE             ACT 0510
      INTEGER J, K, L, MINDX(10,NMAX), MININD(9,5), MXMNK, NUM             ACT 0520
                                                                           ACT 0530
      CHARACTER *  1 TOF, CR                                               ACT 0540
      CHARACTER *  8 PAGE3(NMAX)                                           ACT 0550
      CHARACTER * 40 TITMIX                                                ACT 0560
      CHARACTER * 80 TITLE                                                 ACT 0570
                                                                           ACT 0580
```

```
      DOUBLE PRECISION ATCPRD, ALFA(NMAX), AP(NMAX), C2(2)              ACT 0590
      DOUBLE PRECISION COEF(10), DUMM(2), LOGKT2(NMAX), MCOEF(10,NMAX)  ACT 0600
      DOUBLE PRECISION MINCO(9,5), T, TEMP                              ACT 0610
                                                                        ACT 0620
      INTRINSIC DABS                                                    ACT 0630
                                                                        ACT 0640
      EXTERNAL ATCPRD, PAGE                                             ACT 0650
                                                                        ACT 0660
      COMMON /FMFD  / TOF, CR, TITMIX                                   ACT 0670
      COMMON /FORM  / IPAGE, IPGLN                                      ACT 0680
                                                                        ACT 0690
C ======================================================================|ACT 0700
C ----------------------------------------------------------------------|ACT 0710
C     The following open statement have been changed out by             |ACT 0720
C     Ernie Perkins (ORSD, ARC) in order to allow an command            |ACT 0730
C     proceedure under VMS 4.5 on DEC VAX's to assign the files         |ACT 0740
C     external to the program.                                          |ACT 0750
C ----------------------------------------------------------------------|ACT 0760
C      OPEN (UNR, STATUS = 'OLD', shared, readonly)                     ACT 0770
      OPEN (UNR, FILE = 'RXN.TBL', STATUS = 'OLD')                      ACT 0780
                                                                        ACT 0790
      DO 10 L = 1, MXMNK                                                ACT 0800
        READ (UNR, 900) I, (MCOEF(J,I), MINDX(J,I), J = 1, 10)          ACT 0810
   10 CONTINUE                                                          ACT 0820
                                                                        ACT 0830
      CLOSE (UNR)                                                       ACT 0840
                                                                        ACT 0850
      DO 20 I = 1, MXMNK + 5                                            ACT 0860
        AP(I) = 0.0D0                                                   ACT 0870
   20 CONTINUE                                                          ACT 0880
                                                                        ACT 0890
      T = TEMP + 273.15                                                 ACT 0900
                                                                        ACT 0910
C ----------------------------------------------------------------------|ACT 0920
C     Activity products of phases                                       |ACT 0930
C ----------------------------------------------------------------------|ACT 0940
                                                                        ACT 0950
      DO 40 I = 1, MXMNK                                                ACT 0960
        IC = 0                                                          ACT 0970
        DO 30 J = 1, 10                                                 ACT 0980
          IF (DABS(MCOEF(J,I)) .GT. CPUMIN) THEN                        ACT 0990
            IC = IC + 1                                                 ACT 1000
            COEF(J) = MCOEF(J,I)                                        ACT 1010
            INDX(J) = MINDX(J,I)                                        ACT 1020
          ELSE                                                          ACT 1030
            COEF(J) = 0.0D0                                             ACT 1040
            INDX(J) = MINDX(J,I)                                        ACT 1050
          END IF                                                        ACT 1060
   30   CONTINUE                                                        ACT 1070
        AP(I) = ATCPRD (IC, INDX, COEF, ALFA)                           ACT 1080
   40 CONTINUE                                                          ACT 1090
                                                                        ACT 1100
C ----------------------------------------------------------------------|ACT 1110
C     Calculate activity product for added minerals                     |ACT 1120
C ----------------------------------------------------------------------|ACT 1130
                                                                        ACT 1140
      DO 60 I = 1, 5                                                    ACT 1150
        DO 50 J = 1, 8                                                  ACT 1160
```

```
          IF (DABS(MINCO(J,I)) .GT. CPUMIN) AP(MXMNK+I) =                ACT 1170
     .       AP(MXMNK+I) + MINCO(J,I)*ALFA(MININD(J,I))                  ACT 1180
     50   CONTINUE                                                       ACT 1190
          AP(MXMNK+I) = AP(MXMNK+I) + MINCO(9,I)                         ACT 1200
     60 CONTINUE                                                        ACT 1210
                                                                        ACT 1220
C ------------------------------------------------------------------------|ACT 1230
C     Write out activity products                                       |ACT 1240
C ------------------------------------------------------------------------|ACT 1250
                                                                        ACT 1260
      CALL PAGE                                                         ACT 1270
      WRITE (UNO, 910) TITLE, TEMP, TITMIX                              ACT 1280
      WRITE (UNO, 920)                                                  ACT 1290
      WRITE (UNO, 930) CR                                               ACT 1300
      IPGLN = IPGLN + 4                                                 ACT 1310
      NUM   = 0                                                         ACT 1320
                                                                        ACT 1330
      DO 70 I = 1, MXMNK + 5                                            ACT 1340
        IF (DABS(AP(I))     .LE. 300.0   .AND.                          ACT 1350
     .      DABS(LOGKT2(I)) .LE. 300.0) THEN                            ACT 1360
          NUM = NUM + 1                                                 ACT 1370
          INDEX(NUM) = I                                                ACT 1380
        END IF                                                          ACT 1390
     70 CONTINUE                                                        ACT 1400
                                                                        ACT 1410
      IFIN = (NUM + 1) / 2                                              ACT 1420
      DO 80 I = 1, IFIN                                                 ACT 1430
        L = INDEX(I)                                                    ACT 1440
        C2(1)   = AP(L) - LOGKT2(L)                                     ACT 1450
        DUMM(1) = 2.302585D0 * R * T * C2(1)                            ACT 1460
        J = I + IFIN                                                    ACT 1470
        IF (J .LE. NUM) THEN                                            ACT 1480
          K = INDEX(J)                                                  ACT 1490
          C2(2)   = AP(K) - LOGKT2(K)                                   ACT 1500
          DUMM(2) = 2.302585D0 * R * T * C2(2)                          ACT 1510
        END IF                                                          ACT 1520
                                                                        ACT 1530
        IF (IPGLN .GT. 58) THEN                                         ACT 1540
          CALL PAGE                                                     ACT 1550
          WRITE (UNO, 910) TITLE, TEMP, TITMIX                          ACT 1560
          WRITE (UNO, 920)                                              ACT 1570
          WRITE (UNO, 930) CR                                           ACT 1580
          IPGLN = IPGLN + 4                                             ACT 1590
        END IF                                                          ACT 1600
                                                                        ACT 1610
        IF (J .LE. NUM) THEN                                            ACT 1620
          WRITE (UNO, 940)                                              ACT 1630
     .         L, PAGE3(L), AP(L), LOGKT2(L), C2(1), DUMM(1),           ACT 1640
     .         K, PAGE3(K), AP(K), LOGKT2(K), C2(2), DUMM(2)            ACT 1650
          IPGLN = IPGLN + 1                                             ACT 1660
        ELSE                                                            ACT 1670
          WRITE (UNO, 940)                                              ACT 1680
     .         L, PAGE3(L), AP(L), LOGKT2(L), C2(1), DUMM(1)            ACT 1690
          IPGLN = IPGLN + 1                                             ACT 1700
        END IF                                                          ACT 1710
     80 CONTINUE                                                        ACT 1720
                                                                        ACT 1730
      RETURN                                                            ACT 1740
```

```
                                                                      ACT 1750
  900 FORMAT(I3,/,10(F10.4,I4))                                       ACT 1760
  910 FORMAT('  SAMPLE IDENT - ',A80,4X,'(TEMPERATURE = ',F6.2,')',  ACT 1770
     .           /,20X,A40)                                           ACT 1780
  920 FORMAT(/,6X,'PHASE',5X,'LOG (AP)',4X,'LOG (KT)',2X,             ACT 1790
     .           'LOG (AP/KT)',7X,'DELG', 10X,'PHASE',5X,             ACT 1800
     .           'LOG (AP)',4X,'LOG (KT)',2X,                         ACT 1810
     .           'LOG (AP/KT)',7X,'DELG')                             ACT 1820
  930 FORMAT(A1,6X,'_____',5X,'________',4X,'________',2X,            ACT 1830
     .           '___________',7X,'____', 10X,'_____',5X,             ACT 1840
     .           '________',4X,'________',2X,                         ACT 1850
     .           '___________',7X,'____')                             ACT 1860
  940 FORMAT (1X, I3, 2X, A8, F10.3, 3(2X,F10.3),                     ACT 1870
     .        5X, I3, 2X, A8, F10.3, 3(2X,F10.3))                     ACT 1880
                                                                      ACT 1890
      END                                                             ACT 1900
```

```
      SUBROUTINE ADSORB (TC, Z, OK, ICALL, IEXCH, MXSP, IPRIN2)       ADS 0010
C ==========================================================================|ADS 0020
C     This is the adsorption routine                                      |ADS 0030
C --------------------------------------------------------------------------|ADS 0040
C     Declare constants                                                   |ADS 0050
C ---------------------                                                   |ADS 0060
C     AVOG       DBL   Avogadro's number                                  |ADS 0070
C     BOLTZ      DBL   Boltzman constant                                  |ADS 0080
C     CPUMIN     DBL   Smallest positive real value program uses          |ADS 0090
C     ECHG       DBL   Electron charge                                    |ADS 0100
C     NMAX       INT   General array dimension to allow easy expansion    |ADS 0110
C     UNO        INT   File unit assigned for output file                 |ADS 0120
C     PERMV      DBL   Perm. in a vacuum                                  |ADS 0130
C     TEST       DBL   Value to test against.                             |ADS 0140
C --------------------------------------------------------------------------|ADS 0150
      INTEGER NMAX, UNO                                                   ADS 0160
      DOUBLE PRECISION AVOG, BOLTZ, CPUMIN, DIE, ECHG, PERMV, TEST        ADS 0170
      PARAMETER (NMAX = 340, UNO = 6)                                     ADS 0180
      PARAMETER (AVOG   = 6.022D+23, BOLTZ = 1.38D-23)                    ADS 0190
      PARAMETER (CPUMIN = 1.0D-35, DIE = 78.27, ECHG = 1.6022D-19)        ADS 0200
      PARAMETER (PERMV  = 8.854D-12, TEST = 1.0D-03)                      ADS 0210
                                                                          ADS 0220
C --------------------------------------------------------------------------|ADS 0230
C     Declare variables                                                   |ADS 0240
C ---------------------                                                   |ADS 0250
C     A1MIX      DBL   HTOT, OHTOT, TIC for initial conditions            |ADS 0260
C     ADD        DBL   Amount of component to add/remove from water       |ADS 0270
C     ANALM      DBL   Analyzed molality of species i                     |ADS 0280
C     ANMIX      DBL   Number of moles of initial components              |ADS 0290
C     ANSWER     DBL   Coefficent array used to calculate results         |ADS 0300
C     B2MIX      DBL   HTOT, OHTOT, and TIC for comp 1 of a mixture       |ADS 0310
C     BNMMIX     DBL   Analyzed molality of species i in solution B       |ADS 0320
C     C3MIX      DBL   Temp storage for HTOT, OHTOT, TIC                  |ADS 0330
C     CEC        DBL   Cation Exchange Capacity                           |ADS 0340
C     CNMMIX     DBL   Temp Storage for total mass of each component      |ADS 0350
C     COEF       DBL   Stoichiometric coefficient and Id number           |ADS 0360
C     CROSS      LOG   Have we crossed the root for species adsorption?   |ADS 0370
```

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      BNMMIX(7)  = TOTEL(3)                                                  ADS 1540
      BNMMIX(98) = 0.0                                                       ADS 1550
      DO 40 I = 1, INSP                                                      ADS 1560
        NEUT = 0                                                             ADS 1570
        II   = 0                                                             ADS 1580
        X    = 0.0                                                           ADS 1590
        IBASE(I) = 0                                                         ADS 1600
        DO 25 K = 1, ISCOMP(I)                                               ADS 1610
          J = IDN(I,K)                                                       ADS 1620
          IF (J .EQ. 0) THEN                                                 ADS 1630
            NEUT = K                                                         ADS 1640
          ELSE                                                               ADS 1650
            IF (II .EQ. 0 .OR. II .EQ.  8 .OR.                               ADS 1660
     .          II .EQ. 9 .OR. II .EQ. 10) THEN                             ADS 1670
              II = J                                                         ADS 1680
              X  = 10.0                                                      ADS 1690
            ELSE                                                             ADS 1700
              IF (COEF(I,K) .LT. X) THEN                                     ADS 1710
                X  = COEF(I,K)                                               ADS 1720
                II = J                                                       ADS 1730
              END IF                                                         ADS 1740
            END IF                                                           ADS 1750
          END IF                                                             ADS 1760
25      CONTINUE                                                             ADS 1770
        IBASE(I) = II                                                        ADS 1780
        DO 30 K = 1, ISCOMP(I)                                               ADS 1790
          J = IDN(I,K)                                                       ADS 1800
          IF (J .EQ. 0 .OR. DABS(COEF(I,K)) .LT. CPUMIN) GO TO 30            ADS 1810
          X = CEC * 1.0D-03 * MBASE(I) / (DABS(COEF(I, NEUT)))               ADS 1820
          X = X * (-1.0) * COEF(I,K)                                         ADS 1830
          EQFAC = 0.0                                                        ADS 1840
          IF (J .EQ.   7) EQFAC =  1.0                                       ADS 1850
          IF (J .EQ.   8) EQFAC =  1.0                                       ADS 1860
          IF (J .EQ.   9) EQFAC = -1.0                                       ADS 1870
          IF (J .EQ.  11) J = 12                                             ADS 1880
          IF (J .EQ.  12) EQFAC =  4.0                                       ADS 1890
          IF (J .EQ.  28) EQFAC =  2.0                                       ADS 1900
          IF (J .EQ.  31) EQFAC = -3.0                                       ADS 1910
          IF (J .EQ.  32) EQFAC = -1.0                                       ADS 1920
          IF (J .EQ.  33) EQFAC =  2.0                                       ADS 1930
          IF (J .EQ.  49) EQFAC =  1.0                                       ADS 1940
          IF (J .EQ.  97) EQFAC =  2.0                                       ADS 1950
          EQH = EQH + (X * EQFAC)                                            ADS 1960
                                                                             ADS 1970
          IF (J .EQ.   7) EQC = (X      ) + EQC                              ADS 1980
          IF (J .EQ.  97) EQC = (X      ) + EQC                              ADS 1990
          IF (J .EQ.  98) EQC = (X      ) + EQC                              ADS 2000
          IF (J .EQ. 207) EQC = (X      ) + EQC                              ADS 2010
          IF (J .EQ. 208) EQC = (X * 2.0) + EQC                              ADS 2020
          IF (J .EQ. 209) EQC = (X * 3.0) + EQC                              ADS 2030
          IF (J .EQ.   7 .OR. J .EQ.  97 .OR. J .EQ.  98 .OR.               ADS 2040
     .        J .EQ. 207 .OR. J .EQ. 208 .OR. J .EQ. 209) J = 7              ADS 2050
                                                                             ADS 2060
          BNMMIX(J) = BNMMIX(J) + X                                          ADS 2070
30      CONTINUE                                                             ADS 2080
40    CONTINUE                                                               ADS 2090
                                                                             ADS 2100
      B2MIX(1) = B2MIX(1) + EQH                                              ADS 2110
```

```
        B2MIX(3) = B2MIX(3) + EQC                                          ADS 2120
        IF (B2MIX(3) .GT. 0.0) THEN                                        ADS 2130
          BNMMIX(7)  = B2MIX(3)                                            ADS 2140
          BNMMIX(98) = 0.0                                                 ADS 2150
        ELSE                                                               ADS 2160
          BNMMIX(7)  = 0.0                                                 ADS 2170
          BNMMIX(98) = 0.0                                                 ADS 2180
        END IF                                                             ADS 2190
                                                                           ADS 2200
        DO 50 I = 1, 11                                                    ADS 2210
          ADD(I)  = 0.0D00                                                 ADS 2220
          STEP(I) = 0.0D00                                                 ADS 2230
   50   CONTINUE                                                          ADS 2240
                                                                           ADS 2250
        Y0 = 0.0                                                           ADS 2260
      END IF                                                               ADS 2270
                                                                           ADS 2280
C -----------------------------------------------------------------------|ADS 2290
C     Zero out local arrays                                              |ADS 2300
C -----------------------------------------------------------------------|ADS 2310
                                                                           ADS 2320
      NEUT = 0                                                             ADS 2330
      DO 80 I = 1,11                                                       ADS 2340
        DO 70 J = 1, 11                                                    ADS 2350
          ANSWER(J,I) = 0.0D00                                             ADS 2360
   70   CONTINUE                                                          ADS 2370
        KNOWN(I) = 0.0D00                                                  ADS 2380
   80 CONTINUE                                                           ADS 2390
                                                                           ADS 2400
C -----------------------------------------------------------------------|ADS 2410
C     Set Coefficient array and known column vector                      |ADS 2420
C -----------------------------------------------------------------------|ADS 2430
                                                                           ADS 2440
  100 DO 120 I = 1, INSP                                                   ADS 2450
        KNOWN(I) = DLOG10(KRXN(I))                                         ADS 2460
        DO 110 J = 1, ISCOMP(I)                                            ADS 2470
          IF (IDN(I,J) .EQ. 0) THEN                                        ADS 2480
            ANSWER(I, 11) = COEF(I,J)                                      ADS 2490
          ELSE                                                             ADS 2500
            IF (IEXCH .EQ. 1) THEN                                         ADS 2510
              KNOWN(I) = KNOWN(I) - (COEF(I,J) * DLOG10((M(IDN(I,J)) *     ADS 2520
     .                   DEXP(((-1.0) * Y0 * DBLE(ISCHG(I))))))))         ADS 2530
            ELSE                                                           ADS 2540
              KNOWN(I) = KNOWN(I) - (COEF(I,J) * DLOG10(M(IDN(I,J))))      ADS 2550
            END IF                                                         ADS 2560
          END IF                                                           ADS 2570
  110   CONTINUE                                                         ADS 2580
        ANSWER(I, I) = 1.0D00                                              ADS 2590
        IF (ISCOMP(I) .EQ. 1 .AND. IDN(I,1) .EQ. 0) NEUT = I               ADS 2600
  120 CONTINUE                                                           ADS 2610
                                                                           ADS 2620
      IF (NEUT .EQ. 0) NEUT = INSP + 1                                     ADS 2630
                                                                           ADS 2640
      DO 130 I = 1, INSP                                                   ADS 2650
        ANSWER(NEUT, I)    = 0.0                                         ADS 2660
        ANSWER(I,    NEUT) = ANSWER(I, 11)                               ADS 2670
        ANSWER(I,    11)   = 0.0D00                                      ADS 2680
  130 CONTINUE                                                           ADS 2690
```

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C     CROSSY    LOG   Have we crossed the root for epsilon?                |ADS 0380
C     DIE       DBL   Dielectric constant                                  |ADS 0390
C     DIFF      DBL   Difference from root                                 |ADS 0400
C     DIFYO     DBL   Difference from YO                                   |ADS 0410
C     DONE      LOG   If we are finished, set to .TRUE.                    |ADS 0420
C     DUM       CHA   Dummy character array                                |ADS 0430
C     EQC       DBL   Equivalent carbon in material been added/removed     |ADS 0440
C     EQFAC     DBL   Factor for adding/removing material                  |ADS 0450
C     EQH       DBL   Equivalent Hydrogen in material added/removed        |ADS 0460
C     EXELT     DBL   Total amount of components                           |ADS 0470
C     HTOTI     DBL   Total hydronium                                      |ADS 0480
C     I         INT   Loop Counter                                         |ADS 0490
C     IBASE     INT   ID numbers of the surface for adsorption             |ADS 0500
C     ICALL     INT   Number of calls to this routine                      |ADS 0510
C     IDN       INT   Id numbers of the ISCOMP components adsorption       |ADS 0520
C     IEXCH     INT   Switch for adsorption/ion exchange                   |ADS 0530
C     II        INT   Local pointer used to check for H, OH or H2O         |ADS 0540
C     INSP      INT   Total number of surface sites for adsorption         |ADS 0550
C     IPRIN2    INT   Print switch to print out iterations                 |ADS 0560
C     ISCHG     INT   Charge of each surface site for adsorption           |ADS 0570
C     ISCOMP    INT   Total number of components in dissociation           |ADS 0580
C     IVAL      INT   Number of Iterations                                 |ADS 0590
C     IY        INT   Pointer to last value calculated                     |ADS 0600
C     J         INT   Loop counter                                         |ADS 0610
C     K         INT   Loop counter                                         |ADS 0620
C     KNOWN     DBL   Final value of moles of complex on surface           |ADS 0630
C     KRXN      DBL   K for dissociation reaction of surface species       |ADS 0640
C     M         DBL   Calculated molality of aqueous species               |ADS 0650
C     MAT       DBL   Matrix used for intermediate calculations            |ADS 0660
C     MBASE     DBL   Equivalence Mole Fraction (initial) on surface       |ADS 0670
C     MXSP      INT   Max number of species                                |ADS 0680
C     NEUT      INT   Index for the bare surface complex                   |ADS 0690
C     OHTOTI    DBL   Initial OH total                                     |ADS 0700
C     OK        INT   Normal exit?                                         |ADS 0710
C     PAGE1     CHA   Names of aqueous species                             |ADS 0720
C     SIGD      DBL   Charge density in the difuse layer                   |ADS 0730
C     SIGO      DBL   Charge density at the surface                        |ADS 0740
C     SINGLE    LOG   Switch if all surface comp. have same # of X's       |ADS 0750
C     SPN       CHA   Name of each surface species adsorption              |ADS 0760
C     STEP      DBL   Step size for amount added/sub                       |ADS 0770
C     SUM       DBL   Total of charged species on surface                  |ADS 0780
C     TC        DBL   Temperature in deg C                                 |ADS 0790
C     TITR      DBL   Iteration array in DISTRB, used for guesses          |ADS 0800
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                     |ADS 0810
C     TRYV      DBL   Working storage for mass on surface                  |ADS 0820
C     TRYYO     DBL   Guess for YO                                         |ADS 0830
C     VAL       DBL   Intermediate storage                                 |ADS 0840
C     VECT      DBL   Solution vector for surface complexes                |ADS 0850
C     X         DBL   Temperary storage                                    |ADS 0860
C     YO        DBL   YO                                                   |ADS 0870
C     Z         INT   Charge of aqueous species                            |ADS 0880
C -------------------------------------------------------------------------|ADS 0890
                                                                           ADS 0900
      LOGICAL DONE, CROSS, CROSSY, SINGLE                                  ADS 0910
                                                                           ADS 0920
      CHARACTER*8  PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                   ADS 0930
      CHARACTER*8  DUM(11)                                                 ADS 0940
      CHARACTER*10 SPN(10)                                                 ADS 0950
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                                                                      ADS 0960
      INTEGER I, IBASE(10), ICALL                                     ADS 0970
      INTEGER IDN(10,10), IEXCH, II, IPRIN2, ISCHG(10), INSP          ADS 0980
      INTEGER IPAGE, IPGLN, ISCOMP(10), IVAL, IY, J, K, MXSP          ADS 0990
      INTEGER NEUT, OK, Z(NMAX)                                       ADS 1000
                                                                      ADS 1010
      DOUBLE PRECISION ADD(11), ADENS, ALFA(NMAX), ANALM(NMAX)        ADS 1020
      DOUBLE PRECISION ANMMIX(NMAX), ANSWER(11,11), ATEMP, A1MIX(5)   ADS 1030
      DOUBLE PRECISION BDENS, BNMMIX(NMAX), BTEMP, B2MIX(5)           ADS 1040
      DOUBLE PRECISION CEC, CNMMIX(NMAX), COEF(10,10)                 ADS 1050
      DOUBLE PRECISION CUNITS(NMAX), CO2F, C3MIX(5), DIFF(10)         ADS 1060
      DOUBLE PRECISION DIFY0(10), EQC, EQFAC, EQH                     ADS 1070
      DOUBLE PRECISION EXELT(35), FMIX(10), HTOTI, KNOWN(11)          ADS 1080
      DOUBLE PRECISION KRXN(10), M(NMAX), MAT(10,10), MBASE(10)       ADS 1090
      DOUBLE PRECISION OHTOTI, PH, SAREA, SIGD, SIGO                  ADS 1100
      DOUBLE PRECISION STEP(11), SUM, TAREA, TC, TITR(11)             ADS 1110
      DOUBLE PRECISION TOTEL(5), TRYV(10), TRYY0(10)                  ADS 1120
      DOUBLE PRECISION VAL, VECT(10), X, Y0                           ADS 1130
                                                                      ADS 1140
      EXTERNAL GUESS, SORTA, PAGE                                     ADS 1150
                                                                      ADS 1160
      INTRINSIC DABS, DBLE, DEXP, DLOG10, DSIGN, MAX0, DSQRT          ADS 1170
                                                                      ADS 1180
      COMMON /EXCHAN/ COEF, MBASE, KRXN, CEC, TAREA, SAREA, IDN,      ADS 1190
     .                ISCHG, ISCOMP, INSP                            ADS 1200
      COMMON /EXTOT / EXELT, TOTEL, TITR                              ADS 1210
      COMMON /FORM  / IPAGE, IPGLN                                    ADS 1220
      COMMON /MM    / ANMMIX, A1MIX, B2MIX, FMIX, BNMMIX, ADENS, BDENS, ADS 1230
     .                ATEMP, BTEMP                                   ADS 1240
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                      ADS 1250
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                             ADS 1260
      COMMON /NAMES2/ SPN                                             ADS 1270
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                             ADS 1280
                                                                      ADS 1290
      SAVE ADD, IBASE, KNOWN, STEP, Y0                                ADS 1300
                                                                      ADS 1310
C =====================================================================|ADS 1320
                                                                      ADS 1330
      IY     = 0                                                      ADS 1340
      CROSSY = .FALSE.                                                ADS 1350
                                                                      ADS 1360
C ---------------------------------------------------------------------|ADS 1370
C     Store solution parameters if first call                         |ADS 1380
C     totel: (1) = htot;  (2) = ohtot; (3) = tic                      |ADS 1390
C ---------------------------------------------------------------------|ADS 1400
      IF (ICALL .EQ. 1) THEN                                          ADS 1410
        DO 10 I = 1, 5                                                ADS 1420
          A1MIX(I) = TOTEL(I)                                         ADS 1430
          B2MIX(I) = TOTEL(I)                                         ADS 1440
   10   CONTINUE                                                      ADS 1450
                                                                      ADS 1460
        DO 20 I = 1, MXSP + 44                                        ADS 1470
          ANMMIX(I) = ANALM(I)                                        ADS 1480
          BNMMIX(I) = ANALM(I)                                        ADS 1490
   20   CONTINUE                                                      ADS 1500
                                                                      ADS 1510
        EQC = 0.0                                                     ADS 1520
        EQH = 0.0                                                     ADS 1530
```

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                                                                      ADS 2700
      SINGLE = .TRUE.                                                 ADS 2710
                                                                      ADS 2720
      DO 132 I = 1, (INSP-1)                                          ADS 2730
        IF (DABS(ANSWER(I,NEUT) - ANSWER(INSP,NEUT)) .GT. 1.0E-05)    ADS 2740
     .    SINGLE = .FALSE.                                           ADS 2750
  132 CONTINUE                                                        ADS 2760
                                                                      ADS 2770
      KNOWN(NEUT)       = 0.0                                       ADS 2780
      ANSWER(NEUT,NEUT) = 1.0                                       ADS 2790
                                                                      ADS 2800
C -------------------------------------------------------------------|ADS 2810
C     Now normalize values and get current values                    |ADS 2820
C -------------------------------------------------------------------|ADS 2830
                                                                      ADS 2840
      IF (SINGLE) THEN                                              ADS 2850
        SUM = 0.0                                                   ADS 2860
        DO 150 I = 1, INSP                                          ADS 2870
          KNOWN(I) = 10.0**KNOWN(I)                                 ADS 2880
          SUM = SUM + (KNOWN(I) * DABS(ANSWER(I,NEUT)))             ADS 2890
  150   CONTINUE                                                    ADS 2900
                                                                      ADS 2910
        DO 160 I = 1, INSP                                          ADS 2920
          KNOWN(I) = KNOWN(I) * CEC / (1000.0 * SUM)                ADS 2930
  160   CONTINUE                                                    ADS 2940
                                                                      ADS 2950
      ELSE                                                          ADS 2960
        CROSS = .FALSE.                                             ADS 2970
        IVAL = 0                                                    ADS 2980
        VAL = 0.0D00                                                ADS 2990
  200   DO 220 I = 1, MAX0(INSP, NEUT)                              ADS 3000
          VECT(I) = KNOWN(I)                                        ADS 3010
          DO 210 K = 1, MAX0(INSP, NEUT)                            ADS 3020
            MAT(K,I) = ANSWER(K,I)                                  ADS 3030
  210     CONTINUE                                                  ADS 3040
  220   CONTINUE                                                    ADS 3050
                                                                      ADS 3060
        VECT(NEUT) = VAL                                            ADS 3070
                                                                      ADS 3080
        DO 250 I = 1, MAX0(INSP, NEUT)                              ADS 3090
          IF (I .NE. NEUT) THEN                                     ADS 3100
            X = MAT(I,NEUT) / MAT(NEUT,NEUT)                        ADS 3110
            VECT(I) = VECT(I) - (X * VECT(NEUT))                    ADS 3120
          END IF                                                    ADS 3130
  250   CONTINUE                                                    ADS 3140
                                                                      ADS 3150
        SUM = 0.0                                                   ADS 3160
        DO 260 I = 1, INSP                                          ADS 3170
          SUM = SUM + (10.0**VECT(I))                               ADS 3180
  260   CONTINUE                                                    ADS 3190
                                                                      ADS 3200
        IVAL = IVAL + 1                                             ADS 3210
        TRYV(IVAL) = VAL                                            ADS 3220
        DIFF(IVAL) = SUM - 1.0D00                                   ADS 3230
        IF (DABS(DIFF(IVAL)) .GT. TEST) THEN                        ADS 3240
          IF (IVAL .GT. 1 .AND. .NOT. CROSS) THEN                   ADS 3250
            IF ((DIFF(IVAL) * DIFF(IVAL-1)) .LT. 0.0) CROSS = .TRUE.ADS 3260
          END IF                                                    ADS 3270
```

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        IF (IVAL .GT. 1) THEN                                                ADS 3280
          I = 1                                                              ADS 3290
          CALL SORTA(TRYV, DIFF, IVAL, I)                                    ADS 3300
        END IF                                                               ADS 3310
        IF (CROSS) THEN                                                      ADS 3320
          K = 0                                                              ADS 3330
          DO 270 I = 1, (IVAL-1)                                             ADS 3340
            IF ((DIFF(I) * DIFF(I+1)) .LT. 0.0) K = I                        ADS 3350
270       CONTINUE                                                           ADS 3360
          IF (IVAL .GT. 5) THEN                                              ADS 3370
            IF (K .GT. (IVAL/2)) THEN                                        ADS 3380
              DO 280 I = 1, (IVAL-1)                                         ADS 3390
                DIFF(I) = DIFF(I+1)                                          ADS 3400
                TRYV(I) = TRYV(I+1)                                          ADS 3410
280           CONTINUE                                                       ADS 3420
              K = K - 1                                                      ADS 3430
            END IF                                                           ADS 3440
            IVAL = IVAL - 1                                                  ADS 3450
          END IF                                                             ADS 3460
          CALL GUESS(TRYV, DIFF, VAL, IVAL)                                  ADS 3470
          X = DABS(TRYV(K) - TRYV(K+1)) / 10000.0D00                         ADS 3480
          IF (DABS (TRYV(K)   - VAL) .LT. X    .OR.                          ADS 3490
              DABS (TRYV(K+1) - VAL) .LT. X )  THEN                          ADS 3500
            VAL = (TRYV(K) + TRYV(K+1)) / 2.0                                ADS 3510
          END IF                                                             ADS 3520
        END IF                                                               ADS 3530
        IF (.NOT. CROSS) THEN                                                ADS 3540
          IF (IVAL .GT. 2) THEN                                              ADS 3550
            DO 290 I = 1, (IVAL-1)                                           ADS 3560
              DIFF(I) = DIFF(I+1)                                            ADS 3570
              TRYV(I) = TRYV(I+1)                                            ADS 3580
290         CONTINUE                                                         ADS 3590
            IVAL = IVAL - 1                                                  ADS 3600
          END IF                                                             ADS 3610
          IF (IVAL .EQ. 1) THEN                                              ADS 3620
            VAL = VAL - 1.0D00                                               ADS 3630
          ELSE IF (DABS(DIFF(IVAL)) .LT. DABS(DIFF(IVAL-1))) THEN            ADS 3640
            VAL = (2.0 * TRYV(IVAL)) - TRYV(IVAL-1)                          ADS 3650
          ELSE                                                               ADS 3660
            VAL = (2.0 * TRYV(IVAL-1)) - TRYV(IVAL)                          ADS 3670
          END IF                                                             ADS 3680
        END IF                                                               ADS 3690
        GO TO 200                                                            ADS 3700
      END IF                                                                 ADS 3710
                                                                             ADS 3720
      DO 300 I = 1, INSP                                                     ADS 3730
        KNOWN(I) = (10.0**VECT(I)) * CEC * 1.0D-3 /                          ADS 3740
                   DABS(ANSWER(I,NEUT))                                      ADS 3750
300   CONTINUE                                                               ADS 3760
    END IF                                                                   ADS 3770
                                                                             ADS 3780
    IF (IEXCH .EQ. 1) THEN                                                   ADS 3790
      SIGO = 0.0D00                                                          ADS 3800
      SUM  = 0.0D00                                                          ADS 3810
      DO 330 I = 1, INSP                                                     ADS 3820
        IF (ISCHG(I) .NE. 0) SIGO = (DBLE(ISCHG(I)) * KNOWN(I)) + SIGOADS 3830
        J    = 0                                                           ADS 3840
        DO 320 K = 1, ISCOMP(I)                                            ADS 3850
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          IF (IDN(I,K) .EQ. 0) J = K                                    ADS 3860
320       CONTINUE                                                      ADS 3870
          SUM  = SUM  + (DABS(COEF(I,J)) * KNOWN(I))                    ADS 3880
330     CONTINUE                                                        ADS 3890
        SIGO = ECHG * CEC * AVOG * SIGO / (SUM * 1000.0)                ADS 3900
        SIGD = 0.0D00                                                   ADS 3910
        DO 350 I = 1, MXSP + 44                                         ADS 3920
          SIGD = (M(I) * (DEXP(DBLE(Z(I)) * Y0 * (-1.0D0)) - 1.0D0)) +  ADS 3930
     .           SIGD                                                   ADS 3940
350     CONTINUE                                                        ADS 3950
        SIGD = SIGD * 1000.0D00 * AVOG                                  ADS 3960
        IF (SIGD .GT. CPUMIN) THEN                                      ADS 3970
          SIGD = DSQRT(SIGD)                                            ADS 3980
        ELSE                                                            ADS 3990
          SIGD = 0.0D00                                                 ADS 4000
        END IF                                                          ADS 4010
        SIGD = SIGD * DSQRT(2.0D00 * PERMV * DIE)                       ADS 4020
        SIGD = SIGD * DSQRT(BOLTZ  * (TC + 273.15))                     ADS 4030
        IY = IY + 1                                                     ADS 4040
        TRYY0(IY) = Y0                                                  ADS 4050
        DIFY0(IY) = SIGD + SIGO                                         ADS 4060
        IF (DABS(DIFY0(IY)) .GT. TEST) THEN                             ADS 4070
          IF (IY .GT. 1 .AND. .NOT. CROSSY) THEN                        ADS 4080
            IF ((DIFY0(IY) * DIFY0(IY-1)) .LT. 0.0) CROSSY = .TRUE.     ADS 4090
          END IF                                                        ADS 4100
          IF (CROSSY) THEN                                              ADS 4110
            I = 1                                                       ADS 4120
            CALL SORTA(TRYY0, DIFY0, IY, I)                             ADS 4130
          END IF                                                        ADS 4140
          IF (IY .GT. 6) THEN                                           ADS 4150
            K = 0                                                       ADS 4160
            IF (CROSSY) THEN                                            ADS 4170
              DO 370 I = 1, (IY-1)                                      ADS 4180
                IF ((DIFY0(I) * DIFY0(I+1)) .LT. 0.0) K = I             ADS 4190
370           CONTINUE                                                  ADS 4200
            END IF                                                      ADS 4210
            IF (K .GT. (IY/2) .OR. .NOT. CROSSY) THEN                   ADS 4220
              DO 380 I = 1, (IY-1)                                      ADS 4230
                DIFY0(I) = DIFY0(I+1)                                   ADS 4240
                TRYY0(I) = TRYY0(I+1)                                   ADS 4250
380           CONTINUE                                                  ADS 4260
              K = K - 1                                                 ADS 4270
            END IF                                                      ADS 4280
            IY = IY - 1                                                 ADS 4290
          END IF                                                        ADS 4300
          IF (CROSSY) THEN                                              ADS 4310
            CALL GUESS(TRYY0, DIFY0, Y0, IY)                            ADS 4320
            X = DABS(TRYY0(K) - TRYY0(K+1)) / 10000.0D00                ADS 4330
            IF (DABS (TRYY0(K)   - Y0) .LT. X    .OR.                   ADS 4340
     .          DABS (TRYY0(K+1) - Y0) .LT. X )  THEN                   ADS 4350
              VAL = (TRYY0(K) + TRYY0(K+1)) / 2.0                       ADS 4360
            END IF                                                      ADS 4370
          ELSE                                                          ADS 4380
            IF (DIFY0(IY) .GT. 0.0) THEN                                ADS 4390
              Y0 = Y0 + 0.1D00                                          ADS 4400
            ELSE                                                        ADS 4410
              Y0 = Y0 - 1.0D00                                          ADS 4420
            END IF                                                      ADS 4430
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          END IF                                                          ADS 4440
          GO TO 100                                                       ADS 4450
        END IF                                                            ADS 4460
      END IF                                                              ADS 4470
                                                                          ADS 4480
C ------------------------------------------------------------------------|ADS 4490
C     Check totels, see if we are done, calculate step size.             |ADS 4500
C          Always iterate at least once.                                  |ADS 4510
C ------------------------------------------------------------------------|ADS 4520
                                                                          ADS 4530
  500 DO 505 I = 1, MXSP + 44                                             ADS 4540
        CNMMIX(I) = ANALM(I)                                              ADS 4550
  505 CONTINUE                                                            ADS 4560
                                                                          ADS 4570
      EQC = 0.0                                                           ADS 4580
      EQH = 0.0                                                           ADS 4590
      CNMMIX(7)  = TOTEL(3)                                               ADS 4600
      CNMMIX(98) = 0.0                                                    ADS 4610
      DO 520 I = 1, INSP                                                  ADS 4620
        DO 510 K = 1, ISCOMP(I)                                           ADS 4630
          J = IDN(I,K)                                                    ADS 4640
          IF (J .EQ. 0 .OR. DABS(COEF(I,K)) .LT. CPUMIN) GO TO 510        ADS 4650
          X = KNOWN(I) * COEF(I,K) * (-1.0)                               ADS 4660
          EQFAC = 0.0                                                     ADS 4670
          IF (J .EQ.   7) EQFAC =  1.0                                    ADS 4680
          IF (J .EQ.   8) EQFAC =  1.0                                    ADS 4690
          IF (J .EQ.   9) EQFAC = -1.0                                    ADS 4700
          IF (J .EQ.  11) J = 12                                          ADS 4710
          IF (J .EQ.  12) EQFAC =  4.0                                    ADS 4720
          IF (J .EQ.  28) EQFAC =  2.0                                    ADS 4730
          IF (J .EQ.  31) EQFAC = -3.0                                    ADS 4740
          IF (J .EQ.  32) EQFAC = -1.0                                    ADS 4750
          IF (J .EQ.  33) EQFAC =  2.0                                    ADS 4760
          IF (J .EQ.  49) EQFAC =  1.0                                    ADS 4770
          IF (J .EQ.  97) EQFAC =  2.0                                    ADS 4780
          EQH = EQH + (X * EQFAC)                                         ADS 4790
                                                                          ADS 4800
          IF (J .EQ.   7) EQC = (X      ) + EQC                           ADS 4810
          IF (J .EQ.  97) EQC = (X      ) + EQC                           ADS 4820
          IF (J .EQ.  98) EQC = (X      ) + EQC                           ADS 4830
          IF (J .EQ. 207) EQC = (X      ) + EQC                           ADS 4840
          IF (J .EQ. 208) EQC = (X * 2.0) + EQC                           ADS 4850
          IF (J .EQ. 209) EQC = (X * 3.0) + EQC                           ADS 4860
          IF (J .EQ.   7 .OR. J .EQ.  97 .OR. J .EQ.  98 .OR.            ADS 4870
     .        J .EQ. 207 .OR. J .EQ. 208 .OR. J .EQ. 209) J = 7           ADS 4880
                                                                          ADS 4890
          CNMMIX(J) = CNMMIX(J) + X                                       ADS 4900
  510   CONTINUE                                                          ADS 4910
  520 CONTINUE                                                            ADS 4920
                                                                          ADS 4930
      C3MIX(1) = TOTEL(1) + EQH                                           ADS 4940
      C3MIX(2) = TOTEL(2)                                                 ADS 4950
      C3MIX(3) = TOTEL(3) + EQC                                           ADS 4960
      IF (C3MIX(3) .GT. 0.0) THEN                                         ADS 4970
        CNMMIX(7)  = C3MIX(3)                                             ADS 4980
        CNMMIX(98) = 0.0                                                  ADS 4990
      ELSE                                                                ADS 5000
        CNMMIX(7)  = 0.0                                                  ADS 5010
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      CNMMIX(98) = 0.0                                                  ADS 5020
    END IF                                                              ADS 5030
                                                                        ADS 5040
    IF (ICALL .EQ. 1) THEN                                              ADS 5050
      DONE = .FALSE.                                                    ADS 5060
      DO 530 I = 1, INSP                                                ADS 5070
        J = IBASE(I)                                                    ADS 5080
        IF (J .EQ. 11) J = 12                                           ADS 5090
        IF (J .NE.  0 .AND. J .NE. 8 .AND. J .NE. 9 .AND. J .NE. 10)    ADS 5100
     .    THEN                                                         ADS 5110
          STEP(I) = (BNMMIX(J) - CNMMIX(J)) * 0.25                      ADS 5120
        ELSE IF (J .EQ. 8 .OR. J .EQ. 9) THEN                           ADS 5130
          X = (B2MIX(1) - B2MIX(2)) - (C3MIX(1) - C3MIX(2))             ADS 5140
          IF (DABS(X) .GT. 1.0E-06) STEP(I) = X * 0.1                   ADS 5150
        END IF                                                          ADS 5160
        IF (DABS(STEP(I)) .LT. CPUMIN) THEN                             ADS 5170
          STEP(I) = (CEC / 1000.0) / 100.0                              ADS 5180
        END IF                                                          ADS 5190
530   CONTINUE                                                          ADS 5200
      IF (INSP .EQ. 2) THEN                                             ADS 5210
        X = (DABS(STEP(1)) + DABS(STEP(2))) / 2.0                       ADS 5220
        STEP(1) = DSIGN(X, STEP(1))                                     ADS 5230
        STEP(2) = DSIGN(X, STEP(2))                                     ADS 5240
      END IF                                                            ADS 5250
    ELSE                                                                ADS 5260
      DONE = .TRUE.                                                     ADS 5270
      DO 550 I = 1, INSP                                                ADS 5280
        J = IBASE(I)                                                    ADS 5290
        IF (J .NE. 0 .AND. J .NE.  8 .AND. J .NE. 9 .AND. J .NE. 10)    ADS 5300
     .    THEN                                                         ADS 5310
          IF ((DABS(BNMMIX(J) - CNMMIX(J)) / BNMMIX(J)) .GT. TEST)      ADS 5320
     .      DONE = .FALSE.                                             ADS 5330
          IF ((BNMMIX(J) - CNMMIX(J)) .GT. 0.0) THEN                    ADS 5340
            IF (STEP(I) .LT. 0.0) STEP(I) = STEP(I) * (-0.4)            ADS 5350
          ELSE                                                          ADS 5360
            IF (STEP(I) .GT. 0.0) STEP(I) = STEP(I) * (-0.4)            ADS 5370
          END IF                                                        ADS 5380
        ELSE IF (J .EQ. 8 .OR. J .EQ. 9) THEN                           ADS 5390
          X = (B2MIX(1) - B2MIX(2)) - (C3MIX(1) - C3MIX(2))             ADS 5400
          IF ((DABS(B2MIX(1) - B2MIX(2))) .GT. 1.0D-8)                  ADS 5410
     .      X = X / (B2MIX(1) - B2MIX(2))                               ADS 5420
          IF (DABS(X) .GT. TEST) DONE = .FALSE.                         ADS 5430
          IF (X .GT. 0.0) THEN                                          ADS 5440
            IF (STEP(I) .LT. 0.0) STEP(I) = STEP(I) * (-0.4)            ADS 5450
          ELSE                                                          ADS 5460
            IF (STEP(I) .GT. 0.0) STEP(I) = STEP(I) * (-0.4)            ADS 5470
          END IF                                                        ADS 5480
        END IF                                                          ADS 5490
550   CONTINUE                                                          ADS 5500
    END IF                                                              ADS 5510
                                                                        ADS 5520
    IF (DONE) THEN                                                      ADS 5530
      J = NEUT                                                          ADS 5540
      IF (NEUT .EQ. 0) J = INSP+1                                       ADS 5550
      OK = 0                                                            ADS 5560
      CALL PAGE                                                         ADS 5570
      IPGLN = IPGLN + 26 + (INSP * 3)                                   ADS 5580
      WRITE (UNO, 1005)                                                 ADS 5590
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      WRITE (UNO, 1002)                                                  ADS 5600
      DO 600 I = 1, INSP                                                 ADS 5610
        WRITE (UNO, 1003) SPN(I),                                        ADS 5620
     .       (MBASE(I) * CEC / (1000.0 * DABS(ANSWER(I,J)))),            ADS 5630
     .       (MBASE(I) * CEC / 1000.0), MBASE(I)                         ADS 5640
  600 CONTINUE                                                           ADS 5650
                                                                         ADS 5660
      WRITE (UNO, 1007)                                                  ADS 5670
      DO 620 I = 1, INSP                                                 ADS 5680
        DO 610 K = 1, ISCOMP(I)                                          ADS 5690
          IF (IDN(I,K) .EQ. 0) THEN                                      ADS 5700
            DUM(K) = 'X-      '                                          ADS 5710
          ELSE                                                           ADS 5720
            DUM(K) = PAGE1(IDN(I,K))                                     ADS 5730
          END IF                                                         ADS 5740
  610     CONTINUE                                                       ADS 5750
        WRITE (UNO, 1008) KRXN(I), SPN(I), (DUM(K), COEF(I,K), K=1,      ADS 5760
     .                    ISCOMP(I))                                     ADS 5770
  620 CONTINUE                                                           ADS 5780
                                                                         ADS 5790
      WRITE (UNO, 1001)                                                  ADS 5800
      WRITE (UNO, 1002)                                                  ADS 5810
      DO 650 I = 1, INSP                                                 ADS 5820
        WRITE (UNO, 1003) SPN(I),  KNOWN(I),                             ADS 5830
     .       (KNOWN(I) * DABS(ANSWER(I,J))),                             ADS 5840
     .       (KNOWN(I) * 1000.0 * DABS(ANSWER(I,J)) / CEC)               ADS 5850
  650 CONTINUE                                                           ADS 5860
                                                                         ADS 5870
      WRITE (UNO, 1006) CEC, (CEC / 1000.0)                              ADS 5880
      RETURN                                                             ADS 5890
    END IF                                                               ADS 5900
                                                                         ADS 5910
C ------------------------------------------------------------------------|ADS 5920
C     Change the original solution parameters for the new step and       |ADS 5930
C     go back to calculate species distribution                          |ADS 5940
C ------------------------------------------------------------------------|ADS 5950
                                                                         ADS 5960
  700 EQC = 0.0                                                          ADS 5970
      EQH = 0.0                                                          ADS 5980
      ANALM(7)  = A1MIX(3)                                               ADS 5990
      ANALM(98) = 0.0                                                    ADS 6000
      DO 710 I = 1, INSP                                                 ADS 6010
        ADD(I) = ADD(I) + STEP(I)                                        ADS 6020
  710 CONTINUE                                                           ADS 6030
                                                                         ADS 6040
      DO 730 I = 1, INSP                                                 ADS 6050
        DO 720 K = 1, ISCOMP(I)                                          ADS 6060
          J = IDN(I,K)                                                   ADS 6070
          IF (J .EQ. 0 .OR. DABS(COEF(I,K)) .LT. CPUMIN) GO TO 720       ADS 6080
          X = COEF(I,K) * ADD(I) * (-1.0)                                ADS 6090
          EQFAC = 0.0                                                    ADS 6100
          IF (J .EQ.   7) EQFAC =  1.0                                   ADS 6110
          IF (J .EQ.   8) EQFAC =  1.0                                   ADS 6120
          IF (J .EQ.   9) EQFAC = -1.0                                   ADS 6130
          IF (J .EQ.  11) J = 12                                         ADS 6140
          IF (J .EQ.  12) EQFAC =  4.0                                   ADS 6150
          IF (J .EQ.  28) EQFAC =  2.0                                   ADS 6160
          IF (J .EQ.  31) EQFAC = -3.0                                   ADS 6170
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      IF (J .EQ.  32) EQFAC = -1.0                                      ADS 6180
      IF (J .EQ.  33) EQFAC =  2.0                                      ADS 6190
      IF (J .EQ.  49) EQFAC =  1.0                                      ADS 6200
      IF (J .EQ.  97) EQFAC =  2.0                                      ADS 6210
      EQH = EQH + (X * EQFAC)                                           ADS 6220
                                                                        ADS 6230
      IF (J .EQ.   7) EQC = (X      ) + EQC                             ADS 6240
      IF (J .EQ.  97) EQC = (X      ) + EQC                             ADS 6250
      IF (J .EQ.  98) EQC = (X      ) + EQC                             ADS 6260
      IF (J .EQ. 207) EQC = (X      ) + EQC                             ADS 6270
      IF (J .EQ. 208) EQC = (X * 2.0) + EQC                             ADS 6280
      IF (J .EQ. 209) EQC = (X * 3.0) + EQC                             ADS 6290
      IF (J .EQ.   7 .OR. J .EQ.  97 .OR. J .EQ.  98 .OR.               ADS 6300
     .    J .EQ. 207 .OR. J .EQ. 208 .OR. J .EQ. 209) J = 7              ADS 6310
                                                                        ADS 6320
      ANALM(J) = ANMMIX(J) + X                                          ADS 6330
      IF (J .NE. 8 .AND. J .NE. 9 .AND. J .NE. 10                       ADS 6340
     .                .AND. ANALM(J) .LE. 0.0) THEN                    ADS 6350
        DO 715 J = 1, INSP                                              ADS 6360
          ADD(J)  = ADD(J)  - STEP(J)                                   ADS 6370
          STEP(J) = STEP(J) * (0.5D00)                                  ADS 6380
715       CONTINUE                                                      ADS 6390
          GO TO 700                                                     ADS 6400
        END IF                                                          ADS 6410
720   CONTINUE                                                          ADS 6420
730 CONTINUE                                                            ADS 6430
                                                                        ADS 6440
    TOTEL(1) = A1MIX(1) + EQH                                           ADS 6450
    TOTEL(3) = A1MIX(3) + EQC                                           ADS 6460
    IF (TOTEL(3) .GT. 0.0) THEN                                         ADS 6470
      ANALM(7)  = TOTEL(3)                                              ADS 6480
      ANALM(98) = 0.0                                                   ADS 6490
    ELSE                                                                ADS 6500
      ANALM(7)  = 0.0                                                   ADS 6510
      ANALM(98) = 0.0                                                   ADS 6520
    END IF                                                              ADS 6530
                                                                        ADS 6540
    J = 0                                                               ADS 6550
    DO 800 I = 1, 28                                                    ADS 6560
      J = J + 1                                                         ADS 6570
      IF (J .EQ.   8) J = 12                                            ADS 6580
      IF (J .EQ.  17) J = 18                                            ADS 6590
      IF (J .EQ.  19) J = 21                                            ADS 6600
      IF (J .EQ.  24) J = 25                                            ADS 6610
      IF (J .EQ.  34) J = 48                                            ADS 6620
      IF (J .EQ.  49) J = 169                                           ADS 6630
      IF (J .EQ. 170) J = 210                                           ADS 6640
      EXELT(I)  = ANALM(J)                                              ADS 6650
800 CONTINUE                                                            ADS 6660
    EXELT(29)  = ANALM(7)                                               ADS 6670
    EXELT(30)  = ANALM(246)                                             ADS 6680
    EXELT(31)  = ANALM(265)                                             ADS 6690
    EXELT(32)  = ANALM(136)                                             ADS 6700
    EXELT(33)  = ANALM(MXSP+1)                                          ADS 6710
    EXELT(34)  = ANALM(MXSP+16)                                         ADS 6720
    EXELT(35)  = ANALM(MXSP+31)                                         ADS 6730
                                                                        ADS 6740
    TITR( 1) = EXELT(29)                                                ADS 6750
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      TITR( 2) = EXELT( 6)                                                  ADS 6760
      TITR( 3) = EXELT(22)                                                  ADS 6770
      TITR( 4) = EXELT(21)                                                  ADS 6780
      TITR( 5) = EXELT( 5)                                                  ADS 6790
      TITR( 6) = EXELT(26)                                                  ADS 6800
      TITR( 7) = EXELT(25)                                                  ADS 6810
      TITR( 8) = EXELT(30)                                                  ADS 6820
      TITR( 9) = EXELT(31)                                                  ADS 6830
      TITR(10) = EXELT(33)                                                  ADS 6840
      TITR(11) = EXELT(34)                                                  ADS 6850
                                                                            ADS 6860
      HTOTI  = TOTEL(1)                                                     ADS 6870
      OHTOTI = TOTEL(2)                                                     ADS 6880
                                                                            ADS 6890
      J = NEUT                                                              ADS 6900
      IF (NEUT .EQ. 0) J = INSP+1                                           ADS 6910
      OK = 1                                                                ADS 6920
      IF (IPRIN2 .NE. 0) THEN                                               ADS 6930
        IF ((IPGLN + INSP + 9) .GT. 58) CALL PAGE                           ADS 6940
        IPGLN = IPGLN + INSP + 9                                            ADS 6950
        WRITE (UNO, 1000)                                                   ADS 6960
        WRITE (UNO, 1002)                                                   ADS 6970
        DO 970 I = 1, INSP                                                  ADS 6980
          WRITE (UNO, 1003) SPN(I), KNOWN(I),                               ADS 6990
     .          (KNOWN(I) * DABS(ANSWER(I,J))),                            ADS 7000
     .          (KNOWN(I) * 1000.0 * DABS(ANSWER(I,J)) / CEC)              ADS 7010
  970   CONTINUE                                                            ADS 7020
                                                                            ADS 7030
        WRITE (UNO, 1004)                                                   ADS 7040
      END IF                                                                ADS 7050
                                                                            ADS 7060
      RETURN                                                                ADS 7070
                                                                            ADS 7080
 1000 FORMAT(//,  ' Surface Conditions calculated for the next',            ADS 7090
     .           ' step ..... ')                                            ADS 7100
 1001 FORMAT(///, '  Final Equilibrium Surface Conditions .........')       ADS 7110
 1002 FORMAT( /,3X, 'Surface', 9X, 'Moles on', 11X, 'Moles of',     6X,     ADS 7120
     .              ' Fraction of',                                         ADS 7130
     .        /,3X, 'Complex', 9X, 'Surface',  10X, 'Surface Site', 4X,    ADS 7140
     .              'Surface Sites')                                        ADS 7150
 1003 FORMAT(5X, A, 2X, E12.5, 7X, E12.5, 7X, F6.4)                         ADS 7160
 1004 FORMAT(//)                                                            ADS 7170
 1005 FORMAT(//, '  Initial Surface Conditions .........')                  ADS 7180
 1006 FORMAT(//, '  CEC = ',E12.5,' milli-equivalents ',                    ADS 7190
     .        /, '        ',E12.5,' moles exchange capacity for mono',      ADS 7200
     .                    'valent cations and anions')                    ADS 7210
 1007 FORMAT(//, '    K        Surface Comp.   Species and Coef. .... '     ADS 7220
     .         ,/)                                                        ADS 7230
 1008 FORMAT(E12.5, ' =  ',A, 10(' * (',A,'**',F6.2,')',:))                 ADS 7240
      END                                                                   ADS 7250



      SUBROUTINE AITLIM (X, Y, CROSS)                                       AIT 0010
C ======================================================================|AIT 0020
C     Determines maximum stepsize for convergence on anions              |AIT 0030
```

```
C -------------------------------------------------------------------|AIT 0040
C     CROSS     LOG   Indicates root has been crossed                |AIT 0050
C     RATIO     DBL   Test value based on Y                          |AIT 0060
C     X         DBL   Multiplication factor for stepsize             |AIT 0070
C     Y         DBL   Currently calculated value over mass of        |AIT 0080
C                     component in solution                          |AIT 0090
C -------------------------------------------------------------------|AIT 0100
      DOUBLE PRECISION X, Y, RATIO                                     AIT 0110
      LOGICAL CROSS                                                    AIT 0120
      INTRINSIC DABS                                                   AIT 0130
C ===================================================================|AIT 0140
                                                                       AIT 0150
      RATIO = DABS(1.0D00 - Y)                                         AIT 0160
                                                                       AIT 0170
      IF (CROSS) THEN                                                  AIT 0180
        X = X / 2.0                                                    AIT 0190
        IF (X .LT. 1.0) X = 1.0                                        AIT 0200
      ELSE                                                             AIT 0210
        X = X * 1.3                                                    AIT 0220
      END IF                                                           AIT 0230
                                                                       AIT 0240
      IF (X .GT. 20.0) X = 20.0                                        AIT 0250
                                                                       AIT 0260
      IF (RATIO .GT. 0.02 .AND. X .GT. 10.0) X =10.0                   AIT 0270
      IF (RATIO .GT. 0.05 .AND. X .GT.  5.0) X = 5.0                   AIT 0280
      IF (RATIO .GT. 0.10 .AND. X .GT.  3.0) X = 3.0                   AIT 0290
      IF (RATIO .GT. 0.20 .AND. X .GT.  2.0) X = 2.0                   AIT 0300
      IF (RATIO .GT. 0.3)                    X = 1.0                   AIT 0310
                                                                       AIT 0320
      RETURN                                                           AIT 0330
      END                                                              AIT 0340
```

```
      DOUBLE PRECISION FUNCTION ATCPRD (IC, INDEX, COEF, ALFA)         ATC 0010
C ===================================================================|ATC 0020
C     This function calculates the activity products for reactions     |ATC 0030
C -------------------------------------------------------------------|ATC 0040
C     ALFA      DBL   Activity of aqueous species                    |ATC 0050
C     COEF      DBL   Stoichiometric coefficient for the species     |ATC 0060
C     CPUMIN    DBL   Smallest positive real value program uses      |ATC 0070
C     I         INT   Loop counting variable                         |ATC 0080
C     IC        INT   Number of components                           |ATC 0090
C     INDEX     INT   Index number of the components                 |ATC 0100
C     J         INT   Current index number of this component         |ATC 0110
C -------------------------------------------------------------------|ATC 0120
                                                                       ATC 0130
      DOUBLE PRECISION CPUMIN                                          ATC 0140
      PARAMETER (CPUMIN = 1.0D-35)                                     ATC 0150
                                                                       ATC 0160
      INTEGER I, IC, INDEX(*), J                                       ATC 0170
      DOUBLE PRECISION ALFA(*), COEF(*)                                ATC 0180
      INTRINSIC DLOG10                                                 ATC 0190
                                                                       ATC 0200
C ===================================================================|ATC 0210
                                                                       ATC 0220
```

```
      ATCPRD = 0.0D00                                                    ATC 0230
                                                                         ATC 0240
      DO 100 I=1, IC                                                     ATC 0250
        J = INDEX(I)                                                     ATC 0260
        IF (J .GT. 0) THEN                                               ATC 0270
          IF (ALFA(J) .LT. CPUMIN) THEN                                  ATC 0280
            ATCPRD = -999.99                                             ATC 0290
            RETURN                                                       ATC 0300
          END IF                                                         ATC 0310
          ATCPRD = ATCPRD + (COEF(I) * DLOG10(ALFA(J)))                  ATC 0320
        END IF                                                           ATC 0330
  100 CONTINUE                                                           ATC 0340
                                                                         ATC 0350
      RETURN                                                             ATC 0360
      END                                                                ATC 0370
```

```
      SUBROUTINE CALCUL (A, B, TDS, Y28, DNS, TEMP, HITEMP, PRESS, DENS,CAL 0010
     .                   EHM, EHMC, EMFZSC, GFW, Z, UNITS, MXSP, TIC,  CAL 0020
     .                   ANMTIC, GAMMA, TCO2, BDAT, BDOT, MNACLD,      CAL 0030
     .                   NUFLAG)                                       CAL 0040
C ================================================================================|CAL 0050
C     This routine will do the following:                                          |CAL 0060
C     1) Calculate eh from field data.                                             |CAL 0070
C     2) Calculate analyzed molality.                                              |CAL 0080
C     3) Calculate cation-anion balance.                                           |CAL 0090
C     4) Calc. temp. effects on debye-huckel solvent constants.                    |CAL 0100
C --------------------------------------------------------------------------------|CAL 0110
C     A          DBL   Molal Debye-Huckel coefficient                            |CAL 0120
C     ANALM      DBL   Analyzed molality of species i                            |CAL 0130
C     ANMTIC     DBL   Analyzed TIC                                              |CAL 0140
C     B          DBL   Molal Debye-Huckel coefficient                            |CAL 0150
C     BDAT       DBL   B-dot as a function of temperature                        |CAL 0160
C     BDOT       DBL   Activity coefficient deviation function                   |CAL 0170
C     CADENS     DBL   Calculated density                                        |CAL 0180
C     CPUMIN     DBL   Smallest positive real value program uses                 |CAL 0190
C     CUNITS     DBL   Analytical input concentration                            |CAL 0200
C     CURDEN     DBL   Current density                                           |CAL 0210
C     DENOLD     DBL   Previous density, used for iterations                     |CAL 0220
C     DENS       DBL   Density                                                   |CAL 0230
C     DNS        CHA   Determines if density should be calculated                |CAL 0240
C     EHM        DBL   Measured Eh in volts                                      |CAL 0250
C     EHMC       DBL   Measured Eh using the Calomel electrode                  |CAL 0260
C     EMFZSC     DBL   Measured Eh using the Zobell's solution                  |CAL 0270
C     EXELT      DBL   Total moles of component.                                 |CAL 0280
C     GAMMA      DBL   Activity coef. of species                                 |CAL 0290
C     GFW        DBL   Gram formula weight of aqueous species                    |CAL 0300
C     GFWC       DBL   Gram Formula weight of carbon                             |CAL 0310
C     HITEMP     DBL   In-situ temperature                                       |CAL 0320
C     I          INT   Loop variable                                             |CAL 0330
C     IMIX       INT   Switch used in MIXER routines                             |CAL 0340
C     J          INT   Loop variable                                             |CAL 0350
C     M          DBL   Calculated molality of aqueous species                    |CAL 0360
C     MNACLD     DBL   Sum of Molality * charge / 2                              |CAL 0370
C     MXSP       INT   Total number of aqueous species                           |CAL 0380
```

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C     NMAX       INT   General array dimension to allow easy expansion  |CAL 0390
C     NUFLAG     INT   Sets the activity coefficients of neutral species|CAL 0400
C     PRESS      DBL   Total pressure                                    |CAL 0410
C     S1         DBL   Temperary sum variable                           |CAL 0420
C     S2         DBL   Temperary sum variable                           |CAL 0430
C     S3         DBL   Temperary sum variable                           |CAL 0440
C     T          DBL   Temperature in deg. K                            |CAL 0450
C     TCO2       DBL   Activity coefficients of CO2 with temperature    |CAL 0460
C     TDS        DBL   Total Dissolved Solids    (UNITS = KG/L)         |CAL 0470
C     TEMP       DBL   Temperature of the solution when pH was measured |CAL 0480
C     TIC        DBL   Concentration of total inorganic carbon          |CAL 0490
C     TITR       DBL   Used for convergence in DISTRB                   |CAL 0500
C     TOTEL      DBL   Contains HTOT, OHTOT and Sum CO2                 |CAL 0510
C     UNITS      CHA   Units of concentration                           |CAL 0520
C     Y28        INT   Set at hitemp to skip unneeded calculations      |CAL 0530
C     Z          INT   Charge of aqueous species                        |CAL 0540
C -------------------------------------------------------------------- |CAL 0550
                                                                        CAL 0560
      INTEGER NMAX                                                      CAL 0570
      DOUBLE PRECISION CPUMIN, GFWC                                     CAL 0580
                                                                        CAL 0590
      PARAMETER (NMAX = 340)                                            CAL 0600
      PARAMETER (CPUMIN=1.0D-35, GFWC = 12.011D0)                       CAL 0610
                                                                        CAL 0620
      CHARACTER*1 DNS                                                   CAL 0630
      CHARACTER*5 UNITS                                                 CAL 0640
                                                                        CAL 0650
      INTEGER I, IBMIX, IDMIX(50), IMIX, INMIX, ITMIX                   CAL 0660
      INTEGER J, MXSP, NUFLAG, Y28, Z(NMAX)                             CAL 0670
                                                                        CAL 0680
      DOUBLE PRECISION A, ALFA(NMAX), AMOL(50), ANALM(NMAX), ANMTIC     CAL 0690
      DOUBLE PRECISION B, BDAT(10), BDOT, CADENS, CO2F, CUNITS(NMAX)    CAL 0700
      DOUBLE PRECISION CURDEN, DENOLD, DENS, DFRAC1, DINC, EHM, EHMC    CAL 0710
      DOUBLE PRECISION EMFZSC, EXELT(35), FBOIL, GAMMA(NMAX)            CAL 0720
      DOUBLE PRECISION GFW(NMAX), HITEMP, HTOTI, KHCO2, KHH2S           CAL 0730
      DOUBLE PRECISION M(NMAX), MNACLD, OHTOTI, PH, PRESS, S1, S2, S3   CAL 0740
      DOUBLE PRECISION T, TCO2(10), TDS, TEMP, TIC, TITR(11), TOTEL(5)  CAL 0750
                                                                        CAL 0760
      EXTERNAL KHCO2, KHH2S                                             CAL 0770
                                                                        CAL 0780
      INTRINSIC DABS, DSQRT, IABS                                       CAL 0790
                                                                        CAL 0800
      COMMON /AMM   / IDMIX, AMOL, ITMIX, INMIX, DFRAC1, DINC, FBOIL    CAL 0810
      COMMON /EXTOT / EXELT, TOTEL, TITR                                CAL 0820
      COMMON /IMM   / IBMIX, IMIX                                       CAL 0830
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                        CAL 0840
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                               CAL 0850
                                                                        CAL 0860
      SAVE DENOLD                                                       CAL 0870
                                                                        CAL 0880
C ====================================================================|CAL 0890
                                                                        CAL 0900
      T = TEMP + 273.15D0                                               CAL 0910
      IF (Y28 .EQ. 1) GO TO 70                                          CAL 0920
                                                                        CAL 0930
C -------------------------------------------------------------------- |CAL 0940
C     Calculation of Eh from field data.                                |CAL 0950
C -------------------------------------------------------------------- |CAL 0960
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                                                                      CAL 0970
      IF ((DABS(EMFZSC - 9.0D0)) .LT. 1.0D-10) THEN                   CAL 0980
        S1 = 0.2145D0 - (7.6D-04 * (TEMP - 25.0D0))                   CAL 0990
      ELSE                                                            CAL 1000
        S1 = 4.28D-1  - (2.2D-03 * (TEMP - 25.0D0)) - EMFZSC          CAL 1010
      END IF                                                          CAL 1020
                                                                      CAL 1030
      IF (EHMC .LT. 9.D0) EHM = EHMC + S1                             CAL 1040
                                                                      CAL 1050
C -----------------------------------------------------------------|CAL 1060
C     Calculation of analyzed molality.                            |CAL 1070
C     If no value for density is entered then one will be computed |CAL 1080
C     using the empirical equation:                                |CAL 1090
C      DENSITY = 1.00 + 6.88 X 10 D-7 X TOTAL DISSOLVED SOLIDS     |CAL 1100
C -----------------------------------------------------------------|CAL 1110
                                                                      CAL 1120
      CURDEN = DENS                                                   CAL 1130
      TDS    = 0.0D00                                                 CAL 1140
                                                                      CAL 1150
   10 CONTINUE                                                        CAL 1160
      S1 = 0.0D00                                                     CAL 1170
      DO 20 I = 1, MXSP + 44                                          CAL 1180
        IF      (UNITS .EQ. 'PPM  ') THEN                             CAL 1190
          S1 = S1 + (1.0D-6 * CUNITS(I) * DENS)                       CAL 1200
        ELSE IF (UNITS .EQ. 'MG/L ') THEN                             CAL 1210
          S1 = S1 + (1.0D-6 * CUNITS(I))                              CAL 1220
        ELSE IF (UNITS .EQ. 'MOL/L' .OR. UNITS  .EQ. 'MOL/K') THEN    CAL 1230
          S1 = S1 + (1.0D-3 * CUNITS(I) * GFW(I) * (DENS - TDS))      CAL 1240
        ELSE IF (UNITS .EQ. 'MEQ/L' .AND. Z(I) .NE. 0) THEN           CAL 1250
          S1 = S1 + (1.0D-6 * CUNITS(I) * GFW(I) * (DENS - TDS) /     CAL 1260
     .          IABS(Z(I)))                                           CAL 1270
        END IF                                                        CAL 1280
   20 CONTINUE                                                        CAL 1290
                                                                      CAL 1300
      CADENS = 1.0D0 + (6.88D-7 * (1.0D6 * S1))                       CAL 1310
      IF (DNS .EQ. 'U') THEN                                          CAL 1320
        DENS   = CADENS                                               CAL 1330
        DENOLD = CADENS                                               CAL 1340
      END IF                                                          CAL 1350
                                                                      CAL 1360
      IF (S1 .GT. CPUMIN) THEN                                        CAL 1370
        IF (DABS((TDS - S1) / S1) .LT. 0.0001) THEN                   CAL 1380
          TDS = S1                                                    CAL 1390
        ELSE                                                          CAL 1400
          TDS = S1                                                    CAL 1410
          GO TO 10                                                    CAL 1420
        END IF                                                        CAL 1430
      END IF                                                          CAL 1440
                                                                      CAL 1450
      IF (DNS .EQ. 'N') THEN                                          CAL 1460
        CURDEN = CURDEN + CADENS - DENOLD                             CAL 1470
      ELSE IF (DNS .EQ. 'U') THEN                                     CAL 1480
        CURDEN = DENS                                                 CAL 1490
      END IF                                                          CAL 1500
                                                                      CAL 1510
      DNS    = 'N'                                                    CAL 1520
      DENOLD = CADENS                                                 CAL 1530
      DENS   = CURDEN                                                 CAL 1540
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                                                                      CAL 1550
      IF (IMIX .EQ. 1) GO TO 40                                       CAL 1560
                                                                      CAL 1570
      DO 30 I = 1, MXSP + 44                                          CAL 1580
        M(I) = 0.0D0                                                  CAL 1590
        IF      (UNITS .EQ. 'PPM  ' .AND. GFW(I) .GT. CPUMIN) THEN    CAL 1600
          M(I) = 1.0D-3 * CUNITS(I) * DENS / (GFW(I) * (DENS - TDS))  CAL 1610
        ELSE IF (UNITS .EQ. 'MG/L ' .AND. GFW(I) .GT. CPUMIN) THEN    CAL 1620
          M(I) = 1.0D-3 * CUNITS(I) / (GFW(I) * (DENS - TDS))         CAL 1630
        ELSE IF (UNITS .EQ. 'MOL/L') THEN                             CAL 1640
          M(I) = CUNITS(I) / (DENS - TDS)                             CAL 1650
        ELSE IF (UNITS .EQ. 'MOL/K') THEN                             CAL 1660
          M(I) = CUNITS(I)                                            CAL 1670
        ELSE IF (UNITS .EQ. 'MEQ/L' .AND. Z(I) .NE. 0) THEN           CAL 1680
          M(I) = 1.0D-3 * CUNITS(I) / (IABS(Z(I)) * (DENS - TDS))     CAL 1690
        END IF                                                        CAL 1700
        ANALM(I) = M(I)                                               CAL 1710
   30 CONTINUE                                                        CAL 1720
                                                                      CAL 1730
      IF      (UNITS .EQ. 'PPM  ') THEN                               CAL 1740
        ANMTIC = TIC * 1.0D-3 * DENS / (GFWC * (DENS - TDS))          CAL 1750
      ELSE IF (UNITS .EQ. 'MG/L ') THEN                               CAL 1760
        ANMTIC = TIC * 1.0D-3        / (GFWC * (DENS - TDS))          CAL 1770
      ELSE IF (UNITS .EQ. 'MOL/L') THEN                               CAL 1780
        ANMTIC = TIC                 /         (DENS - TDS)          CAL 1790
      ELSE IF (UNITS .EQ. 'MOL/K') THEN                               CAL 1800
        ANMTIC = TIC                                                  CAL 1810
      END IF                                                          CAL 1820
                                                                      CAL 1830
   40 CONTINUE                                                        CAL 1840
                                                                      CAL 1850
C -----------------------------------------------------------------|CAL 1860
C   Set the mass balance variables to be used in species distribution |CAL 1870
C -----------------------------------------------------------------|CAL 1880
                                                                      CAL 1890
      J = 0                                                           CAL 1900
      DO 60 I = 1, 28                                                 CAL 1910
        J = J + 1                                                     CAL 1920
        IF (J .EQ.   8) J = 12                                        CAL 1930
        IF (J .EQ.  17) J = 18                                        CAL 1940
        IF (J .EQ.  19) J = 21                                        CAL 1950
        IF (J .EQ.  24) J = 25                                        CAL 1960
        IF (J .EQ.  34) J = 48                                        CAL 1970
        IF (J .EQ.  49) J = 169                                       CAL 1980
        IF (J .EQ. 170) J = 210                                       CAL 1990
        EXELT(I)  = M(J)                                              CAL 2000
   60 CONTINUE                                                        CAL 2010
                                                                      CAL 2020
      EXELT(29)  = M(7) + (2.0 * M(98))                               CAL 2030
      EXELT(30)  = M(246)                                             CAL 2040
      EXELT(31)  = M(265)                                             CAL 2050
      EXELT(32)  = M(136)                                             CAL 2060
      EXELT(33)  = M(MXSP+1)                                          CAL 2070
      EXELT(34)  = M(MXSP+16)                                         CAL 2080
      EXELT(35)  = M(MXSP+31)                                         CAL 2090
                                                                      CAL 2100
                                                                      CAL 2110
      TITR( 1) = EXELT(29)                                            CAL 2120
```

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      TITR( 2) = EXELT( 6)                                                  CAL 2130
      TITR( 3) = EXELT(22)                                                  CAL 2140
      TITR( 4) = EXELT(21)                                                  CAL 2150
      TITR( 5) = EXELT( 5)                                                  CAL 2160
      TITR( 6) = EXELT(26)                                                  CAL 2170
      TITR( 7) = EXELT(25)                                                  CAL 2180
      TITR( 8) = EXELT(30)                                                  CAL 2190
      TITR( 9) = EXELT(31)                                                  CAL 2200
      TITR(10) = EXELT(33)                                                  CAL 2210
      TITR(11) = EXELT(34)                                                  CAL 2220
                                                                            CAL 2230
   70 CONTINUE                                                              CAL 2240
                                                                            CAL 2250
                                                                            CAL 2260
      MNACLD = 0.0D0                                                        CAL 2270
      DO 80 I = 1, MXSP + 44                                                CAL 2280
        MNACLD = MNACLD + (ANALM(I) * IABS(Z(I)))                           CAL 2290
   80 CONTINUE                                                              CAL 2300
      MNACLD = 0.5*MNACLD + 1.D0                                            CAL 2310
                                                                            CAL 2320
C -----------------------------------------------------------------------|CAL 2330
C     Calculation of the activity coeffs (gamma) for neutral species.   |CAL 2340
C     Gamma = 1 if nuflag = 1.  If nuflag = 0 then gamma for neutral    |CAL 2350
C     species are equal to gamma(co2) except for gamma(h2s) which is    |CAL 2360
C     calculated separately. Gamma for co2 is calculated by the method  |CAL 2370
C     of drummond (unpublished disert.,1981).                           |CAL 2380
C -----------------------------------------------------------------------|CAL 2390
                                                                            CAL 2400
      S1 = KHCO2(T, MNACLD) / KHCO2(T, 1.0D00)                              CAL 2410
                                                                            CAL 2420
      DO 90 I = 1, MXSP + 44                                                CAL 2430
        IF (IABS(Z(I)) .LT. 1) THEN                                         CAL 2440
          IF (NUFLAG .EQ. 1) THEN                                           CAL 2450
            GAMMA(I) = 1.0D0                                                CAL 2460
          ELSE                                                              CAL 2470
            GAMMA(I) = S1                                                   CAL 2480
          END IF                                                            CAL 2490
        END IF                                                              CAL 2500
   90 CONTINUE                                                              CAL 2510
                                                                            CAL 2520
      IF (ANALM(33) .GT. CPUMIN) THEN                                       CAL 2530
        GAMMA(33) = KHH2S(T,MNACLD) / KHH2S(T, 1.0D00)                      CAL 2540
      ELSE                                                                  CAL 2550
        GAMMA(33) = 1.0D00                                                  CAL 2560
      END IF                                                                CAL 2570
                                                                            CAL 2580
      IF (IMIX .EQ. 1) RETURN                                               CAL 2590
                                                                            CAL 2600
C -----------------------------------------------------------------------|CAL 2610
C     Temperature effects on debye-huckel solvent constants.            |CAL 2620
C -----------------------------------------------------------------------|CAL 2630
                                                                            CAL 2640
      S1 = 374.11D0 - TEMP                                                  CAL 2650
      S2 = S1**0.333333D0                                                   CAL 2660
      S3 = DSQRT((1.0D0 + 0.1342489D0 * S2 - 3.946263D-3 * S1) /            CAL 2670
     .         (3.1975D0 - 0.3151548D0 * S2 - 1.203374D-3 * S1 +          CAL 2680
     .          7.48908D-13 * S1**4))                                     CAL 2690
                                                                            CAL 2700
```

```
      IF ((DABS(HITEMP-TEMP)) .LT. 1.0D-10 .OR. HITEMP .LT. 1.0D-10)    CAL 2710
     .  S3 = DSQRT(S3**2 + 0.0087 * PRESS / (400.0 - TEMP)**0.95)       CAL 2720
                                                                        CAL 2730
      IF (T .LT. 373.16D0) THEN                                         CAL 2740
        S1 = 87.74D0 - TEMP * (TEMP * (1.41D-6 * TEMP -                 CAL 2750
     .                                           9.398D-4) + 0.4008D0)  CAL 2760
      ELSE                                                              CAL 2770
        S1 = 5321D0 / T + 233.76D0 - T * (T * (8.292D-7 * T -           CAL 2780
     .                                           1.417D-3) + 0.9297D0)  CAL 2790
      END IF                                                            CAL 2800
                                                                        CAL 2810
      IF ((DABS(HITEMP-TEMP)) .LT. 1.0D-10 .OR. HITEMP .LT. 1.0D-10)    CAL 2820
     .  S1 = S1 + 0.053 * PRESS / (400.0 - TEMP)**0.5                   CAL 2830
                                                                        CAL 2840
      S1 = DSQRT(S1 * T)                                                CAL 2850
      A  = 18246D2 * S3 / S1**3                                         CAL 2860
      B  = 50.29   * S3 / S1                                            CAL 2870
                                                                        CAL 2880
C -------------------------------------------------------------------|CAL 2890
C     Calculate bdot                                                  |CAL 2900
C -------------------------------------------------------------------|CAL 2910
                                                                        CAL 2920
      IF (TEMP .GT. 300.0D0) THEN                                       CAL 2930
        BDOT = 0.0D0                                                    CAL 2940
      ELSE                                                              CAL 2950
        DO 120 J = 1, 9                                                 CAL 2960
          IF ((DABS(TEMP-TCO2(J))) .LT. 1.0D-10) THEN                   CAL 2970
            BDOT = BDAT(J)                                              CAL 2980
            GO TO 130                                                   CAL 2990
          ELSE IF (TEMP .LT. TCO2(J)) THEN                              CAL 3000
            BDOT = BDAT(J-1) + (TEMP-TCO2(J-1)) * (BDAT(J) -            CAL 3010
     .             BDAT(J-1)) / (TCO2(J)-TCO2(J-1))                     CAL 3020
            GO TO 130                                                   CAL 3030
          END IF                                                        CAL 3040
  120   CONTINUE                                                        CAL 3050
  130   CONTINUE                                                        CAL 3060
      END IF                                                            CAL 3070
                                                                        CAL 3080
      RETURN                                                            CAL 3090
      END                                                               CAL 3100
```

```
      SUBROUTINE CO2OPT (TEMP, HITEMP, GAMMA, ICO2, IMCO3, FCCSAT,      CO2 0010
     .                   MNACLD, ITIC, ISAT, IPRIN2, *)                 CO2 0020
C ===================================================================|CO2 0030
C     Titrates co2 to a given criterion (pH, pco2, m(h2co3), or       |CO2 0040
C     saturation with calcite, siderite, or dolomite)                 |CO2 0050
C -------------------------------------------------------------------|CO2 0060
C     ALFA      DBL   Activity of aqueous species i                   |CO2 0070
C     ANALM     DBL   Analyzed molality of species i                  |CO2 0080
C     CO2F      DBL   Sum of CO2 plus CO2 lost from solution          |CO2 0090
C     CO2INC    DBL   Amount of CO2 to be added/removed               |CO2 0100
C     CO2SAT    DBL   Saturation indices/test for various options     |CO2 0110
C     CPUMIN    DBL   Smallest positive real value program uses       |CO2 0120
C     CROSS     LOG   Have we crossed root?                           |CO2 0130
```

```
C     DCH4       DBL   Concentration of CH4 lost up annulus                |CO2 0140
C     DDCH4      DBL   Concentration of CH4 lost before pH measurement      |CO2 0150
C     DCO2       DBL   Concentration of CO2 lost up annulus                |CO2 0160
C     DDCO2      DBL   Concentration of CO2 lost before pH measurement      |CO2 0170
C     DH2S       DBL   Concentration of H2S lost up annulus                |CO2 0180
C     DDH2S      DBL   Concentration of H2S lost before pH measurement      |CO2 0190
C     DNH3       DBL   Concentration of NH3 lost up annulus                |CO2 0200
C     DDNH3      DBL   Concentration of NH3 lost before pH measurement      |CO2 0210
C     DONE       LOG   Switch indicating DONE                              |CO2 0220
C     EXELT      DBL   Total amount of components                          |CO2 0230
C     FCCSAT     DBL   Zero test value                                     |CO2 0240
C     FIXIT      DBL   Fixing value in the CO2 option                      |CO2 0250
C     GAMMA      DBL   Activity coef. of aqueous species                   |CO2 0260
C     HFAC       DBL   Amount of H to be added to hydronium balance        |CO2 0270
C     HITEMP     DBL   In-situ temperature                                 |CO2 0280
C     HTOT       DBL   Current total hydronium                             |CO2 0290
C     HTOTI      DBL   Initial hydronium                                   |CO2 0300
C     I          INT   Loop variable                                       |CO2 0310
C     ICO2       INT   Switch for CO2 option                               |CO2 0320
C     IIC        INT   Index pointer to select carbonate species           |CO2 0330
C     IMCO3      INT   Selects CO2 option                                  |CO2 0340
C     IOPT       INT   Switch for CO2 option                               |CO2 0350
C     IPAGE      INT   Current page number of output file                  |CO2 0360
C     IPGLN      INT   Current line number of the output file              |CO2 0370
C     IPRIN2     INT   Switch for printing                                 |CO2 0380
C     ISAT       INT   Counter for storing things in the position          |CO2 0390
C     ITIC       INT   Hitemp distribution of carbonate species            |CO2 0400
C     JCO3       INT   Switch to control printing of some headings         |CO2 0410
C     KH         DBL   Henry's law constant for CO2 at T                   |CO2 0420
C     KHCO2      DBL   Function to Calculate the Henry's law K for CO2     |CO2 0430
C     KT1        DBL   Equilibrium constant of the aqueous reactions       |CO2 0440
C     KTFAC      DBL   Correction for number of CO2 groups                 |CO2 0450
C     LOGKT1     DBL   Log K for aqueous species at specified temp.        |CO2 0460
C     LOGKT2     DBL   Log K for minerals at specified temperature         |CO2 0470
C     LTCSAT     DBL   Value used for testing                              |CO2 0480
C     M          DBL   Calculated molality of aqueous species              |CO2 0490
C     MAXCO2     DBL   Determines which carbonate species has the          |CO2 0500
C                        largest molality                                  |CO2 0510
C     MNACLD     DBL   Sum of Molality * charge / 2                        |CO2 0520
C     NDIM       INT   Parameter for dimension                             |CO2 0530
C     NMAX       INT   General array dimension to allow easy expansion     |CO2 0540
C     OHTOT      DBL   Total OH in solution                                |CO2 0550
C     OHTOTI     DBL   Total OH in solution .. initially                   |CO2 0560
C     PH         DBL   Measured pH of the solution                         |CO2 0570
C     PHHIT      INT   HITEMP switch, used to control PHCALC               |CO2 0580
C     PPHHIT     INT   Switch to control calling PHCALC                    |CO2 0590
C     SATNAM     CHA   Name used for this option, Cal, Dol, ....           |CO2 0600
C     TEMP       DBL   Temperature of the solution when pH was measured    |CO2 0610
C     TIAP       DBL   Temporary activity product                          |CO2 0620
C     TITR       DBL   Used for convergence in DISTRB                      |CO2 0630
C     TK         DBL   Temperature in deg K                                |CO2 0640
C     TKT        DBL   Temporary thermodynamic log k                       |CO2 0650
C     TOTEL      DBL   Total amount of each element                        |CO2 0660
C     UNO        INT   File unit assigned for output file                  |CO2 0670
C ---------------------------------------------------------------------    |CO2 0680
                                                                           CO2 0690
      INTEGER NDIM, NMAX, UNO                                              CO2 0700
      DOUBLE PRECISION CPUMIN                                              CO2 0710
```

```
      PARAMETER (CPUMIN = 1.0D-35, NDIM = 7, NMAX = 340, UNO = 6)        CO2 0720
                                                                         CO2 0730
      INTEGER I, ICO2, IIC, IMCO3, IOPT, IPAGE, IPGLN, IPRIN2, ISAT      CO2 0740
      INTEGER ITIC, JCO3, PHHIT, PPHHIT                                  CO2 0750
                                                                         CO2 0760
      LOGICAL CROSS, DONE                                                CO2 0770
                                                                         CO2 0780
      CHARACTER *  1 TOF, CR                                             CO2 0790
      CHARACTER *  8 SATNAM(6)                                           CO2 0800
      CHARACTER * 40 TITMIX                                              CO2 0810
                                                                         CO2 0820
      DOUBLE PRECISION ALFA(NMAX), ANALM(NMAX)                           CO2 0830
      DOUBLE PRECISION CO2F, CO2SAT(NDIM), CO2INC(NDIM), CUNITS(NMAX)    CO2 0840
      DOUBLE PRECISION DCH4, DDCH4, DCO2, DDCO2, DH2S, DDH2S             CO2 0850
      DOUBLE PRECISION DNH3, DDNH3, EXELT(35), FCCSAT, FIXIT             CO2 0860
      DOUBLE PRECISION GAMMA(NMAX), HFAC, HITEMP, HTOT, HTOTI            CO2 0870
      DOUBLE PRECISION KH, KHCO2, KT1(NMAX), KTFAC                       CO2 0880
      DOUBLE PRECISION LOGKT1(NMAX), LOGKT2(NMAX), LTCSAT                CO2 0890
      DOUBLE PRECISION M(NMAX), MAXCO2, MNACLD, OHTOT, OHTOTI, PH        CO2 0900
      DOUBLE PRECISION SCO2, TEMP, TIAP, TITR(11), TK, TKT, TOTEL(5)     CO2 0910
                                                                         CO2 0920
      EXTERNAL GUESS, KHCO2, PAGE, SORTA                                 CO2 0930
                                                                         CO2 0940
      INTRINSIC DABS, DLOG10                                             CO2 0950
                                                                         CO2 0960
      COMMON /ALOGK / LOGKT1, LOGKT2                                     CO2 0970
      COMMON /EXTOT / EXELT, TOTEL, TITR                                 CO2 0980
      COMMON /FMFD  / TOF, CR, TITMIX                                    CO2 0990
      COMMON /FORM  / IPAGE, IPGLN                                       CO2 1000
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,             CO2 1010
     .                DCH4, DDCH4, IOPT, FIXIT                          CO2 1020
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                         CO2 1030
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                                CO2 1040
      COMMON /TTK   / KT1                                                CO2 1050
      COMMON /ZPH   / PHHIT, PPHHIT, JCO3, SCO2, HTOT, OHTOT             CO2 1060
                                                                         CO2 1070
      SAVE CO2SAT, CO2INC, CROSS, DONE                                   CO2 1080
                                                                         CO2 1090
      DATA SATNAM/ 'CALCITE ', 'DOLOMITE', 'SIDERITE', ' AQ CO2',        CO2 1100
     .             '  PH',  '  PCO2'/                                   CO2 1110
                                                                         CO2 1120
C ========================================================================|CO2 1130
                                                                         CO2 1140
C -------------------------------------------------------------------------|CO2 1150
C     If CO2, H2S, NH3 or CH4 are being added                            |CO2 1160
C -------------------------------------------------------------------------|CO2 1170
                                                                         CO2 1180
      IF (ICO2 .EQ. 0) THEN                                              CO2 1190
        DCO2 = DDCO2                                                     CO2 1200
        DH2S = DDH2S                                                     CO2 1210
        DNH3 = DDNH3                                                     CO2 1220
        DCH4 = DDCH4                                                     CO2 1230
        CALL PAGE                                                        CO2 1240
        WRITE (UNO, 1001) DCO2, DH2S, DNH3, DCH4                         CO2 1250
        IPGLN = IPGLN + 6                                                CO2 1260
                                                                         CO2 1270
        IF (DABS(HITEMP-TEMP) .GT. CPUMIN) HITEMP = TEMP                 CO2 1280
                                                                         CO2 1290
```

```
        JCO3 = 1                                                        CO2 1300
        ITIC = 2                                                        CO2 1310
        IOPT   = 0                                                      CO2 1320
        PHHIT  = 1                                                      CO2 1330
        PPHHIT = 0                                                      CO2 1340
        HTOTI  = HTOT                                                   CO2 1350
        OHTOTI = OHTOT                                                  CO2 1360
                                                                        CO2 1370
        EXELT(25)  = EXELT(25) + DDH2S                                  CO2 1380
        TITR(7)    = EXELT(25)                                          CO2 1390
        EXELT(24)  = EXELT(24) + DDNH3                                  CO2 1400
        EXELT(29)  = EXELT(29) + DDCO2                                  CO2 1410
        TITR(1)    = EXELT(29)                                          CO2 1420
        M(285)     = M(285)    + DDCH4                                  CO2 1430
        ANALM(285) = M(285)    + DDCH4                                  CO2 1440
                                                                        CO2 1450
        DDCO2 = 0.0                                                     CO2 1460
        DDH2S = 0.0                                                     CO2 1470
        DDNH3 = 0.0                                                     CO2 1480
        DDCH4 = 0.0                                                     CO2 1490
                                                                        CO2 1500
        RETURN                                                          CO2 1510
      END IF                                                            CO2 1520
                                                                        CO2 1530
C -----------------------------------------------------------------------|CO2 1540
C     Add the amount of CO2                                             |CO2 1550
C          required for saturation with CALCITE  (IMCO3=1)              |CO2 1560
C          required for saturation with DOLOMITE (IMCO3=2)              |CO2 1570
C          required for saturation with SIDERITE (IMCO3=3)              |CO2 1580
C          required to reach a specified m H2CO3 (IMCO3=4)              |CO2 1590
C               which is stored in FIXIT                                |CO2 1600
C          required to reach a specified pH      (IMCO3=5)              |CO2 1610
C               which is stored in FIXIT                                |CO2 1620
C          required to reach a specified p CO2   (IMCO3=6)              |CO2 1630
C               which is stored in FIXIT                                |CO2 1640
C                                                                       |CO2 1650
C     ICO2 must be greater than zero for this option to be used.        |CO2 1660
C -----------------------------------------------------------------------|CO2 1670
                                                                        CO2 1680
      IF (ISAT .EQ. 0) THEN                                             CO2 1690
        CROSS = .FALSE.                                                 CO2 1700
        DONE  = .FALSE.                                                 CO2 1710
                                                                        CO2 1720
        IF (DABS(HITEMP-TEMP) .GT. 1.0D-10) HITEMP = TEMP               CO2 1730
                                                                        CO2 1740
        PHHIT  = 1                                                      CO2 1750
        PPHHIT = 0                                                      CO2 1760
        HTOTI  = HTOT                                                   CO2 1770
        OHTOTI = OHTOT                                                  CO2 1780
        JCO3   = 1                                                      CO2 1790
        ITIC   = 2                                                      CO2 1800
      END IF                                                            CO2 1810
                                                                        CO2 1820
      ISAT = ISAT + 1                                                   CO2 1830
                                                                        CO2 1840
C -----------------------------------------------------------------------|CO2 1850
C     Scan for the most abundant species of CO2 and use it later to     |CO2 1860
C     minimize round-off errors in calculations.                        |CO2 1870
```

```
C ------------------------------------------------------------------|CO2 1880
                                                                    CO2 1890
      MAXCO2 = M(7)                                                 CO2 1900
      HFAC   = ALFA(8)                                              CO2 1910
      IIC    = 7                                                    CO2 1920
                                                                    CO2 1930
      DO 10 I = 97, 98                                              CO2 1940
        IF (M(I) .GT. MAXCO2) THEN                                  CO2 1950
          MAXCO2 = M(I)                                             CO2 1960
          IIC    = I                                                CO2 1970
        END IF                                                      CO2 1980
   10 CONTINUE                                                      CO2 1990
                                                                    CO2 2000
      IF (IIC .EQ. 97) HFAC = ALFA(8)**2                            CO2 2010
      IF (IIC .EQ. 98) HFAC = 1.0                                   CO2 2020
                                                                    CO2 2030
C ------------------------------------------------------------------|CO2 2040
C     Set up TEST for each of the options                           |CO2 2050
C ------------------------------------------------------------------|CO2 2060
                                                                    CO2 2070
      IF (IMCO3 .EQ. 1) THEN                                        CO2 2080
        TKT = LOGKT2(24)                                            CO2 2090
        KTFAC = 1.0                                                 CO2 2100
        TIAP  = ALFA(1) * ALFA(IIC) / HFAC                          CO2 2110
      ELSE IF (IMCO3 .EQ. 2) THEN                                   CO2 2120
        TKT = LOGKT2(41)                                            CO2 2130
        KTFAC = 2.0                                                 CO2 2140
        TIAP  = ALFA(1) * ALFA(2) * ALFA(IIC)**2 / HFAC**2          CO2 2150
      ELSE IF (IMCO3 .EQ. 3) THEN                                   CO2 2160
        TKT = LOGKT2(146)                                           CO2 2170
        KTFAC = 1.0                                                 CO2 2180
        TIAP  = ALFA(18) * ALFA(IIC) / HFAC                         CO2 2190
      ELSE IF (IMCO3 .EQ. 4) THEN                                   CO2 2200
        LTCSAT = DLOG10(FIXIT) - DLOG10(M(97))                      CO2 2210
      ELSE IF (IMCO3 .EQ. 5) THEN                                   CO2 2220
        LTCSAT = PH - FIXIT                                         CO2 2230
      ELSE IF (IMCO3 .EQ. 6) THEN                                   CO2 2240
        TK  = TEMP + 273.15                                         CO2 2250
        KH  = KHCO2 (TK, MNACLD)                                    CO2 2260
        LTCSAT = DLOG10((FIXIT/KH)) - DLOG10(M(97))                 CO2 2270
      END IF                                                        CO2 2280
                                                                    CO2 2290
      IF (IMCO3 .EQ. 1 .OR. IMCO3 .EQ. 2 .OR. IMCO3 .EQ. 3) THEN    CO2 2300
        IF (IIC .EQ. 7) THEN                                        CO2 2310
          TKT = TKT - KTFAC * LOGKT1(1)                             CO2 2320
        ELSE IF (IIC .EQ. 97) THEN                                  CO2 2330
          TKT = TKT - KTFAC * (LOGKT1(1) + LOGKT1(72))              CO2 2340
        END IF                                                      CO2 2350
        LTCSAT = DLOG10(TIAP) - TKT                                 CO2 2360
      END IF                                                        CO2 2370
                                                                    CO2 2380
      IF (DABS(LTCSAT) .LT. FCCSAT) DONE = .TRUE.                   CO2 2390
                                                                    CO2 2400
      IF (DONE) THEN                                                CO2 2410
        IOPT     = 0                                                CO2 2420
        PHHIT    = 0                                                CO2 2430
        PPHHIT   = 1                                                CO2 2440
        ISAT     = 0                                                CO2 2450
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```
      JCO3     = 0                                                    CO2 2460
      HTOTI    = HTOTI    + (2.D0 * DCO2)                             CO2 2470
      TOTEL(1) = HTOTI                                                CO2 2480
      TOTEL(3) = TOTEL(3) + DCO2                                      CO2 2490
      CO2F     = CO2F     + DCO2                                      CO2 2500
                                                                      CO2 2510
      IF (IPGLN .GT. 55 .OR. IPRIN2 .EQ. 0) CALL PAGE                 CO2 2520
      IF      (IMCO3 .LE. 3) THEN                                     CO2 2530
        WRITE (UNO,1007) SATNAM(IMCO3), DCO2                          CO2 2540
      ELSE IF (IMCO3 .EQ. 4) THEN                                     CO2 2550
        WRITE (UNO,1008) SATNAM(IMCO3), FIXIT, DCO2                   CO2 2560
      ELSE IF (IMCO3 .EQ. 5) THEN                                     CO2 2570
        WRITE (UNO,1009) FIXIT, DCO2                                  CO2 2580
      ELSE IF (IMCO3 .EQ. 6) THEN                                     CO2 2590
        WRITE (UNO,1008) SATNAM(IMCO3), FIXIT, DCO2                   CO2 2600
      END IF                                                          CO2 2610
      IPGLN = IPGLN + 5                                               CO2 2620
      DCO2  = 0.D0                                                    CO2 2630
      RETURN 1                                                        CO2 2640
    END IF                                                            CO2 2650
                                                                      CO2 2660
    IF (ISAT .EQ. 1) THEN                                             CO2 2670
      CO2SAT(1) = LTCSAT                                              CO2 2680
      CO2INC(1) = 0.0                                                 CO2 2690
      IF      (IMCO3 .EQ. 1) THEN                                     CO2 2700
        DCO2 = M(IIC) * ((1.0/(10.0**LTCSAT)) -1.0)                   CO2 2710
        IF (DCO2 .LT. 0.0)  DCO2 = 0.01                               CO2 2720
        IF (DCO2 .GT. 0.05) DCO2 = 0.01                               CO2 2730
      ELSE IF (IMCO3 .EQ. 2) THEN                                     CO2 2740
        DCO2 = M(IIC) * ((1.0/(10.0**LTCSAT)) -1.0)                   CO2 2750
        DCO2 = DCO2 / 2.0                                             CO2 2760
        IF (DCO2 .LT. 0.0)  DCO2 = 0.01                               CO2 2770
        IF (DCO2 .GT. 0.05) DCO2 = 0.01                               CO2 2780
      ELSE IF (IMCO3 .EQ. 3) THEN                                     CO2 2790
        DCO2 = M(IIC) * ((1.0/(10.0**LTCSAT)) -1.0)                   CO2 2800
        IF (DCO2 .LT. 0.0)  DCO2 = 0.01                               CO2 2810
        IF (DCO2 .GT. 0.05) DCO2 = 0.01                               CO2 2820
      ELSE IF (IMCO3 .EQ. 4) THEN                                     CO2 2830
        IF (IIC .EQ. 7) THEN                                          CO2 2840
          DCO2 = FIXIT * KT1(72) * GAMMA(97) / ALFA(8)                CO2 2850
          DCO2 = DCO2 / GAMMA(7)                                      CO2 2860
          DCO2 = (DCO2 - M(7)) / 3.0                                  CO2 2870
        ELSE IF (IIC .EQ. 97) THEN                                    CO2 2880
          DCO2 = FIXIT - M(97)                                        CO2 2890
        ELSE IF (IIC .EQ. 98) THEN                                    CO2 2900
          DCO2 = FIXIT * KT1(72) * GAMMA(97) / ALFA(8)                CO2 2910
          DCO2 = DCO2 * KT1(1) / (GAMMA(98) * ALFA(8))                CO2 2920
          DCO2 = (DCO2 - M(98)) / 3.0                                 CO2 2930
        END IF                                                        CO2 2940
      ELSE IF (IMCO3 .EQ. 5) THEN                                     CO2 2950
        DCO2 = 10.0**(-FIXIT) - 10.0**(-PH)                           CO2 2960
        DCO2 = DCO2 / 2.0                                             CO2 2970
      ELSE IF (IMCO3 .EQ. 6) THEN                                     CO2 2980
        IF (IIC .EQ. 7) THEN                                          CO2 2990
          DCO2 = (FIXIT/KH) * KT1(72) * GAMMA(97) / ALFA(8)           CO2 3000
          DCO2 = DCO2 / GAMMA(7)                                      CO2 3010
          DCO2 = (DCO2 - M(7)) / 3.0                                  CO2 3020
        ELSE IF (IIC .EQ. 97) THEN                                    CO2 3030
```

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            DCO2 = (FIXIT/KH) - M(97)                                    CO2 3040
          ELSE IF (IIC .EQ. 98) THEN                                     CO2 3050
            DCO2 = (FIXIT/KH) * KT1(72) * GAMMA(97) / ALFA(8)            CO2 3060
            DCO2 = DCO2 * KT1(1) / (GAMMA(98) * ALFA(8))                 CO2 3070
            DCO2 = (DCO2 - M(98)) / 3.0                                  CO2 3080
          END IF                                                         CO2 3090
        END IF                                                           CO2 3100
      ELSE IF (ISAT .GE. 2) THEN                                         CO2 3110
        CO2SAT(ISAT) = LTCSAT                                            CO2 3120
        CO2INC(ISAT) = DCO2                                              CO2 3130
        IF ((LTCSAT * CO2SAT(1)) .LT. 0.0) CROSS = .TRUE.                CO2 3140
                                                                         CO2 3150
C ---------------------------------------------------------------------|CO2 3160
C     Sort if Root has been crossed                                      |CO2 3170
C ---------------------------------------------------------------------|CO2 3180
                                                                         CO2 3190
        I = 1                                                            CO2 3200
        IF (CROSS) CALL SORTA (CO2INC, CO2SAT, ISAT, I)                  CO2 3210
                                                                         CO2 3220
C ---------------------------------------------------------------------|CO2 3230
C     Due to size of guess routine, keep only last NDIM-1 pts            |CO2 3240
C ---------------------------------------------------------------------|CO2 3250
                                                                         CO2 3260
        IF (ISAT .EQ. NDIM) THEN                                         CO2 3270
          IF (.NOT. CROSS) THEN                                          CO2 3280
            DO 20 I = 1, (NDIM-1)                                        CO2 3290
              CO2INC(I) = CO2INC(I+1)                                    CO2 3300
              CO2SAT(I) = CO2SAT(I+1)                                    CO2 3310
   20       CONTINUE                                                     CO2 3320
          END IF                                                         CO2 3330
          IF (CROSS) THEN                                                CO2 3340
            IF (CO2SAT(1) * CO2SAT(2) .LT. 0.0) THEN                     CO2 3350
              ISAT = NDIM-1                                              CO2 3360
            ELSE IF (CO2SAT(NDIM-1)*CO2SAT(NDIM) .LT. 0.0) THEN          CO2 3370
              DO 30 I = 1,(NDIM-1)                                       CO2 3380
                CO2INC(I) = CO2INC(I+1)                                  CO2 3390
                CO2SAT(I) = CO2SAT(I+1)                                  CO2 3400
   30         CONTINUE                                                   CO2 3410
            ELSE IF (DABS(CO2SAT(1)) .GT. DABS(CO2SAT(NDIM))) THEN       CO2 3420
              DO 40 I = 1,(NDIM-1)                                       CO2 3430
                CO2INC(I) = CO2INC(I+1)                                  CO2 3440
                CO2SAT(I) = CO2SAT(I+1)                                  CO2 3450
   40         CONTINUE                                                   CO2 3460
            END IF                                                       CO2 3470
          END IF                                                         CO2 3480
          ISAT = NDIM - 1                                                CO2 3490
        END IF                                                           CO2 3500
                                                                         CO2 3510
C ---------------------------------------------------------------------|CO2 3520
C     If root not yet crossed, keep on trucking                          |CO2 3530
C ---------------------------------------------------------------------|CO2 3540
                                                                         CO2 3550
        IF (.NOT. CROSS) THEN                                            CO2 3560
          DCO2 = DCO2 * 2.0                                              CO2 3570
          IF ((CO2F + DCO2) .LT. CPUMIN) DCO2 = 1.0D-10 - CO2F           CO2 3580
        END IF                                                           CO2 3590
                                                                         CO2 3600
C ---------------------------------------------------------------------|CO2 3610
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C     If ROOT crossed, go and get it                                    |CO2 3620
C -------------------------------------------------------------------- |CO2 3630
                                                                        CO2 3640
        IF (CROSS) THEN                                                 CO2 3650
          CALL GUESS (CO2INC, CO2SAT, DCO2, ISAT)                       CO2 3660
        END IF                                                          CO2 3670
      END IF                                                            CO2 3680
                                                                        CO2 3690
      IF (IPRIN2 .GT. 0) THEN                                           CO2 3700
        IF (IMCO3 .LE. 3) THEN                                          CO2 3710
          WRITE (UNO,1004) SATNAM(IMCO3), LTCSAT                        CO2 3720
        ELSE                                                            CO2 3730
          WRITE (UNO,1002) SATNAM(IMCO3), LTCSAT                        CO2 3740
        END IF                                                          CO2 3750
        IPGLN = IPGLN + 2                                               CO2 3760
        IF (IPGLN .GT. 57) CALL PAGE                                    CO2 3770
        WRITE (UNO,1003) DCO2                                           CO2 3780
        IPGLN = IPGLN + 2                                               CO2 3790
      END IF                                                            CO2 3800
                                                                        CO2 3810
                                                                        CO2 3820
      IF (ISAT .EQ. 1) THEN                                             CO2 3830
        EXELT(29) = DCO2 + EXELT(29)                                    CO2 3840
        TITR(1)   = EXELT(29)                                           CO2 3850
      END IF                                                            CO2 3860
                                                                        CO2 3870
      RETURN                                                            CO2 3880
                                                                        CO2 3890
 1001 FORMAT(/,' Adding gases to the analyses using the DCO2/DH2S/DNH3',CO2 3900
     .          '/DCH4 ',                                              CO2 3910
     .       /,' option.  Moles of CO2 added = ', E14.6,               CO2 3920
     .       /,'                of H2S added = ', E14.6,               CO2 3930
     .       /,'                of NH3 added = ', E14.6,               CO2 3940
     .       /,'                of CH4 added = ', E14.6,               CO2 3950
     .       /)                                                       CO2 3960
 1002 FORMAT(/,5X,'LOG (CALCULATED-DESIRED) ',A8,' = ',E10.4)          CO2 3970
 1003 FORMAT(/,5X,'VALUE OF DCO2 FOR THIS ITERATION = ',E10.4)         CO2 3980
 1004 FORMAT(/,5X,'LOG SI (',A8,') = ', E10.4)                         CO2 3990
 1005 FORMAT(/,' *** DESIRED EQUILIBRIUM DOES NOT SEEM TO ',           CO2 4000
     .          ' CONVERGE WITHIN THE LIMITS OF',                      CO2 4010
     .          ' .5 AND 1.0E5 PPM AQ CO2 ***',                        CO2 4020
     .       /,'    SI = ', D16.8, '   TIC = ', D16.8,                 CO2 4030
     .          '  MOLS/KG WATER')                                     CO2 4040
 1006 FORMAT(/,' *** DESIRED EQUILIBRIUM DOES NOT SEEM TO',            CO2 4050
     .          ' CONVERGE ***', /)                                    CO2 4060
 1007 FORMAT(//,5X,'CO2 added to achieve equilibrium with ', A8, ' = ', CO2 4070
     .          E10.4, 'Moles/Kg Water',//)                           CO2 4080
 1008 FORMAT(//,' CO2 added to achieve saturation with ',A8,' of ',    CO2 4090
     .          E10.4,' = ', E10.4, ' Moles/Kg water',//)             CO2 4100
 1009 FORMAT(//,' CO2 added to achieve pH of ', F10.4, ' = ',          CO2 4110
     .          E13.4, ' Moles/Kg water',//)                          CO2 4120
                                                                       CO2 4130
      END                                                              CO2 4140
```

```
      DOUBLE PRECISION FUNCTION DEBYE (CHARGE, DNA)                      DEB 0010
C ================================================================================|DEB 0020
C     This function returns the value of the ion size parameter based  |DEB 0030
C     upon the charge of the species                                   |DEB 0040
C --------------------------------------------------------------------------------|DEB 0050
C     CHARGE     INT   Charge of the aqueous species                   |DEB 0060
C     CPUMIN     DBL   Smallest positive real value program uses       |DEB 0070
C     DNA        DBL   Read-in value of the ion size parameter         |DEB 0080
C --------------------------------------------------------------------------------|DEB 0090
                                                                                  DEB 0100
      DOUBLE PRECISION CPUMIN                                                     DEB 0110
      PARAMETER (CPUMIN = 1.0D-35)                                                DEB 0120
                                                                                  DEB 0130
      INTEGER CHARGE                                                              DEB 0140
      DOUBLE PRECISION DNA                                                        DEB 0150
                                                                                  DEB 0160
      INTRINSIC IABS                                                              DEB 0170
                                                                                  DEB 0180
C ================================================================================|DEB 0190
                                                                                  DEB 0200
      IF (DNA .GT. CPUMIN) THEN                                                   DEB 0210
        DEBYE = DNA                                                               DEB 0220
      ELSE IF (IABS(CHARGE) .EQ. 0) THEN                                          DEB 0230
        DEBYE = 0.0D00                                                            DEB 0240
      ELSE IF (IABS(CHARGE) .EQ. 1) THEN                                          DEB 0250
        DEBYE = 4.0D00                                                            DEB 0260
      ELSE IF (IABS(CHARGE) .EQ. 2) THEN                                          DEB 0270
        DEBYE = 6.0D00                                                            DEB 0280
      ELSE IF (IABS(CHARGE) .EQ. 3) THEN                                          DEB 0290
        DEBYE = 9.0D00                                                            DEB 0300
      ELSE IF (IABS(CHARGE) .GE. 4) THEN                                          DEB 0310
        DEBYE = 12.0D00                                                           DEB 0320
      END IF                                                                      DEB 0330
                                                                                  DEB 0340
      RETURN                                                                      DEB 0350
      END                                                                         DEB 0360




      SUBROUTINE DISTRB (NUFLAG, FLAGS, GAMMA, Z, DHA, TEMP, HITEMP,  DIS 0010
     .                   EHM, ALK, TITLE, A, B, MXSP, MXAQK, MU,      DIS 0020
     .                   IPRIN1, IPIT, TK, CONV1, ANMTIC, ITIC, HTOT, DIS 0030
     .                   OHTOT, SCO2, JCO3, ITWR, BDOT)               DIS 0040
C ================================================================================|DIS 0050
C     This routine iterates and distributes the species                |DIS 0060
C --------------------------------------------------------------------------------|DIS 0070
C     A          DBL   Molal Debye-Huckel coefficient                  |DIS 0080
C     ALFA       DBL   Activity of aqueous species i                   |DIS 0090
C     ALK        INT   Flag for distribution of carbonate species      |DIS 0100
C     ANALCO     DBL   Inorganic Carbon  ... initially alk or tic      |DIS 0110
C     ANALM      DBL   Analyzed molality of species i                  |DIS 0120
C     ANMTIC     DBL   Analyzed total inorganic carbon                 |DIS 0130
C     B          DBL   Molal Debye-Huckel coefficient                  |DIS 0140
C     BDOT       DBL   Activity coefficient deviation function         |DIS 0150
C     C1         DBL   TDS * 1000.0                                    |DIS 0160
C     CO2F       DBL   Sum of CO2 plus CO2 lost from solution          |DIS 0170
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C     CONV1     DBL   Tolerance factor for convergence of anions          |DIS 0180
C     CPUMIN    DBL   Smallest positive real value program uses          |DIS 0190
C     CR        CHA   Inserts carriage returns in output                |DIS 0200
C     CROSS     LOG   Local logical variable for crossing root          |DIS 0210
C     CUNITS    DBL   Analytical input concentration                    |DIS 0220
C     DHA       DBL   Ion size parameter                                |DIS 0230
C     DIFF      DBL   Difference used in convergence                    |DIS 0240
C     DONE      LOG   Have we crossed root                              |DIS 0250
C     EHM       DBL   Measured Eh in volts                              |DIS 0260
C     EXELT     DBL   Total amount of each component                    |DIS 0270
C     F         DBL   Faraday constant                                  |DIS 0280
C     FACTOR    DBL   Factor used in convergence                        |DIS 0290
C     FIXIT     DBL   Fixing value in the CO2 option                    |DIS 0300
C     FLAGS     INT   Selection flags for calculation of redox equil.   |DIS 0310
C     GAMMA     DBL   Activity coefficient of species i                 |DIS 0320
C     HITEMP    DBL   In-situ temperature                               |DIS 0330
C     HTOT      DBL   Total hydronium (current)                         |DIS 0340
C     HTOTI     DBL   Total hydronium (initial)                         |DIS 0350
C     I         INT   Loop counter                                      |DIS 0360
C     IFL1      INT   Switch sets activity coeffs of non-pitzer species |DIS 0370
C     IOPT      INT   H+ option                                         |DIS 0380
C     IPAGE     INT   Current page number of output file                |DIS 0390
C     IPGLN     INT   Current line number of the output file            |DIS 0400
C     IPIT      INT   Flag to use pitzer activity coefficients          |DIS 0410
C     IPRIN1    INT   Flag for printing iteration of anions             |DIS 0420
C     ITER      INT   Iteration count                                   |DIS 0430
C     ITIC      INT   Hitemp distribution of carbonate species          |DIS 0440
C     ITWR      INT   Printing Flag                                     |DIS 0450
C     JCO3      INT   Switch to control printing of some headings       |DIS 0460
C     KT1       DBL   Equilibrium constant of the aqueous reactions     |DIS 0470
C     LOGKT1    DBL   Log K for aqueous species at specified temp.      |DIS 0480
C     LOGKT2    DBL   Log K for minerals at specified temperature       |DIS 0490
C     M         DBL   Calculated molality of aqueous species            |DIS 0500
C     MU        DBL   Ionic strength of aqueous solution                |DIS 0510
C     MXAQK     INT   Total number of aqueous log k values              |DIS 0520
C     MXSP      INT   Total number of aqueous species                   |DIS 0530
C     NMAX      INT   General array dimension to allow easy expansion   |DIS 0540
C     NUFLAG    INT   Sets the activity coefficients of neutral species |DIS 0550
C     OHTOT     DBL   OH total                                          |DIS 0560
C     OHTOTI    DBL   Initial OH total                                  |DIS 0570
C     PAGE1     CHA   Names of aqueous species                          |DIS 0580
C     PAGE2     CHA   Names of equilibrium constants                    |DIS 0590
C     PAGE3     CHA   Names of solubility constants                     |DIS 0600
C     PALFA     DBL   Pitzer alpha's                                    |DIS 0610
C     PG        DBL   Pitzer gamma's                                    |DIS 0620
C     PGDCA     DBL   Pitzer gamma for Ca                               |DIS 0630
C     PGDNA     DBL   Pitzer gamma for Na                               |DIS 0640
C     PH        DBL   Measured pH of the solution                       |DIS 0650
C     R         DBL   Gas constant                                      |DIS 0660
C     S         DBL   Sum of anions complexes                           |DIS 0670
C     SCO2      DBL   Sum of carbonate in solution                      |DIS 0680
C     T         DBL   Temperature                                       |DIS 0690
C     TEMP      DBL   Temperature of the solution when pH was measured  |DIS 0700
C     TITLE     CHA   Name of the sample                                |DIS 0710
C     TITMIX    CHA   Title for Mixtures                                |DIS 0720
C     TITR      DBL   Convergence (vector) for each component           |DIS 0730
C     TK        DBL   Temperature steps used by program                 |DIS 0740
C     TOTEL     DBL   Total amount of each component                    |DIS 0750
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C     UNO       INT   File unit assigned for output file                    |DIS 0760
C     VERSN     CHA   Version Number                                        |DIS 0770
C     X         DBL   Temperary variable                                    |DIS 0780
C     Z         INT   Charge of aqueous species                             |DIS 0790
C -------------------------------------------------------------------------|DIS 0800
                                                                            DIS 0810
      INTEGER NMAX, UNO                                                     DIS 0820
      DOUBLE PRECISION CPUMIN, F, R                                         DIS 0830
                                                                            DIS 0840
      PARAMETER (NMAX = 340, UNO = 6)                                       DIS 0850
      PARAMETER (CPUMIN = 1.0D-35, F = 2.30603D+1, R = 1.98719D-3)          DIS 0860
                                                                            DIS 0870
      INTEGER ALK, FLAGS(6), I, IFL1, IOPT, IPAGE, IPGLN                    DIS 0880
      INTEGER IPIT, IPRIN1, ITER, ITIC, ITWR                                DIS 0890
      INTEGER JCO3, MXAQK, MXSP, NUFLAG, Z(NMAX)                            DIS 0900
                                                                            DIS 0910
      LOGICAL DONE, CROSS                                                   DIS 0920
                                                                            DIS 0930
      CHARACTER *  1 TOF, CR                                                DIS 0940
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                  DIS 0950
      CHARACTER * 14 VERSN                                                  DIS 0960
      CHARACTER * 40 TITMIX                                                 DIS 0970
      CHARACTER * 80 TITLE                                                  DIS 0980
                                                                            DIS 0990
      DOUBLE PRECISION A, ALFA(NMAX), ANALCO, ANALM(NMAX), ANMTIC           DIS 1000
      DOUBLE PRECISION B, BDOT, C1, CO2F, CONV1, CUNITS(NMAX)               DIS 1010
      DOUBLE PRECISION DCH4, DCO2, DDCH4, DDCO2, DDH2S, DDNH3               DIS 1020
      DOUBLE PRECISION DH2S, DHA(NMAX), DIFF(11), DNH3                      DIS 1030
      DOUBLE PRECISION EHM, EXELT(35), FACTOR(11), FIXIT, GAMMA(NMAX)       DIS 1040
      DOUBLE PRECISION HITEMP, HTOT, HTOTI, INC, KT1(NMAX)                  DIS 1050
      DOUBLE PRECISION LALFA(NMAX), LOGKT1(NMAX), LOGKT2(NMAX)              DIS 1060
      DOUBLE PRECISION M(NMAX), MU, OHTOT, OHTOTI                           DIS 1070
      DOUBLE PRECISION PALFA(NMAX), PG(NMAX), PGDCA, PGDNA, PH              DIS 1080
      DOUBLE PRECISION S(11), SCO2, SEXP10, SLOG10, T, TEMP, TITR(11)       DIS 1090
      DOUBLE PRECISION TK(11), TOTEL(5), X                                  DIS 1100
                                                                            DIS 1110
      EXTERNAL AITLIM, PAGE, PITZER, SEXP10, SLOG10                         DIS 1120
                                                                            DIS 1130
      INTRINSIC DABS, DLOG10, DSQRT, IABS, MOD                              DIS 1140
                                                                            DIS 1150
      COMMON /ALOGK / LOGKT1, LOGKT2                                        DIS 1160
      COMMON /EXTOT / EXELT, TOTEL, TITR                                    DIS 1170
      COMMON /FMFD  / TOF, CR, TITMIX                                       DIS 1180
      COMMON /FORM  / IPAGE, IPGLN                                          DIS 1190
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,                DIS 1200
     .                DCH4, DDCH4, IOPT, FIXIT                             DIS 1210
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                            DIS 1220
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                   DIS 1230
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                                   DIS 1240
      COMMON /TTK   / KT1                                                   DIS 1250
                                                                            DIS 1260
      SAVE DIFF, PGDCA, PGDNA                                               DIS 1270
                                                                            DIS 1280
C =========================================================================|DIS 1290
                                                                            DIS 1300
      VERSN ='USGS-ARC-88-8'                                                DIS 1310
                                                                            DIS 1320
      T = TEMP + 273.15                                                     DIS 1330
```

```
                                                                      DIS 1340
C -----------------------------------------------------------------|DIS 1350
C     Initialize activities to 0                                   |DIS 1360
C -----------------------------------------------------------------|DIS 1370
                                                                      DIS 1380
      DO 10 I = 1, NMAX                                               DIS 1390
        ALFA(I) = 0.0D0                                               DIS 1400
        PG(I)   = 0.0D0                                               DIS 1410
   10 CONTINUE                                                        DIS 1420
                                                                      DIS 1430
      ALFA(8)  = 10.0**(-PH)                                          DIS 1440
                                                                      DIS 1450
      IFL1 = 0                                                        DIS 1460
                                                                      DIS 1470
      DO 20 I = 1, 11                                                 DIS 1480
        DIFF(I)   = 0.0                                               DIS 1490
        FACTOR(I) = 1.0                                               DIS 1500
   20 CONTINUE                                                        DIS 1510
                                                                      DIS 1520
C -----------------------------------------------------------------|DIS 1530
C     Write titles etc.                                            |DIS 1540
C -----------------------------------------------------------------|DIS 1550
                                                                      DIS 1560
      IF (JCO3 .EQ. 0 .AND. ITWR .EQ. 0) THEN                         DIS 1570
        IF (IPRIN1 .NE. 0) THEN                                       DIS 1580
          IF (IPGLN .GE. 45) CALL PAGE                                DIS 1590
          WRITE (UNO, 1000) VERSN, CR                                 DIS 1600
          WRITE (UNO, 1001) TITLE, TITMIX                             DIS 1610
          WRITE (UNO, 1002) TEMP                                      DIS 1620
          WRITE (UNO, 1003)                                           DIS 1630
          WRITE (UNO, 1004) CR                                        DIS 1640
          IPGLN = IPGLN + 14                                          DIS 1650
        END IF                                                        DIS 1660
      END IF                                                          DIS 1670
                                                                      DIS 1680
C -----------------------------------------------------------------|DIS 1690
C     Iterative loop                                               |DIS 1700
C     iter2 counts ph loop; iter counts species distribution       |DIS 1710
C -----------------------------------------------------------------|DIS 1720
                                                                      DIS 1730
      ITER  = 0                                                       DIS 1740
                                                                      DIS 1750
   30 CONTINUE                                                        DIS 1760
      ITER = ITER + 1                                                 DIS 1770
                                                                      DIS 1780
C -----------------------------------------------------------------|DIS 1790
C     Calculation of total molality & ah2o.                        |DIS 1800
C -----------------------------------------------------------------|DIS 1810
                                                                      DIS 1820
      C1 = 0.0D0                                                      DIS 1830
      DO 40 I = 1, MXSP + 44                                          DIS 1840
        IF (I .NE. 10 .AND. I .NE. 12 .AND. I .NE. 32) C1 = C1 + M(I) DIS 1850
   40 CONTINUE                                                        DIS 1860
                                                                      DIS 1870
      IF (C1 .GT. 10.0) C1 = 10.0                                     DIS 1880
      ALFA(10) = 1.0D0 - (1.7D-2 * C1)                                DIS 1890
                                                                      DIS 1900
C -----------------------------------------------------------------|DIS 1910
```

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C     Calculation of the ionic strength (i), equivalent mnacle=i.      |DIS 1920
C ---------------------------------------------------------------------|DIS 1930
                                                                        DIS 1940
      MU = 0.0D0                                                        DIS 1950
      DO 50 I = 1, MXSP + 44                                            DIS 1960
        IF (M(I) .LT. CPUMIN) THEN                                      DIS 1970
          M(I) = 0.0D0                                                  DIS 1980
        ELSE IF (I .EQ. 163 .AND. M(I) .GT. 2.0) THEN                   DIS 1990
          MU = MU + (1.0 * Z(I)**2)                                     DIS 2000
        ELSE                                                            DIS 2010
          MU = MU + (M(I) * Z(I)**2)                                    DIS 2020
        END IF                                                          DIS 2030
   50 CONTINUE                                                          DIS 2040
                                                                        DIS 2050
      MU = 0.5D0 * MU                                                   DIS 2060
      IF (MU .GT. 10.0) MU = 10.0                                       DIS 2070
                                                                        DIS 2080
C ---------------------------------------------------------------------|DIS 2090
C     Only call pitzer the first time each temperature is done         |DIS 2100
C ---------------------------------------------------------------------|DIS 2110
                                                                        DIS 2120
      IF (IPIT .EQ. 1 .AND. ITER .EQ. 1) THEN                           DIS 2130
        CALL PITZER (A, MU, MXSP, TEMP, PGDCA, PGDNA, PG, TK, PALFA,    DIS 2140
     .               EXELT(29), Z, IFL1)                                DIS 2150
      END IF                                                            DIS 2160
                                                                        DIS 2170
      IFL1 = 1                                                          DIS 2180
                                                                        DIS 2190
   60 CONTINUE                                                          DIS 2200
      IF (IPIT .EQ. 1) THEN                                             DIS 2210
        IF (IFL1 .EQ. 1) I = 3                                          DIS 2220
        IF (IFL1 .EQ. 2) I = 1                                          DIS 2230
        IF (IFL1 .EQ. 1) GAMMA(I) = PGDNA                               DIS 2240
        IF (IFL1 .EQ. 2) GAMMA(I) = PGDCA                               DIS 2250
                                                                        DIS 2260
C ---------------------------------------------------------------------|DIS 2270
C     The following statement when enabled may give improved results   |DIS 2280
C     at lower temperatures and salinities.  When high temperatures or |DIS 2290
C     salinities are involved this statement should be disabled since  |DIS 2300
C     it will cause the program to return activity coefficients which  |DIS 2310
C     are too high.                                                    |DIS 2320
C       IF (M(I) .GT. CPUMIN) GAMMA(I) = GAMMA(I) * EXELT(I) / M(I)     DIS 2330
C ---------------------------------------------------------------------|DIS 2340
                                                                        DIS 2350
        BDOT = DLOG10(GAMMA(I)) + ((A * Z(I)**2 * DSQRT(MU)) /          DIS 2360
     .         (1.0 + DHA(I) * B * DSQRT(MU)))                          DIS 2370
        BDOT = BDOT / MU                                                DIS 2380
      END IF                                                            DIS 2390
                                                                        DIS 2400
C ---------------------------------------------------------------------|DIS 2410
C     Calculation of the activity coefficients (gamma) for charged     |DIS 2420
C     species by the bdot method (helgeson,1969).  If pitzer equations |DIS 2430
C     are being used, bdot is not the same as in helgeson.             |DIS 2440
C ---------------------------------------------------------------------|DIS 2450
                                                                        DIS 2460
      DO 70 I = 1, MXSP + 44                                            DIS 2470
        IF (Z(I).EQ.0) GO TO 70                                         DIS 2480
        IF (IFL1.EQ.1 .AND. (IABS(Z(I))).NE.1) GO TO 70                 DIS 2490
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        IF (IFL1.EQ.2 .AND. (IABS(Z(I))).LT.2) GO TO 70                  DIS 2500
        GAMMA(I) = A * DSQRT(MU) * Z(I)**2                               DIS 2510
        GAMMA(I) = GAMMA(I) / (1.0 + (DHA(I) * B * DSQRT(MU)))           DIS 2520
        GAMMA(I) = (BDOT * MU) - GAMMA(I)                                DIS 2530
        GAMMA(I) = 10.0**GAMMA(I)                                        DIS 2540
   70 CONTINUE                                                           DIS 2550
                                                                         DIS 2560
C ---------------------------------------------------------------------|DIS 2570
C     Calculation of a number of anion activities.                       |DIS 2580
C ---------------------------------------------------------------------|DIS 2590
                                                                         DIS 2600
      IF (NUFLAG .EQ. 0) THEN                                            DIS 2610
        GAMMA(11) = 10.0**(0.00978 * 10.0**(280.0 / T) * (MU + 1.0D0))   DIS 2620
        GAMMA(12) = GAMMA(11)                                            DIS 2630
      END IF                                                             DIS 2640
                                                                         DIS 2650
      IF (IFL1 .EQ. 1) THEN                                              DIS 2660
        IFL1 = 2                                                         DIS 2670
        GO TO 60                                                         DIS 2680
      END IF                                                             DIS 2690
                                                                         DIS 2700
      IFL1 = 3                                                           DIS 2710
                                                                         DIS 2720
      DO 80 I = 1, MXSP + 44                                             DIS 2730
        IF (ALFA(I) .LT. CPUMIN) THEN                                    DIS 2740
            ALFA(I)  = 0.0D0                                             DIS 2750
            LALFA(I) = -999.9                                            DIS 2760
        ELSE                                                             DIS 2770
            LALFA(I) = DLOG10(ALFA(I))                                   DIS 2780
        END IF                                                           DIS 2790
        IF (I .NE. 6 .AND. PG(I) .GT. CPUMIN) GAMMA(I) = PG(I)           DIS 2800
   80 CONTINUE                                                           DIS 2810
                                                                         DIS 2820
C ---------------------------------------------------------------------|DIS 2830
C     Activity of H+ and OH-                                             |DIS 2840
C -------------------------                                             |DIS 2850
                                                                         DIS 2860
      ALFA(8)  = 10.0**(-PH)                                             DIS 2870
      LALFA(8) = -PH                                                     DIS 2880
      M(8)     = ALFA(8) / GAMMA(8)                                      DIS 2890
                                                                         DIS 2900
      ALFA(9)  = ALFA(10) * KT1(2) / ALFA(8)                             DIS 2910
      LALFA(9) = DLOG10(ALFA(9))                                         DIS 2920
      M(9)     = ALFA(9) / GAMMA(9)                                      DIS 2930
                                                                         DIS 2940
C ---------------------------------------------------------------------|DIS 2950
C     Chloride species                                                   |DIS 2960
C --------------------                                                  |DIS 2970
                                                                         DIS 2980
      IF (EXELT(5) .GT. CPUMIN) THEN                                     DIS 2990
   90   CONTINUE                                                        DIS 3000
        M(5)     = TITR(5)                                               DIS 3010
        ALFA(5)  = M(5) * GAMMA(5)                                       DIS 3020
        LALFA(5) = SLOG10(ALFA(5))                                       DIS 3030
                                                                         DIS 3040
        IF (IPIT .EQ. 1 .AND. PG(5) .GT. CPUMIN                          DIS 3050
     .                  .AND. GAMMA(5) .LE. 10) THEN                    DIS 3060
          IF (DABS(PALFA(5) - ALFA(5)) .GT. 1.0D-2 * PALFA(5)) THEN      DIS 3070
```

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            IF (PALFA(5) .GT. ALFA(5)) THEN                                  DIS 3080
              INC=0.1                                                        DIS 3090
            ELSE                                                             DIS 3100
              INC=-0.01                                                      DIS 3110
            END IF                                                           DIS 3120
            GAMMA(5)=GAMMA(5)*(1.0+INC)                                      DIS 3130
            GO TO 90                                                         DIS 3140
          END IF                                                             DIS 3150
        END IF                                                               DIS 3160
        IF (IPIT .EQ. 1 .AND. GAMMA(5) .GT. 10.0)  GAMMA(5) = 10.0           DIS 3170
        IF (IPIT .EQ. 1 .AND. GAMMA(5) .LT. PG(5)) GAMMA(5) = PG(5)          DIS 3180
      END IF                                                                 DIS 3190
                                                                             DIS 3200
C -------------------------------------------------------------------------|DIS 3210
C     Acetate species                                                        |DIS 3220
C -------------------                                                       |DIS 3230
                                                                             DIS 3240
      IF (EXELT(26) .GT. CPUMIN) THEN                                        DIS 3250
        M(228)    = TITR(6) / (1.0D0 + ((GAMMA(228) * KT1(25)) /           DIS 3260
     .                        (ALFA(8) * GAMMA(48))))                      DIS 3270
        ALFA(228) = M(228) * GAMMA(228)                                      DIS 3280
        LALFA(228) = SLOG10(ALFA(228))                                       DIS 3290
                                                                             DIS 3300
        M(48) = LOGKT1(25) + LALFA(228) - DLOG10(GAMMA(48)) - LALFA(8)       DIS 3310
        M(48) = SEXP10(M(48))                                                DIS 3320
        ALFA(48)  = M(48) * GAMMA(48)                                        DIS 3330
        LALFA(48) = SLOG10(ALFA(48))                                         DIS 3340
      END IF                                                                 DIS 3350
                                                                             DIS 3360
C -------------------------------------------------------------------------|DIS 3370
C     Oxalate species                                                        |DIS 3380
C -------------------                                                       |DIS 3390
                                                                             DIS 3400
      IF (EXELT(30) .GT. CPUMIN) THEN                                        DIS 3410
        M(247)    = TITR(8) / (1.0D0 + ((GAMMA(247) * ALFA(8) /            DIS 3420
     .              KT1(224) * GAMMA(248)) + ((KT1(223) * GAMMA(247)) /    DIS 3430
     .             (GAMMA(246) * ALFA(8)))))                               DIS 3440
                                                                             DIS 3450
        ALFA(247)  = M(247) * GAMMA(247)                                     DIS 3460
        LALFA(247) = SLOG10(ALFA(247))                                       DIS 3470
                                                                             DIS 3480
        M(248)     = LALFA(247) + LALFA(8) - LOGKT1(224)                     DIS 3490
     .                          - DLOG10(GAMMA(248))                        DIS 3500
        M(248)     = SEXP10(M(248))                                          DIS 3510
                                                                             DIS 3520
        ALFA(248)  = M(248) * GAMMA(248)                                     DIS 3530
        LALFA(248) = SLOG10(ALFA(248))                                       DIS 3540
                                                                             DIS 3550
        M(246)     = LOGKT1(223) + LALFA(247) - DLOG10(GAMMA(246))           DIS 3560
     .                          - LALFA(8)                                  DIS 3570
        M(246)     = SEXP10(M(246))                                          DIS 3580
        ALFA(246)  = M(246) * GAMMA(246)                                     DIS 3590
        LALFA(246) = SLOG10(ALFA(246))                                       DIS 3600
      END IF                                                                 DIS 3610
                                                                             DIS 3620
C -------------------------------------------------------------------------|DIS 3630
C     Succinate species                                                      |DIS 3640
C --------------------                                                      |DIS 3650
```

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                                                                      DIS 3660
      IF (EXELT(31) .GT. CPUMIN) THEN                                 DIS 3670
        M(266)    = TITR(9) / (1.0D0 + ((GAMMA(266) * ALFA(8) /       DIS 3680
     .              KT1(242) * GAMMA(267)) + ((KT1(241) * GAMMA(266)) / DIS 3690
     .             (GAMMA(265) * ALFA(8)))))                          DIS 3700
                                                                      DIS 3710
        ALFA(266)  = M(266) * GAMMA(266)                              DIS 3720
        LALFA(266) = SLOG10(ALFA(266))                                DIS 3730
                                                                      DIS 3740
        M(267)    = LALFA(266) + LALFA(8) - LOGKT1(242)               DIS 3750
        M(267)    = SEXP10(M(267))                                    DIS 3760
        M(267)    = M(267) / GAMMA(267)                               DIS 3770
                                                                      DIS 3780
        ALFA(267) = M(267) * GAMMA(267)                               DIS 3790
        LALFA(267) = SLOG10(ALFA(267))                                DIS 3800
                                                                      DIS 3810
        M(265)    = LOGKT1(241) + LALFA(266) - LALFA(8)               DIS 3820
        M(265)    = SEXP10(M(265))                                    DIS 3830
        M(265)    = M(265) / GAMMA(265)                               DIS 3840
                                                                      DIS 3850
        ALFA(265)  = M(265) * GAMMA(265)                              DIS 3860
        LALFA(265) = SLOG10(ALFA(265))                                DIS 3870
      END IF                                                          DIS 3880
                                                                      DIS 3890
                                                                      DIS 3900
C -----------------------------------------------------------------|DIS 3910
C     User defined anion #1                                         |DIS 3920
C ------------------------                                         |DIS 3930
                                                                      DIS 3940
      IF (EXELT(33) .GT. CPUMIN) THEN                                 DIS 3950
        M(MXSP+2)    = TITR(10) / (1.0D0 + ((GAMMA(MXSP+2) * ALFA(8)) / DIS 3960
     .                 (KT1(MXAQK+2) * GAMMA(MXSP+3)) +              DIS 3970
     .                ((KT1(MXAQK+1) * GAMMA(MXSP+2)) /              DIS 3980
     .                 (GAMMA(MXSP+1) * ALFA(8)))))                  DIS 3990
        ALFA(MXSP+2) = M(MXSP+2) * GAMMA(MXSP+2)                      DIS 4000
                                                                      DIS 4010
        M(MXSP+3)    = (ALFA(MXSP+2) * ALFA(8)) / (KT1(MXAQK+2) *     DIS 4020
     .                   GAMMA(MXSP+3))                               DIS 4030
        ALFA(MXSP+3) = M(MXSP+3) * GAMMA(MXSP+3)                      DIS 4040
                                                                      DIS 4050
        M(MXSP+1)    = (KT1(MXAQK+1) * ALFA(MXSP+2)) /                DIS 4060
     .                 (GAMMA(MXSP+1) * ALFA(8))                     DIS 4070
        ALFA(MXSP+1) = M(MXSP+1) * GAMMA(MXSP+1)                      DIS 4080
      END IF                                                          DIS 4090
                                                                      DIS 4100
C -----------------------------------------------------------------|DIS 4110
C     User defined anion #2                                         |DIS 4120
C --------------------                                             |DIS 4130
                                                                      DIS 4140
      IF (EXELT(34) .GT. CPUMIN) THEN                                 DIS 4150
        M(MXSP+17)    = TITR(11) / (1.0D0 + ((GAMMA(MXSP+17) *        DIS 4160
     .                  ALFA(8)) / (KT1(MXAQK+16) * GAMMA(MXSP+18)) +  DIS 4170
     .                 ((KT1(MXAQK+15) * GAMMA(MXSP+17)) /           DIS 4180
     .                  (GAMMA(MXSP+16) * ALFA(8)))))                DIS 4190
        ALFA(MXSP+17) = M(MXSP+17) * GAMMA(MXSP+17)                   DIS 4200
                                                                      DIS 4210
        M(MXSP+18)    = (ALFA(MXSP+17) * ALFA(8)) / (KT1(MXAQK+16) *  DIS 4220
     .                    GAMMA(MXSP+18))                             DIS 4230
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        ALFA(MXSP+18) = M(MXSP+18) * GAMMA(MXSP+18)                          DIS 4240
                                                                             DIS 4250
        M(MXSP+16)    = (KT1(MXAQK+15) * ALFA(MXSP+17)) /                    DIS 4260
     .                    (GAMMA(MXSP+16) * ALFA(8))                        DIS 4270
        ALFA(MXSP+16) = M(MXSP+16) * GAMMA(MXSP+16)                          DIS 4280
      END IF                                                                 DIS 4290
                                                                             DIS 4300
C ---------------------------------------------------------------------|DIS 4310
C     Fluoride species                                                 |DIS 4320
C -------------------                                                  |DIS 4330
                                                                             DIS 4340
      IF (EXELT(22) .GT. CPUMIN) THEN                                        DIS 4350
        M(30)     = TITR(3) / (1.0D0 + ((GAMMA(30) * ALFA(8)) /            DIS 4360
     .                          (KT1(71) * GAMMA(96))))                    DIS 4370
        ALFA(30)  = M(30) * GAMMA(30)                                        DIS 4380
        LALFA(30) = SLOG10(ALFA(30))                                         DIS 4390
                                                                             DIS 4400
        M(96)     = (ALFA(30) * ALFA(8)) / (KT1(71) * GAMMA(96))             DIS 4410
        ALFA(96)  = M(96) * GAMMA(96)                                        DIS 4420
        LALFA(96) = SLOG10(ALFA(96))                                         DIS 4430
      END IF                                                                 DIS 4440
                                                                             DIS 4450
C ---------------------------------------------------------------------|DIS 4460
C     CO2 species                                                      |DIS 4470
C --------------                                                       |DIS 4480
                                                                             DIS 4490
      IF (EXELT(29) .GT. CPUMIN) THEN                                        DIS 4500
        M(7)      = TITR(1) / (1.0D0 + ((GAMMA(7) * KT1(1) * 2) /          DIS 4510
     .              (GAMMA(98) * ALFA(8))))                                DIS 4520
        ALFA(7)   = M(7) * GAMMA(7)                                          DIS 4530
        LALFA(7)  = SLOG10(ALFA(7))                                          DIS 4540
                                                                             DIS 4550
        M(98)     = (KT1(1) * ALFA(7)) / (GAMMA(98) * ALFA(8))               DIS 4560
        ALFA(98)  = M(98) * GAMMA(98)                                        DIS 4570
        LALFA(98) = SLOG10(ALFA(98))                                         DIS 4580
                                                                             DIS 4590
        M(97)     = (ALFA(7) * ALFA(8)) / (KT1(72) * GAMMA(97))              DIS 4600
        ALFA(97)  = M(97) * GAMMA(97)                                        DIS 4610
        LALFA(97) = SLOG10(ALFA(97))                                         DIS 4620
      END IF                                                                 DIS 4630
                                                                             DIS 4640
C ---------------------------------------------------------------------|DIS 4650
C     Sulfur species                                                   |DIS 4660
C -----------------                                                    |DIS 4670
                                                                             DIS 4680
      IF (EXELT(25) .GT. CPUMIN) THEN                                        DIS 4690
        M(101)     = TITR(7) / (1.0D0 + ((GAMMA(101) * ALFA(8)) /          DIS 4700
     .               (KT1(10) * GAMMA(33)) + ((KT1(75) * GAMMA(101)) /     DIS 4710
     .               (GAMMA(102) * ALFA(8)))))                             DIS 4720
        ALFA(101)  = GAMMA(101) * M(101)                                     DIS 4730
        LALFA(101) = SLOG10(ALFA(101))                                       DIS 4740
                                                                             DIS 4750
        M(33)      = (ALFA(101) * ALFA(8)) / (KT1(10) * GAMMA(33))           DIS 4760
        ALFA(33)   = M(33) * GAMMA(33)                                       DIS 4770
        LALFA(33)  = SLOG10(ALFA(33))                                        DIS 4780
                                                                             DIS 4790
        M(102)     = (KT1(75) * ALFA(101)) / (GAMMA(102) * ALFA(8))          DIS 4800
        ALFA(102)  = M(102) * GAMMA(102)                                     DIS 4810
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        LALFA(102) = SLOG10(ALFA(102))                                    DIS 4820
      END IF                                                              DIS 4830
                                                                          DIS 4840
  100 CONTINUE                                                            DIS 4850
      IF (EXELT(6) .GE. CPUMIN) THEN                                      DIS 4860
        M(103)     = TITR(2) / (1.0D0 + (((KT1(76) * GAMMA(103)) /        DIS 4870
     .               (GAMMA(6) * ALFA(8)))))                            DIS 4880
        ALFA(103)  = M(103) * GAMMA(103)                                  DIS 4890
        LALFA(103) = SLOG10(ALFA(103))                                    DIS 4900
                                                                          DIS 4910
        M(6)       = (KT1(76) * ALFA(103)) / (GAMMA(6) * ALFA(8))         DIS 4920
        ALFA(6)    = M(6) * GAMMA(6)                                      DIS 4930
        LALFA(6)   = SLOG10(ALFA(6))                                      DIS 4940
                                                                          DIS 4950
        IF (IPIT .EQ. 1 .AND. PG(6) .GT. CPUMIN                           DIS 4960
     .                  .AND. GAMMA(6) .LE. 10.0) THEN                   DIS 4970
          IF (DABS(PALFA(6)-ALFA(6)) .GT. 1.0D-2*PALFA(6)) THEN           DIS 4980
            IF (PALFA(6) .GT. ALFA(6)) THEN                               DIS 4990
              INC=0.1                                                     DIS 5000
            ELSE                                                          DIS 5010
              INC=-0.01                                                   DIS 5020
            END IF                                                        DIS 5030
            GAMMA(6)=GAMMA(6)*(1.0+INC)                                   DIS 5040
            GO TO 100                                                     DIS 5050
          END IF                                                          DIS 5060
        END IF                                                            DIS 5070
        IF (IPIT.EQ.1 .AND. GAMMA(6) .GT. 10.0)  GAMMA(6) = 10.0          DIS 5080
        IF (IPIT.EQ.1 .AND. GAMMA(6) .LT. PG(6)) GAMMA(6) = PG(6)         DIS 5090
      END IF                                                              DIS 5100
                                                                          DIS 5110
C -------------------------------------------------------------------    |DIS 5120
C     Silica species                                                      |DIS 5130
C -----------------                                                       |DIS 5140
                                                                          DIS 5150
      IF (EXELT(8) .GT. CPUMIN) THEN                                      DIS 5160
        M(91)      = EXELT(8) / (1.0D0 + ((GAMMA(91) * ALFA(8)) /         DIS 5170
     .               (KT1(3) * GAMMA(11)) + ((KT1(66) * GAMMA(91)) /     DIS 5180
     .               (GAMMA(90) * ALFA(8)))))                            DIS 5190
        ALFA(91)   = GAMMA(91) * M(91)                                    DIS 5200
        LALFA(91)  = SLOG10(ALFA(91))                                     DIS 5210
                                                                          DIS 5220
        M(11)      = (ALFA(91) * ALFA(8)) / (KT1(3) * GAMMA(11))          DIS 5230
        ALFA(11)   = M(11) * GAMMA(11)                                    DIS 5240
        LALFA(11)  = SLOG10(ALFA(11))                                     DIS 5250
                                                                          DIS 5260
        M(90)      = (KT1(66) * ALFA(91)) / (GAMMA(90) * ALFA(8))         DIS 5270
        ALFA(90)   = M(90) * GAMMA(90)                                    DIS 5280
        LALFA(90)  = SLOG10(ALFA(90))                                     DIS 5290
                                                                          DIS 5300
        M(12)      = M(11)                                                DIS 5310
        ALFA(12)   = M(12) * GAMMA(12)                                    DIS 5320
        LALFA(12)  = SLOG10(ALFA(12))                                     DIS 5330
                                                                          DIS 5340
        M(284)     = (ALFA(11) * ALFA(30)**2 * (ALFA(30) / ALFA(9))       DIS 5350
     .             * (ALFA(30) / ALFA(9))    * (ALFA(30) / ALFA(9))     DIS 5360
     .             * (ALFA(30) / ALFA(9)))   / KT1(257)                  DIS 5370
                                                                          DIS 5380
        ALFA(284)  = M(284) * GAMMA(284)                                  DIS 5390
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        LALFA(284) = SLOG10(ALFA(284))                                    DIS 5400
      END IF                                                              DIS 5410
                                                                          DIS 5420
C -----------------------------------------------------------------------|DIS 5430
C     Boron Species                                                       |DIS 5440
C ----------------                                                       |DIS 5450
                                                                          DIS 5460
      IF (EXELT(23) .GT. CPUMIN) THEN                                     DIS 5470
        M(31)     = EXELT(23) / (1.0D0 + ((GAMMA(31) * ALFA(9)) /         DIS 5480
     .                          (KT1(64) * GAMMA(89))))                  DIS 5490
        ALFA(31)  = M(31) * GAMMA(31)                                     DIS 5500
        LALFA(31) = SLOG10(ALFA(31))                                      DIS 5510
                                                                          DIS 5520
        M(89)     = (ALFA(31) * ALFA(9)) / (KT1(64) * GAMMA(89))          DIS 5530
        ALFA(89)  = M(89) * GAMMA(89)                                     DIS 5540
        LALFA(89) = SLOG10(ALFA(89))                                      DIS 5550
      END IF                                                              DIS 5560
                                                                          DIS 5570
C -----------------------------------------------------------------------|DIS 5580
C     Phosphate species                                                   |DIS 5590
C --------------------                                                   |DIS 5600
                                                                          DIS 5610
      IF (EXELT(21) .GT. CPUMIN) THEN                                     DIS 5620
        M(29)     = TITR(4) / (1.0D0 + GAMMA(29) * ((ALFA(8) /            DIS 5630
     .              (KT1(73) * GAMMA(99))) + (ALFA(8)**2 / (KT1(74) *    DIS 5640
     .              GAMMA(100))) + (ALFA(8)**3 / (KT1(49) *              DIS 5650
     .              GAMMA(74)))))                                        DIS 5660
        ALFA(29)  = M(29) * GAMMA(29)                                     DIS 5670
        LALFA(29) = SLOG10(ALFA(29))                                      DIS 5680
                                                                          DIS 5690
        M(74)     = (ALFA(29) * ALFA(8)**3) / (KT1(49) * GAMMA(74))       DIS 5700
        ALFA(74)  = M(74) * GAMMA(74)                                     DIS 5710
        LALFA(74) = SLOG10(ALFA(74))                                      DIS 5720
                                                                          DIS 5730
        M(99)     = (ALFA(29) * ALFA(8)) / (KT1(73) * GAMMA(99))          DIS 5740
        ALFA(99)  = M(99) * GAMMA(99)                                     DIS 5750
        LALFA(99) = SLOG10(ALFA(99))                                      DIS 5760
                                                                          DIS 5770
        M(100)     = (ALFA(29) * ALFA(8)**2) / (KT1(74) * GAMMA(100))     DIS 5780
        ALFA(100)  = M(100) * GAMMA(100)                                  DIS 5790
        LALFA(100) = SLOG10(ALFA(100))                                    DIS 5800
      END IF                                                              DIS 5810
                                                                          DIS 5820
C -----------------------------------------------------------------------|DIS 5830
C     Nitrogen species                                                    |DIS 5840
C -------------------                                                    |DIS 5850
                                                                          DIS 5860
      IF (EXELT(24) .GT. CPUMIN) THEN                                     DIS 5870
        M(147)     = ALFA(9) / (KT1(118) * GAMMA(147))                    DIS 5880
                                                                          DIS 5890
        M(146)     = EXELT(24) / (1.0D0 + GAMMA(146) * M(147))            DIS 5900
        ALFA(146)  = M(146) * GAMMA(146)                                  DIS 5910
        LALFA(146) = SLOG10(ALFA(146))                                    DIS 5920
                                                                          DIS 5930
        M(147)     = M(147) * ALFA(146)                                   DIS 5940
        ALFA(147)  = M(147) * GAMMA(147)                                  DIS 5950
        LALFA(147) = SLOG10(ALFA(147))                                    DIS 5960
                                                                          DIS 5970
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        M(32)     = M(147)                                                  DIS 5980
        ALFA(32)  = M(32) * GAMMA(32)                                       DIS 5990
        LALFA(32) = SLOG10(ALFA(32))                                        DIS 6000
      END IF                                                                DIS 6010
                                                                            DIS 6020
      IF (EXELT(32) .GT. CPUMIN) THEN                                       DIS 6030
        M(136)    = EXELT(32) / (1.0D0 + ((GAMMA(136) * ALFA(8)) /          DIS 6040
     .              (KT1(77) * GAMMA(104))))                              DIS 6050
        ALFA(136) = M(136) * GAMMA(136)                                     DIS 6060
        LALFA(136) = SLOG10(ALFA(136))                                      DIS 6070
                                                                            DIS 6080
        M(104)     = (ALFA(8) * ALFA(136)) / (KT1(77) * GAMMA(104))         DIS 6090
        ALFA(104)  = M(104) * GAMMA(104)                                    DIS 6100
        LALFA(104) = SLOG10(ALFA(104))                                      DIS 6110
      END IF                                                                DIS 6120
                                                                            DIS 6130
C -------------------------------------------------------------------------|DIS 6140
C     User defined cation                                                   |DIS 6150
C -----------------------                                                   |DIS 6160
                                                                            DIS 6170
      IF (EXELT(35) .GT. CPUMIN) THEN                                       DIS 6180
        M(MXSP+32) = ALFA(  5)     / (KT1(MXAQK+29) * GAMMA(MXSP+32))       DIS 6190
        M(MXSP+33) = ALFA(  6)     / (KT1(MXAQK+30) * GAMMA(MXSP+33))       DIS 6200
        M(MXSP+34) = ALFA(  7)     / (KT1(MXAQK+31) * GAMMA(MXSP+34))       DIS 6210
        M(MXSP+35) = ALFA(  9)     / (KT1(MXAQK+32) * GAMMA(MXSP+35))       DIS 6220
        M(MXSP+36) = ALFA( 29)     / (KT1(MXAQK+33) * GAMMA(MXSP+36))       DIS 6230
        M(MXSP+37) = ALFA( 30)     / (KT1(MXAQK+34) * GAMMA(MXSP+37))       DIS 6240
        M(MXSP+38) = ALFA( 48)     / (KT1(MXAQK+35) * GAMMA(MXSP+38))       DIS 6250
        M(MXSP+39) = ALFA( 98)     / (KT1(MXAQK+36) * GAMMA(MXSP+39))       DIS 6260
        M(MXSP+40) = ALFA(101)     / (KT1(MXAQK+37) * GAMMA(MXSP+40))       DIS 6270
        M(MXSP+41) = ALFA(246)     / (KT1(MXAQK+38) * GAMMA(MXSP+41))       DIS 6280
        M(MXSP+42) = ALFA(265)     / (KT1(MXAQK+39) * GAMMA(MXSP+42))       DIS 6290
        M(MXSP+43) = ALFA(MXSP+ 1) / (KT1(MXAQK+40) * GAMMA(MXSP+43))       DIS 6300
        M(MXSP+44) = ALFA(MXSP+16) / (KT1(MXAQK+41) * GAMMA(MXSP+44))       DIS 6310
                                                                            DIS 6320
        M(MXSP+31)    = EXELT(35) / (1.0D0 + GAMMA(MXSP+31)  *              DIS 6330
     .                  (M(MXSP+32) + M(MXSP+33) + M(MXSP+34) +             DIS 6340
     .                   M(MXSP+35) + M(MXSP+36) + M(MXSP+37) +             DIS 6350
     .                   M(MXSP+38) + M(MXSP+39) + M(MXSP+40) +             DIS 6360
     .                   M(MXSP+41) + M(MXSP+42) + M(MXSP+43) +             DIS 6370
     .                   M(MXSP+44)))                                       DIS 6380
        ALFA(MXSP+31)  = M(MXSP+31) * GAMMA(MXSP+31)                        DIS 6390
        LALFA(MXSP+31) = SLOG10(ALFA(MXSP+31))                              DIS 6400
                                                                            DIS 6410
        DO 110 I = 32, 44                                                   DIS 6420
          M(MXSP+I)     = M(MXSP+I) * ALFA(MXSP+31)                         DIS 6430
          ALFA(MXSP+I)  = M(MXSP+I) * GAMMA(MXSP+I)                         DIS 6440
          LALFA(MXSP+I) = SLOG10(ALFA(MXSP+I))                              DIS 6450
  110   CONTINUE                                                            DIS 6460
      END IF                                                                DIS 6470
                                                                            DIS 6480
C -------------------------------------------------------------------------|DIS 6490
C     Calcium species                                                       |DIS 6500
C ------------------                                                        |DIS 6510
                                                                            DIS 6520
  120 CONTINUE                                                              DIS 6530
      IF (EXELT(1) .GT. CPUMIN) THEN                                        DIS 6540
        M( 55) = ALFA( 98)    / (KT1( 30) * GAMMA(55))                      DIS 6550
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      M( 56) = ALFA(  7)    / (KT1( 31) * GAMMA(56))                  DIS 6560
      M( 57) = ALFA(  9)    / (KT1( 32) * GAMMA(57))                  DIS 6570
      M( 58) = ALFA( 29)    / (KT1( 33) * GAMMA(58))                  DIS 6580
      M( 59) = ALFA( 99)    / (KT1( 34) * GAMMA(59))                  DIS 6590
      M( 60) = ALFA(100)    / (KT1( 35) * GAMMA(60))                  DIS 6600
      M( 61) = ALFA(  6)    / (KT1( 36) * GAMMA(61))                  DIS 6610
      M(231) = ALFA( 48)    / (KT1(211) * GAMMA(231))                 DIS 6620
      M(252) = ALFA(246)    / (KT1(228) * GAMMA(252))                 DIS 6630
      M(271) = ALFA(265)    / (KT1(246) * GAMMA(271))                 DIS 6640
      M(281) = ALFA(  5)    / (KT1(146) * GAMMA(281))                 DIS 6650
      M(282) = ALFA(  5)**2 / (KT1(147) * GAMMA(282))                 DIS 6660
      M(MXSP+ 6) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 5) * GAMMA(MXSP+ 6))   DIS 6670
      M(MXSP+21) = ALFA(MXSP+16) / (KT1(MXAQK+19) * GAMMA(MXSP+21))   DIS 6680
                                                                      DIS 6690
      M(1) = EXELT(1) / (1.0D0 + GAMMA(1) * (M(55) + M(56) + M(57) +  DIS 6700
     .       M(58) + M(59) + M(60) + M(61) + M(231) + M(252) +        DIS 6710
     .       M(271) + M(281) + M(282) + M(MXSP+6) + M(MXSP+21)))      DIS 6720
      ALFA(1)  = M(1) * GAMMA(1)                                      DIS 6730
      LALFA(1) = SLOG10(ALFA(1))                                      DIS 6740
                                                                      DIS 6750
      DO 130 I = 55, 61                                               DIS 6760
        M(I)     = M(I) * ALFA(1)                                     DIS 6770
        ALFA(I)  = M(I) * GAMMA(I)                                    DIS 6780
        LALFA(I) = SLOG10(ALFA(I))                                    DIS 6790
  130 CONTINUE                                                        DIS 6800
                                                                      DIS 6810
      M(231)         = M(231) * ALFA(1)                             DIS 6820
      ALFA(231)      = M(231) * GAMMA(231)                          DIS 6830
      LALFA(231)     = SLOG10(ALFA(231))                            DIS 6840
                                                                      DIS 6850
      M(252)         = M(252) * ALFA(1)                             DIS 6860
      ALFA(252)      = M(252) * GAMMA(252)                          DIS 6870
      LALFA(252)     = SLOG10(ALFA(252))                            DIS 6880
                                                                      DIS 6890
      M(271)         = M(271) * ALFA(1)                             DIS 6900
      ALFA(271)      = M(271) * GAMMA(271)                          DIS 6910
      LALFA(271)     = SLOG10(ALFA(271))                            DIS 6920
                                                                      DIS 6930
      M(281)         = M(281) * ALFA(1)                             DIS 6940
      ALFA(281)      = M(281) * GAMMA(281)                          DIS 6950
      LALFA(281)     = SLOG10(ALFA(281))                            DIS 6960
                                                                      DIS 6970
      M(282)         = M(282) * ALFA(1)                             DIS 6980
      ALFA(282)      = M(282) * GAMMA(282)                          DIS 6990
      LALFA(282)     = SLOG10(ALFA(282))                            DIS 7000
                                                                      DIS 7010
      M(MXSP+6)      = M(MXSP+6) * ALFA(1)                          DIS 7020
      ALFA(MXSP+6)   = M(MXSP+6) * GAMMA(MXSP+6)                    DIS 7030
      LALFA(MXSP+6)  = SLOG10(ALFA(MXSP+6))                         DIS 7040
                                                                      DIS 7050
      M(MXSP+21)      = M(MXSP+21) * ALFA(1)                        DIS 7060
      ALFA(MXSP+21)   = M(MXSP+21) * GAMMA(MXSP+21)                 DIS 7070
      LALFA(MXSP+21)  = SLOG10(ALFA(MXSP+21))                       DIS 7080
                                                                      DIS 7090
      IF (IPIT.EQ.1 .AND. PG(1).GT.CPUMIN                           DIS 7100
     .              .AND. GAMMA(1).LE.10.0) THEN                    DIS 7110
        IF (DABS(PALFA(1) - ALFA(1)) .GT. 1.0D-2*PALFA(1)) THEN     DIS 7120
          IF (PALFA(1) .GT. ALFA(1)) THEN                           DIS 7130
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            INC = 0.1                                                          DIS 7140
          ELSE                                                                 DIS 7150
            INC = -0.01                                                        DIS 7160
          END IF                                                               DIS 7170
          GAMMA(1) = GAMMA(1) * (1 + INC)                                      DIS 7180
          GO TO 120                                                            DIS 7190
        END IF                                                                 DIS 7200
      END IF                                                                   DIS 7210
                                                                               DIS 7220
      IF (IPIT.EQ.1 .AND. GAMMA(1).GT.10.0) GAMMA(1) = 10.0                    DIS 7230
      IF (IPIT.EQ.1 .AND. GAMMA(1).LT.PG(1)) GAMMA(1) = PG(1)                  DIS 7240
    END IF                                                                     DIS 7250
                                                                               DIS 7260
C ---------------------------------------------------------------------------|DIS 7270
C     Magnesium species                                                        |DIS 7280
C --------------------                                                        |DIS 7290
  140 CONTINUE                                                                 DIS 7300
      IF (EXELT(2) .GT. CPUMIN) THEN                                           DIS 7310
        M(120) = ALFA( 98) / (KT1( 93) * GAMMA(120))                           DIS 7320
        M(121) = ALFA(  7) / (KT1( 94) * GAMMA(121))                           DIS 7330
        M(122) = ALFA( 30) / (KT1( 95) * GAMMA(122))                           DIS 7340
        M(123) = ALFA(  9) / (KT1( 96) * GAMMA(123))                           DIS 7350
        M(124) = ALFA(  6) / (KT1( 97) * GAMMA(124))                           DIS 7360
        M(125) = ALFA( 29) / (KT1( 98) * GAMMA(125))                           DIS 7370
        M(126) = ALFA( 99) / (KT1( 99) * GAMMA(126))                           DIS 7380
        M(127) = ALFA(100) / (KT1(100) * GAMMA(127))                           DIS 7390
        M(236) = ALFA( 48) / (KT1(216) * GAMMA(236))                           DIS 7400
        M(256) = ALFA(246) / (KT1(232) * GAMMA(256))                           DIS 7410
        M(275) = ALFA(265) / (KT1(250) * GAMMA(275))                           DIS 7420
        M(MXSP+10) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 9) *                          DIS 7430
     .                GAMMA(MXSP+10))                                          DIS 7440
        M(MXSP+25) = ALFA(MXSP+16) / (KT1(MXAQK+23) *                          DIS 7450
     .                GAMMA(MXSP+25))                                          DIS 7460
                                                                               DIS 7470
        M(2)     = EXELT(2) / (1.0D0 + GAMMA(2) * (M(120) + M(121) +           DIS 7480
     .             M(122) + M(123) + M(124) + M(125) + M(126) + M(127) +       DIS 7490
     .             M(236) + M(256) + M(275) + M(MXSP+10) + M(MXSP+25)))        DIS 7500
        ALFA(2)  = M(2) * GAMMA(2)                                             DIS 7510
        LALFA(2) = SLOG10(ALFA(2))                                             DIS 7520
                                                                               DIS 7530
        DO 150 I = 120, 127                                                    DIS 7540
          M(I)     = M(I) * ALFA(2)                                            DIS 7550
          ALFA(I)  = M(I) * GAMMA(I)                                           DIS 7560
          LALFA(I) = SLOG10(ALFA(I))                                           DIS 7570
  150   CONTINUE                                                               DIS 7580
                                                                               DIS 7590
        M(236)          = M(236) * ALFA(2)                                     DIS 7600
        ALFA(236)       = M(236) * GAMMA(236)                                  DIS 7610
        LALFA(236)      = SLOG10(ALFA(236))                                    DIS 7620
                                                                               DIS 7630
        M(256)          = M(256) * ALFA(2)                                     DIS 7640
        ALFA(256)       = M(256) * GAMMA(256)                                  DIS 7650
        LALFA(256)      = SLOG10(ALFA(256))                                    DIS 7660
                                                                               DIS 7670
        M(275)          = M(275) * ALFA(2)                                     DIS 7680
        ALFA(275)       = M(275) * GAMMA(275)                                  DIS 7690
        LALFA(275)      = SLOG10(ALFA(275))                                    DIS 7700
                                                                               DIS 7710
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                                                                      DIS 7720
        M(MXSP+10)      = M(MXSP+10) * ALFA(2)                        DIS 7730
        ALFA(MXSP+10)   = M(MXSP+10) * GAMMA(MXSP+10)                 DIS 7740
        LALFA(MXSP+10) = SLOG10(ALFA(MXSP+10))                        DIS 7750
                                                                      DIS 7760
        M(MXSP+25)      = M(MXSP+25) * ALFA(2)                        DIS 7770
        ALFA(MXSP+25)   = M(MXSP+25) * GAMMA(MXSP+25)                 DIS 7780
        LALFA(MXSP+25) = SLOG10(ALFA(MXSP+25))                        DIS 7790
                                                                      DIS 7800
        IF (IPIT.EQ.1 .AND. PG(2).GT.CPUMIN                           DIS 7810
     .                .AND. GAMMA(2).LE.50.0) THEN                   DIS 7820
          IF (DABS(PALFA(2)-ALFA(2)) .GT. 1.0D-2*PALFA(2)) THEN       DIS 7830
            IF (PALFA(2) .GT. ALFA(2)) THEN                           DIS 7840
              INC=0.1                                                 DIS 7850
            ELSE                                                      DIS 7860
              INC=-0.01                                               DIS 7870
            END IF                                                    DIS 7880
            GAMMA(2)=GAMMA(2)*(1.0+INC)                               DIS 7890
            GO TO 140                                                 DIS 7900
          END IF                                                      DIS 7910
        END IF                                                        DIS 7920
                                                                      DIS 7930
        IF (IPIT.EQ.1 .AND. GAMMA(2) .GT. 10.0)  GAMMA(2) = 10.0      DIS 7940
        IF (IPIT.EQ.1 .AND. GAMMA(2) .LT. PG(2)) GAMMA(2) = PG(2)     DIS 7950
      END IF                                                          DIS 7960
                                                                      DIS 7970
C -------------------------------------------------------------------|DIS 7980
C     Sodium species                                                  |DIS 7990
C -----------------                                                   |DIS 8000
                                                                      DIS 8010
  160 CONTINUE                                                        DIS 8020
      IF (EXELT(3) .GT. CPUMIN) THEN                                  DIS 8030
        M(137) = ALFA(  5) / (KT1(110) * GAMMA(137))                  DIS 8040
        M(138) = ALFA( 98) / (KT1(111) * GAMMA(138))                  DIS 8050
        M(139) = ALFA(  7) / (KT1(112) * GAMMA(139))                  DIS 8060
        M(140) = (M(3) * GAMMA(3) * ALFA(98)) / (KT1(113) * GAMMA(140)) DIS 8070
        M(141) = (M(3) * GAMMA(3) * ALFA(6))  / (KT1(114) * GAMMA(141)) DIS 8080
        M(142) = ALFA(  6) / (KT1(115) * GAMMA(142))                  DIS 8090
        M(143) = ALFA( 99) / (KT1(116) * GAMMA(143))                  DIS 8100
        M(144) = ALFA( 30) / (KT1(120) * GAMMA(144))                  DIS 8110
        M(145) = ALFA(101) / (KT1(119) * GAMMA(145))                  DIS 8120
        M(237) = ALFA( 48) / (KT1(217) * GAMMA(237))                  DIS 8130
        M(261) = ALFA(246) / (KT1(237) * GAMMA(261))                  DIS 8140
        M(277) = ALFA(265) / (KT1(252) * GAMMA(277))                  DIS 8150
        M(MXSP+12) = ALFA(MXSP+ 1) / (KT1(MXAQK+11) * GAMMA(MXSP+12))  DIS 8160
        M(MXSP+27) = ALFA(MXSP+16) / (KT1(MXAQK+25) * GAMMA(MXSP+27))  DIS 8170
                                                                      DIS 8180
        M(3)    = EXELT(3) / (1.0D0 + GAMMA(3) * (M(137) + M(138) +   DIS 8190
     .            M(139) + M(140) + M(141) + M(142) + M(143) + M(144) + DIS 8200
     .            M(145) + M(237) + M(261) + M(277) + M(MXSP+12)      + DIS 8210
     .            M(MXSP+27)))                                       DIS 8220
        ALFA(3)  = M(3) * GAMMA(3)                                    DIS 8230
        LALFA(3) = SLOG10(ALFA(3))                                    DIS 8240
                                                                      DIS 8250
        DO 170 I = 137, 145                                           DIS 8260
          M(I)     = M(I) * ALFA(3)                                   DIS 8270
          ALFA(I)  = M(I) * GAMMA(I)                                  DIS 8280
          LALFA(I) = SLOG10(ALFA(I))                                  DIS 8290
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  170   CONTINUE                                                          DIS 8300
                                                                          DIS 8310
        M(237)          = M(237) * ALFA(3)                              DIS 8320
        ALFA(237)       = M(237) * GAMMA(237)                           DIS 8330
        LALFA(237)      = SLOG10(ALFA(237))                             DIS 8340
                                                                          DIS 8350
        M(261)          = M(261) * ALFA(3)                              DIS 8360
        ALFA(261)       = M(261) * GAMMA(261)                           DIS 8370
        LALFA(261)      = SLOG10(ALFA(261))                             DIS 8380
                                                                          DIS 8390
        M(277)          = M(277) * ALFA(3)                              DIS 8400
        ALFA(277)       = M(277) * GAMMA(277)                           DIS 8410
        LALFA(277)      = SLOG10(ALFA(277))                             DIS 8420
                                                                          DIS 8430
        M(MXSP+12)      = M(MXSP+12) * ALFA(3)                          DIS 8440
        ALFA(MXSP+12)   = M(MXSP+12) * GAMMA(MXSP+12)                   DIS 8450
        LALFA(MXSP+12)  = SLOG10(ALFA(MXSP+12))                         DIS 8460
                                                                          DIS 8470
        M(MXSP+27)      = M(MXSP+27) * ALFA(3)                          DIS 8480
        ALFA(MXSP+27)   = M(MXSP+27) * GAMMA(MXSP+27)                   DIS 8490
        LALFA(MXSP+27)  = SLOG10(ALFA(MXSP+27))                         DIS 8500
                                                                          DIS 8510
        IF (IPIT.EQ.1 .AND. PG(3).GT.CPUMIN                             DIS 8520
     .                .AND. GAMMA(3).LE.10.0) THEN                       DIS 8530
          IF (DABS(PALFA(3)-ALFA(3)) .GT. 1.0D-2*PALFA(3)) THEN         DIS 8540
            IF (PALFA(3) .GT. ALFA(3)) THEN                             DIS 8550
              INC = 0.1                                                 DIS 8560
            ELSE                                                        DIS 8570
              INC = -0.01                                               DIS 8580
            END IF                                                      DIS 8590
           GAMMA(3)=GAMMA(3)*(1+INC)                                    DIS 8600
           GO TO 160                                                    DIS 8610
          END IF                                                        DIS 8620
        END IF                                                          DIS 8630
                                                                          DIS 8640
        IF (IPIT .EQ. 1 .AND. GAMMA(3) .GT. 10.0)  GAMMA(3) = 10.0      DIS 8650
        IF (IPIT .EQ. 1 .AND. GAMMA(3) .LT. PG(3)) GAMMA(3) = PG(3)     DIS 8660
      END IF                                                            DIS 8670
                                                                          DIS 8680
C -----------------------------------------------------------------------|DIS 8690
C     Potassium species                                                  |DIS 8700
C ---------------------                                                  |DIS 8710
                                                                          DIS 8720
  180 CONTINUE                                                          DIS 8730
      IF (EXELT(4) .GT. CPUMIN) THEN                                    DIS 8740
        M(113) = ALFA(  5) / (KT1( 86) * GAMMA(113))                    DIS 8750
        M(114) = ALFA( 98) / (KT1( 87) * GAMMA(114))                    DIS 8760
        M(115) = ALFA(103) / (KT1( 88) * GAMMA(115))                    DIS 8770
        M(116) = ALFA(  6) / (KT1( 89) * GAMMA(116))                    DIS 8780
        M(117) = ALFA( 99) / (KT1( 90) * GAMMA(117))                    DIS 8790
        M(235) = ALFA( 48) / (KT1(215) * GAMMA(235))                    DIS 8800
        M(255) = ALFA(246) / (KT1(231) * GAMMA(255))                    DIS 8810
        M(274) = ALFA(265) / (KT1(249) * GAMMA(274))                    DIS 8820
                                                                          DIS 8830
        M(MXSP+ 9) = ALFA(MXSP+ 1) / (KT1(MXAQK+8)  * GAMMA(MXSP+ 9))   DIS 8840
        M(MXSP+24) = ALFA(MXSP+16) / (KT1(MXAQK+22) * GAMMA(MXSP+24))   DIS 8850
                                                                          DIS 8860
        M(4)    = EXELT(4) / (1.0D0 + GAMMA(4) * (M(113) + M(114) +     DIS 8870
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     .           M(115) + M(116) + M(117) + M(235) + M(255) +          DIS 8880
     .           M(274) + M(MXSP+9) + M(MXSP+24)))                     DIS 8890
         ALFA(4) = M(4) * GAMMA(4)                                     DIS 8900
                                                                       DIS 8910
         DO 190 I = 113, 117                                           DIS 8920
           M(I)    = M(I) * ALFA(4)                                    DIS 8930
           ALFA(I) = M(I) * GAMMA(I)                                   DIS 8940
  190    CONTINUE                                                      DIS 8950
                                                                       DIS 8960
         M(235)         = M(235)     * ALFA(4)                       DIS 8970
         ALFA(235)      = M(235)     * GAMMA(235)                    DIS 8980
                                                                       DIS 8990
         M(255)         = M(255)     * ALFA(4)                       DIS 9000
         ALFA(255)      = M(255)     * GAMMA(255)                    DIS 9010
                                                                       DIS 9020
         M(274)         = M(274)     * ALFA(4)                       DIS 9030
         ALFA(274)      = M(274)     * GAMMA(274)                    DIS 9040
                                                                       DIS 9050
         M(MXSP+ 9)     = M(MXSP+ 9) * ALFA(4)                       DIS 9060
         ALFA(MXSP+ 9) = M(MXSP+ 9) * GAMMA(MXSP+ 9)                  DIS 9070
                                                                       DIS 9080
         M(MXSP+24)     = M(MXSP+24) * ALFA(4)                       DIS 9090
         ALFA(MXSP+24) = M(MXSP+24) * GAMMA(MXSP+24)                  DIS 9100
                                                                       DIS 9110
         IF (IPIT.EQ.1 .AND. PG(4).GT.CPUMIN                           DIS 9120
                       .AND. GAMMA(4).LE.10.0) THEN                    DIS 9130
           IF (DABS(PALFA(4)-ALFA(4)) .GT. 1.0D-2*PALFA(4)) THEN       DIS 9140
             IF (PALFA(4) .GT. ALFA(4)) THEN                           DIS 9150
               INC =0.1                                                DIS 9160
             ELSE                                                      DIS 9170
               INC =-0.01                                              DIS 9180
             END IF                                                    DIS 9190
             GAMMA(4)=GAMMA(4)*(1.0+INC)                               DIS 9200
             GO TO 180                                                 DIS 9210
           END IF                                                      DIS 9220
         END IF                                                        DIS 9230
                                                                       DIS 9240
         IF (IPIT .EQ. 1 .AND. GAMMA(4) .GT. 10.0)  GAMMA(4) = 10.0    DIS 9250
         IF (IPIT .GT. 1 .AND. GAMMA(4) .LT. PG(4)) GAMMA(4) = PG(4)   DIS 9260
       END IF                                                          DIS 9270
                                                                       DIS 9280
C ---------------------------------------------------------------------|DIS 9290
C     Silver species                                                   |DIS 9300
C -----------------                                                    |DIS 9310
                                                                       DIS 9320
       IF (EXELT(9) .GT. CPUMIN) THEN                                  DIS 9330
         M(43) = 0.0D00                                                DIS 9340
         M(44) = 0.0D00                                                DIS 9350
         M(45) = 0.0D00                                                DIS 9360
         M(46) = 0.0D00                                                DIS 9370
         M(47) = 0.0D00                                                DIS 9380
         IF (DABS(KT1(20)) .GT. 1.0D-30)                               DIS 9390
     .     M(43) = ALFA(5)    / (KT1(20) * GAMMA(43))                  DIS 9400
         IF (DABS(KT1(21)) .GT. 1.0D-30)                               DIS 9410
     .     M(44) = ALFA(5)**2 / (KT1(21) * GAMMA(44))                  DIS 9420
         IF (DABS(KT1(22)) .GT. 1.0D-30)                               DIS 9430
     .     M(45) = ALFA(5)**3 / (KT1(22) * GAMMA(45))                  DIS 9440
         IF (DABS(KT1(23)) .GT. 1.0D-30)                               DIS 9450
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     .      M(46) = ALFA(5)**4 / (KT1(23) * GAMMA(46))                    DIS 9460
            IF (DABS(KT1(24)) .GT. 1.0D-30)                               DIS 9470
     .      M(47) = ALFA(6)    / (KT1(24) * GAMMA(47))                    DIS 9480
                                                                          DIS 9490
            M(13)    = EXELT(9) / (1.0D0 + GAMMA(13) * (M(42) + M(44) +   DIS 9500
     .                 M(45) + M(46) + M(47)))                           DIS 9510
            ALFA(13) = M(13) * GAMMA(13)                                  DIS 9520
                                                                          DIS 9530
            DO 200 I = 43, 47                                             DIS 9540
              M(I)    = M(I) * ALFA(13)                                   DIS 9550
              ALFA(I) = M(I) * GAMMA(I)                                   DIS 9560
      200   CONTINUE                                                      DIS 9570
          END IF                                                          DIS 9580
                                                                          DIS 9590
C ---------------------------------------------------------------------  |DIS 9600
C     Aluminum species                                                    |DIS 9610
C ---------------------                                                   |DIS 9620
                                                                          DIS 9630
          IF (EXELT(10) .GT. CPUMIN) THEN                                 DIS 9640
            M( 34) = ALFA( 30)    / (KT1( 11) * GAMMA( 34))               DIS 9650
            M( 35) = ALFA( 30)**2 / (KT1( 12) * GAMMA( 35))               DIS 9660
            M( 36) = ALFA( 30)**3 / (KT1( 13) * GAMMA( 36))               DIS 9670
            M( 37) = 0.0                                                  DIS 9680
            IF (DABS(KT1(15)) .GT. 1.0D-30)                               DIS 9690
     .        M( 37) = ALFA( 30)**4 / (KT1( 14) * GAMMA( 37))             DIS 9700
                                                                          DIS 9710
            M( 38) =      LALFA(9)  - LOGKT1(15) - DLOG10(GAMMA(38))      DIS 9720
            M( 38) = SEXP10( M(38))                                       DIS 9730
            M( 39) = (2.0*LALFA(9)) - LOGKT1(16) - DLOG10(GAMMA(39))      DIS 9740
            M( 39) = SEXP10( M(39))                                       DIS 9750
            M( 40) = (4.0*LALFA(9)) - LOGKT1(17) - DLOG10(GAMMA(40))      DIS 9760
            M( 40) = SEXP10( M(40))                                       DIS 9770
                                                                          DIS 9780
            M( 41) = ALFA(  6)    / (KT1( 18) * GAMMA( 41))               DIS 9790
            M( 42) = ALFA(  6)**2 / (KT1( 19) * GAMMA( 42))               DIS 9800
            M(163) = 0.0D00                                               DIS 9810
            IF (DABS(KT1(9)) .GT. 1.0D-30) M(163) = ALFA( 30)**5          DIS 9820
     .                                    / (KT1(  9) * GAMMA(163))      DIS 9830
            M(164) = 0.0D00                                               DIS 9840
            IF (DABS(KT1(65)) .GT. 1.0D-30) M(164) = ALFA( 30)**6         DIS 9850
     .                                    / (KT1( 65) * GAMMA(164))      DIS 9860
            M(229) = ALFA( 48)    / (KT1(209) * GAMMA(229))               DIS 9870
            M(249) = ALFA(246)    / (KT1(225) * GAMMA(249))               DIS 9880
            M(250) = ALFA(246)**2 / (KT1(226) * GAMMA(250))               DIS 9890
            M(268) = ALFA(265)    / (KT1(243) * GAMMA(268))               DIS 9900
            M(269) = ALFA(265)**2 / (KT1(244) * GAMMA(269))               DIS 9910
            M(MXSP+ 4) = ALFA(MXSP+ 1) / (KT1(MXAQK+3)  * GAMMA(MXSP+ 4)) DIS 9920
            M(MXSP+19) = ALFA(MXSP+16) / (KT1(MXAQK+17) * GAMMA(MXSP+19)) DIS 9930
                                                                          DIS 9940
            M(14)    = EXELT(10) / (1.0D0 + GAMMA(14) * (M(34) + M(35) +  DIS 9950
     .                 M( 36) + M( 37) + M( 38) + M( 39) + M( 40) + M(41) + DIS 9960
     .                 M( 42) + M(163) + M(164) + M(229) + M(249) +       DIS 9970
     .                 M(250) + M(268) + M(269) + M(MXSP+4) + M(MXSP+19))) DIS 9980
            ALFA(14) = M(14) * GAMMA(14)                                  DIS 9990
                                                                          DIS10000
            IF (M(163) .GT. 3.0) M(163) = 3.0                             DIS10010
                                                                          DIS10020
            DO 210 I = 34, 42                                             DIS10030
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        M(I)     = M(I) * ALFA(14)                                          DIS10040
        ALFA(I) = M(I) * GAMMA(I)                                           DIS10050
  210   CONTINUE                                                            DIS10060
                                                                            DIS10070
        DO 220 I = 163, 164                                                 DIS10080
          M(I)     = M(I) * ALFA(14)                                        DIS10090
          ALFA(I) = M(I) * GAMMA(I)                                         DIS10100
  220   CONTINUE                                                            DIS10110
                                                                            DIS10120
        M(229)          = M(229)      * ALFA(14)                            DIS10130
        ALFA(229)       = M(229)      * GAMMA(229)                          DIS10140
                                                                            DIS10150
        M(249)          = M(249)      * ALFA(14)                            DIS10160
        ALFA(249)       = M(249)      * GAMMA(249)                          DIS10170
                                                                            DIS10180
        M(250)          = M(250)      * ALFA(14)                            DIS10190
        ALFA(250)       = M(250)      * GAMMA(250)                          DIS10200
                                                                            DIS10210
        M(268)          = M(268)      * ALFA(14)                            DIS10220
        ALFA(268)       = M(268)      * GAMMA(268)                          DIS10230
                                                                            DIS10240
        M(269)          = M(269)      * ALFA(14)                            DIS10250
        ALFA(269)       = M(269)      * GAMMA(269)                          DIS10260
                                                                            DIS10270
        M(MXSP+ 4)      = M(MXSP+ 4) * ALFA(14)                             DIS10280
        ALFA(MXSP+4)    = M(MXSP+ 4) * GAMMA(MXSP+ 4)                       DIS10290
                                                                            DIS10300
        M(MXSP+19)      = M(MXSP+19) * ALFA(14)                             DIS10310
        ALFA(MXSP+19) = M(MXSP+19) * GAMMA(MXSP+19)                         DIS10320
      END IF                                                                DIS10330
                                                                            DIS10340
C -------------------------------------------------------------------------|DIS10350
C     Iron species                                                          |DIS10360
C ---------------                                                           |DIS10370
                                                                            DIS10380
      IF (EXELT(13) .GT. CPUMIN) THEN                                       DIS10390
        M( 71) = ALFA(  5)     / (KT1( 46) * GAMMA( 71))                    DIS10400
        M( 72) = ALFA(  5)**2 / (KT1( 47) * GAMMA( 72))                     DIS10410
        M( 73) = ALFA( 99)     / (KT1( 48) * GAMMA( 73))                    DIS10420
        M( 75) = ALFA(  9)     / (KT1( 50) * GAMMA( 75))                    DIS10430
        M( 76) = ALFA(  9)**2 / (KT1( 51) * GAMMA( 76))                     DIS10440
        M( 77) = ALFA( 10)**2  / (KT1( 52) * GAMMA( 77) * ALFA(8)**3)       DIS10450
        M( 78) = ALFA(  6)     / (KT1( 53) * GAMMA( 78))                    DIS10460
        M(233) = ALFA( 48)     / (KT1(213) * GAMMA(233))                    DIS10470
        M(234) = ALFA( 48)**2 / (KT1(214) * GAMMA(234))                     DIS10480
        M(253) = ALFA(246)     / (KT1(229) * GAMMA(253))                    DIS10490
        M(272) = ALFA(265)     / (KT1(247) * GAMMA(272))                    DIS10500
        M(MXSP+ 8) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 7) * GAMMA(MXSP+ 8))      DIS10510
        M(MXSP+23) = ALFA(MXSP+16) / (KT1(MXAQK+21) * GAMMA(MXSP+23))      DIS10520
                                                                            DIS10530
C -------------------------------------------------------------------------|DIS10540
C     If fe+3 is to be calculated from eh measurements then put             |DIS10550
C     flags(1) = 1.  If from the reaction:                                  |DIS10560
C         fe+3 + 1/2h2o + 1/8hs- = fe++ + 1/8so4 + 9/8h+                    |DIS10570
C     then flags(1) = 0.                                                    |DIS10580
C -------------------------------------------------------------------------|DIS10590
                                                                            DIS10600
        IF (EHM .LT. 9.0D0 .AND. FLAGS(1) .EQ. 1) THEN                      DIS10610
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        C1    = 10.0**((EHM * F - LOGKT1(138)) / (2.303 * R * T))      DIS10620
        M(19) = C1 / GAMMA(19)                                         DIS10630
      ELSE IF (EXELT(25) .LT. CPUMIN) THEN                             DIS10640
        M(19) = 0.0                                                    DIS10650
      ELSE IF (FLAGS(1) .EQ. 0) THEN                                   DIS10660
        M(19) = (ALFA(6)**0.125  * ALFA(8)**1.125) / (KT1(5) *         DIS10670
     .           DSQRT(ALFA(10)) * ALFA(101)**0.125 * GAMMA(19))       DIS10680
      END IF                                                           DIS10690
                                                                       DIS10700
      M( 79) = ALFA(  5)    / (KT1( 54) * GAMMA( 79))                  DIS10710
      M( 80) = ALFA(  5)**2 / (KT1( 55) * GAMMA( 80))                  DIS10720
      M( 81) = 0.0D00                                                  DIS10730
      IF (DABS(KT1(56)) .GT. 1.0D-30)                                  DIS10740
     .    M( 81) = ALFA(  5)**3 / (KT1( 56) * GAMMA( 81))              DIS10750
      M( 82) = 0.0D00                                                  DIS10760
      IF (DABS(KT1(57)) .GT. 1.0D-30)                                  DIS10770
     .    M( 82) = ALFA(  5)**4 / (KT1( 57) * GAMMA( 82))              DIS10780
      M( 83) = ALFA(  6)    / (KT1( 58) * GAMMA( 83))                  DIS10790
      M( 84) = ALFA(  6)**2 / (KT1( 59) * GAMMA( 84))                  DIS10800
      M( 85) = ALFA(  9)    / (KT1( 60) * GAMMA( 85))                  DIS10810
      M( 86) = ALFA(  9)**2 / (KT1( 61) * GAMMA( 86))                  DIS10820
      M( 87) = 0.0D00                                                  DIS10830
      IF (DABS(KT1(62)) .GT. 1.0D-30)                                  DIS10840
     .    M( 87) = ALFA(  9)**3 / (KT1( 62) * GAMMA( 87))              DIS10850
      M( 88) = 0.0D00                                                  DIS10860
      IF (DABS(KT1(53)) .GT. 1.0D-30)                                  DIS10870
     .    M( 88) = ALFA(  9)**4 / (KT1( 63) * GAMMA( 88))              DIS10880
      M(254) = ALFA(246)    / (KT1(230) * GAMMA(253))                  DIS10890
      M(273) = ALFA(265)    / (KT1(248) * GAMMA(273))                  DIS10900
      M(283) = ALFA( 30)    / (KT1(256) * GAMMA(283))                  DIS10910
                                                                       DIS10920
      DO 230 I = 79, 88                                                DIS10930
        M(I) = M(I) * M(19) * GAMMA(19)                                DIS10940
230   CONTINUE                                                         DIS10950
                                                                       DIS10960
      M(254) = M(254) * M(19) * GAMMA(19)                              DIS10970
      M(273) = M(273) * M(19) * GAMMA(19)                              DIS10980
      M(283) = M(283) * M(19) * GAMMA(19)                              DIS10990
                                                                       DIS11000
      M(18)   = EXELT(13) / (1.0D0 + GAMMA(18) * (M(19) + M(71) +      DIS11010
     .           M( 72) + M( 73) + M( 75) + M( 76) + M( 77) + M( 78) + DIS11020
     .           M( 79) + M( 80) + M( 81) + M( 82) + M( 83) + M( 84) + DIS11030
     .           M( 85) + M( 86) + M( 87) + M( 88) + M(233) + M(234) + DIS11040
     .           M(253) + M(254) + M(272) + M(273) + M(283) +          DIS11050
     .           M(MXSP+8) + M(MXSP+23)))                              DIS11060
      ALFA(18) = M(18) * GAMMA(18)                                     DIS11070
                                                                       DIS11080
      M(19)    = M(19) * ALFA(18)                                      DIS11090
      ALFA(19) = M(19) * GAMMA(19)                                     DIS11100
                                                                       DIS11110
      DO 240 I = 71, 88                                                DIS11120
        IF (I .EQ. 74) GO TO 240                                       DIS11130
        M(I)    = M(I) * ALFA(18)                                      DIS11140
        ALFA(I) = M(I) * GAMMA(I)                                      DIS11150
240   CONTINUE                                                         DIS11160
                                                                       DIS11170
      M(233)        = M(233)     * ALFA(18)                            DIS11180
      ALFA(233)     = M(233)     * GAMMA(233)                          DIS11190
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                                                                      DIS11200
        M(234)         = M(234)      * ALFA(18)                       DIS11210
        ALFA(234)      = M(234)      * GAMMA(234)                     DIS11220
                                                                      DIS11230
        M(253)         = M(253)      * ALFA(18)                       DIS11240
        ALFA(253)      = M(253)      * GAMMA(253)                     DIS11250
                                                                      DIS11260
        M(254)         = M(254)      * ALFA(18)                       DIS11270
        ALFA(254)      = M(254)      * GAMMA(254)                     DIS11280
                                                                      DIS11290
        M(272)         = M(272)      * ALFA(18)                       DIS11300
        ALFA(272)      = M(272)      * GAMMA(272)                     DIS11310
                                                                      DIS11320
        M(273)         = M(273)      * ALFA(18)                       DIS11330
        ALFA(273)      = M(273)      * GAMMA(273)                     DIS11340
                                                                      DIS11350
        M(283)         = M(283)      * ALFA(18)                       DIS11360
        ALFA(283)      = M(283)      * GAMMA(283)                     DIS11370
                                                                      DIS11380
        M(MXSP+ 8)     = M(MXSP+ 8) * ALFA(18)                        DIS11390
        ALFA(MXSP+ 8) = M(MXSP+ 8) * GAMMA(MXSP+ 8)                   DIS11400
                                                                      DIS11410
        M(MXSP+23)     = M(MXSP+23) * ALFA(18)                        DIS11420
        ALFA(MXSP+23) = M(MXSP+23) * GAMMA(MXSP+23)                   DIS11430
      END IF                                                          DIS11440
                                                                      DIS11450
C -----------------------------------------------------------------------DIS11460
C     Barium species                                                  |DIS11470
C -----------------                                                   |DIS11480
                                                                      DIS11490
      IF (EXELT(11) .GT. CPUMIN) THEN                                 DIS11500
        M( 51) = ALFA( 98) / (KT1( 26) * GAMMA( 51))                  DIS11510
        M( 52) = ALFA(  7) / (KT1( 27) * GAMMA( 52))                  DIS11520
        M( 53) = ALFA(  9) / (KT1( 28) * GAMMA( 53))                  DIS11530
        M( 54) = ALFA(  6) / (KT1( 29) * GAMMA( 54))                  DIS11540
        M(230) = ALFA( 48) / (KT1(210) * GAMMA(230))                  DIS11550
        M(251) = ALFA(246) / (KT1(227) * GAMMA(251))                  DIS11560
        M(270) = ALFA(265) / (KT1(245) * GAMMA(270))                  DIS11570
        M(MXSP+ 5) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 4) * GAMMA(MXSP+ 5)) DIS11580
        M(MXSP+20) = ALFA(MXSP+16) / (KT1(MXAQK+18) * GAMMA(MXSP+20)) DIS11590
                                                                      DIS11600
        M(15)    = EXELT(11) / (1.0D0 + GAMMA(15) * (M(51) + M(52) +  DIS11610
     .             M(53) + M(54) + M(230) + M(251) + M(270) +         DIS11620
     .             M(MXSP+5) + M(MXSP+20)))                           DIS11630
        ALFA(15) = M(15) * GAMMA(15)                                  DIS11640
                                                                      DIS11650
        DO 250 I =  51, 54                                            DIS11660
          M(I)    = M(I) * ALFA(15)                                   DIS11670
          ALFA(I) = M(I) * GAMMA(I)                                   DIS11680
  250   CONTINUE                                                      DIS11690
                                                                      DIS11700
        M(230)         = M(230)      * ALFA(15)                       DIS11710
        ALFA(230)      = M(230)      * GAMMA(230)                     DIS11720
                                                                      DIS11730
        M(251)         = M(251)      * ALFA(15)                       DIS11740
        ALFA(251)      = M(251)      * GAMMA(251)                     DIS11750
                                                                      DIS11760
        M(270)         = M(270)      * ALFA(15)                       DIS11770
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        ALFA(270)      = M(270)      * GAMMA(270)                          DIS11780
                                                                           DIS11790
        M(MXSP+5)      = M(MXSP+5)   * ALFA(15)                            DIS11800
        ALFA(MXSP+5)   = M(MXSP+5)   * GAMMA(MXSP+5)                       DIS11810
                                                                           DIS11820
        M(MXSP+20)     = M(MXSP+20)  * ALFA(15)                            DIS11830
        ALFA(MXSP+20)  = M(MXSP+20)  * GAMMA(MXSP+20)                      DIS11840
      END IF                                                               DIS11850
                                                                           DIS11860
C -----------------------------------------------------------------------|DIS11870
C     Copper species                                                       |DIS11880
C -----------------                                                       |DIS11890
                                                                           DIS11900
      IF (EXELT(12) .GE. CPUMIN) THEN                                      DIS11910
        M(62)  = ALFA( 5)    / (KT1( 37) * GAMMA( 62))                     DIS11920
        M(63)  = ALFA( 5)**2 / (KT1( 38) * GAMMA( 63))                     DIS11930
        M(64)  = ALFA( 5)**3 / (KT1( 39) * GAMMA( 64))                     DIS11940
        M(232) = ALFA(48)    / (KT1(212) * GAMMA(232))                     DIS11950
        M(MXSP+ 7) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 6) * GAMMA(MXSP+ 7))      DIS11960
        M(MXSP+22) = ALFA(MXSP+16) / (KT1(MXAQK+20) * GAMMA(MXSP+22))      DIS11970
                                                                           DIS11980
C -----------------------------------------------------------------------|DIS11990
C     If cu++ is to be calculated from eh measurements then                |DIS12000
C     flags(2) = 1.  If from cu++ + fe++ = cu+ + fe+3, then                |DIS12010
C     flags(2) = 0.                                                        |DIS12020
C -----------------------------------------------------------------------|DIS12030
                                                                           DIS12040
        IF (EHM .LT. 9.0 .AND. FLAGS(2) .EQ. 1) THEN                       DIS12050
          C1    = 1.0D1**((EHM * F - LOGKT1(139)) / (2.303 * R * T))       DIS12060
          M(17) = C1 / GAMMA(19)                                           DIS12070
        ELSE IF (EXELT(25) .LT. CPUMIN) THEN                               DIS12080
          M(17) = 0.0D0                                                    DIS12090
        ELSE IF (FLAGS(2) .EQ. 0) THEN                                     DIS12100
          M(17) = ALFA(19) / (KT1(4) * ALFA(18) * GAMMA(17))               DIS12110
        END IF                                                             DIS12120
                                                                           DIS12130
        M(65) = ALFA(5)    / (KT1(40) * GAMMA(65))                         DIS12140
        M(66) = ALFA(5)**2 / (KT1(41) * GAMMA(66))                         DIS12150
        M(67) = 0.0D00                                                     DIS12160
        IF (DABS(KT1(42)) .GT. 1.0D-30)                                    DIS12170
     .     M(67) = ALFA(5)**3 / (KT1(42) * GAMMA(67))                      DIS12180
        M(68) = 0.0D00                                                     DIS12190
        IF (DABS(KT1(43)) .GT. 1.0D-30)                                    DIS12200
     .     M(68) = ALFA(5)**4 / (KT1(43) * GAMMA(68))                      DIS12210
        M(69) = ALFA(9)    / (KT1(44) * GAMMA(69))                         DIS12220
        M(70) = ALFA(6)    / (KT1(45) * GAMMA(70))                         DIS12230
                                                                           DIS12240
        DO 260 I = 65, 70                                                  DIS12250
          M(I) = M(I) * M(17) * GAMMA(17)                                  DIS12260
  260   CONTINUE                                                           DIS12270
                                                                           DIS12280
        M(16)    = EXELT(12) / (1.0D0 + GAMMA(16) * (M(17) + M(62) +       DIS12290
     .             M(63) + M(64) + M(65) + M(66) + M(67) + M(68) +         DIS12300
     .             M(69) + M(70) + M(232) + M(MXSP+7) + M(MXSP+22)))       DIS12310
        ALFA(16) = M(16) * GAMMA(16)                                       DIS12320
                                                                           DIS12330
        M(17)    = M(17)  * ALFA(16)                                       DIS12340
        ALFA(17) = M(17)  * GAMMA(17)                                      DIS12350
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                                                                      DIS12360
      DO 270 I = 62, 70                                               DIS12370
        M(I)    = M(I) * ALFA(16)                                     DIS12380
        ALFA(I) = M(I) * GAMMA(I)                                     DIS12390
  270 CONTINUE                                                        DIS12400
                                                                      DIS12410
      M(232)        = M(232)     * ALFA(16)                         DIS12420
      ALFA(232)     = M(232)     * GAMMA(232)                       DIS12430
                                                                      DIS12440
      M(MXSP+ 7)    = M(MXSP+ 7) * ALFA(16)                         DIS12450
      ALFA(MXSP+ 7) = M(MXSP+ 7) * GAMMA(MXSP+7)                    DIS12460
                                                                      DIS12470
      M(MXSP+22)    = M(MXSP+22) * ALFA(16)                         DIS12480
      ALFA(MXSP+22) = M(MXSP+22) * GAMMA(MXSP+22)                   DIS12490
    END IF                                                            DIS12500
                                                                      DIS12510
C -------------------------------------------------------------------|DIS12520
C     Mercury species                                                 |DIS12530
C -----------------                                                   |DIS12540
                                                                      DIS12550
      IF (EXELT(14) .GT. CPUMIN) THEN                                 DIS12560
        M(105) = ALFA(5)      / (KT1(78)  * GAMMA(105))               DIS12570
        M(106) = ALFA(5)**2   / (KT1(79)  * GAMMA(106))               DIS12580
        M(107) = ALFA(5)**3   / (KT1(80)  * GAMMA(107))               DIS12590
        M(108) = ALFA(5)**4   / (KT1(81)  * GAMMA(108))               DIS12600
        M(109) = ALFA(6)      / (KT1(82)  * GAMMA(109))               DIS12610
                                                                      DIS12620
C -------------------------------------------------------------------|DIS12630
C     The k values for hgsh2s)2 are so small a divide by zero error   |DIS12640
C     will occur is the reason for the following statement.           |DIS12650
C -------------------------------------------------------------------|DIS12660
        M(110) = 0.0                                                  DIS12670
        IF (DABS(KT1(83)) .GT. 1.0D-30) M(110) = ALFA(33)**2          DIS12680
     .           * ALFA(101) / (KT1(83) * GAMMA(110) * ALFA(8))       DIS12690
        M(111) = ALFA(101)**3 / (KT1(84)  * GAMMA(111))               DIS12700
        M(165) = ALFA(9)      / (KT1(117) * GAMMA(165))               DIS12710
        M(166) = ALFA(9)**2   / (KT1(137) * GAMMA(166))               DIS12720
                                                                      DIS12730
C -------------------------------------------------------------------|DIS12740
C     If hg++ is to be calculated from eh then flags(3) = 1.          |DIS12750
C     If from 2hg++ + 2fe++ = hg++ + 2fe+3 then flags(3) = 0.         |DIS12760
C -------------------------------------------------------------------|DIS12770
                                                                      DIS12780
        IF (EHM .LT. 9.0 .AND. FLAGS(3) .EQ. 1) THEN                  DIS12790
          C1    = 10.0**(((EHM*F - LOGKT1(140))*2) / (2.303*R*T))     DIS12800
          M(20) = C1 * M(21) * GAMMA(21) / GAMMA(20)                  DIS12810
        ELSE IF (EXELT(25) .LT. CPUMIN  .OR. EXELT(13) .LT. CPUMIN    DIS12820
     .      .OR.  ALFA(18)  .LT. 1.0D-30 .OR. ALFA(19)  .LT. 1.0D-30) DIS12830
     .        THEN                                                     DIS12840
          M(20)  = 0.0                                                DIS12850
          M(112) = 0.0                                                DIS12860
        ELSE IF (FLAGS(3) .EQ. 0) THEN                                DIS12870
          M(20)  = 2.0 * DLOG10(ALFA(18)) - 2.0 * DLOG10(ALFA(19))    DIS12880
     .             + DLOG10(M(21)) + DLOG10(GAMMA(21)) + DLOG10(KT1(6)) DIS12890
     .             - DLOG10(GAMMA(20))                                DIS12900
          IF (M(20) .GT. -30.0 .AND. M(20) .LT. +30.0) THEN           DIS12910
            M(20) = 10.0**M(20)                                       DIS12920
          ELSE                                                        DIS12930
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            M(20) = 0.0D00                                                    DIS12940
          END IF                                                              DIS12950
                                                                              DIS12960
          M(112) = 2.0 * DLOG10(ALFA(18)) - 2.0 * DLOG10(ALFA(19))            DIS12970
     .           + DLOG10(KT1(85)) - DLOG10(GAMMA(112))                       DIS12980
          IF (M(112) .GT. -30.0 .AND. M(112) .LT. +30.0) THEN                 DIS12990
            M(112) = 10.0**M(112)                                             DIS13000
          ELSE                                                                DIS13010
            M(112) = 0.0                                                      DIS13020
          END IF                                                              DIS13030
        END IF                                                                DIS13040
                                                                              DIS13050
        M(21)    = EXELT(14) / (1.0D0 + GAMMA(21) * (M(20) + M(105) +         DIS13060
     .             M(106) + M(107) + M(108) + M(109) + M(110) +               DIS13070
     .             M(111) + M(112) + M(165) + M(166)))                        DIS13080
        ALFA(21) = M(21) * GAMMA(21)                                          DIS13090
                                                                              DIS13100
        M(20)    = M(20) * ALFA(21)                                           DIS13110
        ALFA(20) = M(20) * GAMMA(20)                                          DIS13120
                                                                              DIS13130
        DO 280 I = 105, 112                                                   DIS13140
          M(I)    = M(I) * ALFA(21)                                           DIS13150
          ALFA(I) = M(I) * GAMMA(I)                                           DIS13160
280     CONTINUE                                                              DIS13170
                                                                              DIS13180
        DO 290 I = 165, 166                                                   DIS13190
          M(I)    = M(I) * ALFA(21)                                           DIS13200
          ALFA(I) = M(I) * GAMMA(I)                                           DIS13210
290     CONTINUE                                                              DIS13220
      END IF                                                                  DIS13230
                                                                              DIS13240
C -------------------------------------------------------------------------|DIS13250
C     Lithium species                                                        |DIS13260
C -------------------                                                        |DIS13270
                                                                              DIS13280
      IF (EXELT(15) .GT. CPUMIN) THEN                                         DIS13290
        M(118) = ALFA(9) / (KT1(91) * GAMMA(118))                             DIS13300
        M(119) = ALFA(6) / (KT1(92) * GAMMA(119))                             DIS13310
                                                                              DIS13320
        M(22)    = EXELT(15) / (1.0D0 + GAMMA(22) * (M(118) + M(119)))        DIS13330
        ALFA(22) = M(22) * GAMMA(22)                                          DIS13340
                                                                              DIS13350
        DO 300 I = 118, 119                                                   DIS13360
          M(I)    = M(I) * ALFA(22)                                           DIS13370
          ALFA(I) = M(I) * GAMMA(I)                                           DIS13380
300     CONTINUE                                                              DIS13390
      END IF                                                                  DIS13400
                                                                              DIS13410
C -------------------------------------------------------------------------|DIS13420
C     Manganese species                                                      |DIS13430
C --------------------                                                       |DIS13440
                                                                              DIS13450
      IF (EXELT(16) .GT. CPUMIN) THEN                                         DIS13460
        M(128) = ALFA(  5)    / (KT1(101) * GAMMA(128))                       DIS13470
        M(129) = ALFA(  5)**2 / (KT1(102) * GAMMA(129))                       DIS13480
        M(130) = ALFA(  5)**3 / (KT1(103) * GAMMA(130))                       DIS13490
        M(131) = 0.0D00                                                       DIS13500
        IF (DABS(KT1(104)) .GT. 1.0D-30)                                      DIS13510
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     .      M(131) = ALFA(  5)**4 / (KT1(104) * GAMMA(131))            DIS13520
           M(132) = ALFA(  7)    / (KT1(105) * GAMMA(132))             DIS13530
           M(133) = ALFA(  6)    / (KT1(106) * GAMMA(133))             DIS13540
           M(134) = ALFA( 99)    / (KT1(108) * GAMMA(134))             DIS13550
           M(135) = ALFA(  9)    / (KT1(109) * GAMMA(135))             DIS13560
           M(257) = ALFA(246)    / (KT1(233) * GAMMA(257))             DIS13570
           M(258) = ALFA(246)**2 / (KT1(234) * GAMMA(258))             DIS13580
           M(259) = ALFA(246)**3 / (KT1(235) * GAMMA(259))             DIS13590
           M(276) = ALFA(265)    / (KT1(251) * GAMMA(276))             DIS13600
           M(MXSP+11) = ALFA(MXSP+ 1) / (KT1(MXAQK+10) * GAMMA(MXSP+11))  DIS13610
           M(MXSP+26) = ALFA(MXSP+16) / (KT1(MXAQK+24) * GAMMA(MXSP+26))  DIS13620
                                                                        DIS13630
C ------------------------------------------------------------------------|DIS13640
C     If mn+++ is to be calculated from eh then flags(4) = 1.           |DIS13650
C     If from mn+3 + fe++ = mn++ + fe+3 then flags(4) = 0.               |DIS13660
C ------------------------------------------------------------------------|DIS13670
                                                                        DIS13680
           IF (EHM.LT.9.0D0 .AND. FLAGS(4) .EQ. 1) THEN                 DIS13690
             C1    = 1.0D1**((EHM * F - LOGKT1(141)) / (2.303 * R * T))  DIS13700
             M(24) = C1 / GAMMA(23)                                     DIS13710
           ELSE IF (EXELT(25) .LT. CPUMIN) THEN                         DIS13720
             M(24) = 0.0D0                                              DIS13730
           ELSE IF (EXELT(13) .LT. CPUMIN) THEN                         DIS13740
             M(24) = 0.0D0                                              DIS13750
           ELSE IF (FLAGS(4) .EQ. 0) THEN                               DIS13760
             M(24) = ALFA(19) / (KT1(7) * ALFA(18) * GAMMA(24))         DIS13770
           END IF                                                       DIS13780
                                                                        DIS13790
           M(153) = ALFA(  5)    / (KT1(107) * GAMMA(153))              DIS13800
           M(153) = M(153) * M(24) * GAMMA(24)                          DIS13810
                                                                        DIS13820
           M(260) = ALFA(246)    / (KT1(236) * GAMMA(258))              DIS13830
           M(260) = M(260) * M(24) * GAMMA(24)                          DIS13840
                                                                        DIS13850
           M(23)    = EXELT(16) / (1.0D0 + GAMMA(23) * (M(24) + M(128) +  DIS13860
     .                M(129) + M(130) + M(131) + M(132) + M(133) +      DIS13870
     .                M(134) + M(135) + M(153) + M(257) + M(258) +      DIS13880
     .                M(259) + M(260) + M(276) + M(MXSP+11) + M(MXSP+26))) DIS13890
           ALFA(23) = M(23) * GAMMA(23)                                 DIS13900
                                                                        DIS13910
           M(24)    = M(24) * ALFA(23)                                  DIS13920
           ALFA(24) = M(24) * GAMMA(24)                                 DIS13930
                                                                        DIS13940
           DO 310 I = 128, 135                                          DIS13950
             M(I)    = M(I) * ALFA(23)                                  DIS13960
             ALFA(I) = M(I) * GAMMA(I)                                  DIS13970
    310    CONTINUE                                                     DIS13980
                                                                        DIS13990
           M(153)         = M(153)     * ALFA(23)                       DIS14000
           ALFA(153)      = M(153)     * GAMMA(153)                     DIS14010
                                                                        DIS14020
           DO 320 I = 257, 260                                          DIS14030
             M(I)    = M(I) * ALFA(23)                                  DIS14040
             ALFA(I) = M(I) * GAMMA(I)                                  DIS14050
    320    CONTINUE                                                     DIS14060
                                                                        DIS14070
           M(276)         = M(276)     * ALFA(23)                       DIS14080
           ALFA(276)      = M(276)     * GAMMA(276)                     DIS14090
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                                                                        DIS14100
        M(MXSP+11)     = M(MXSP+11) * ALFA(23)                          DIS14110
        ALFA(MXSP+11) = M(MXSP+11) * GAMMA(MXSP+11)                     DIS14120
                                                                        DIS14130
        M(MXSP+26)     = M(MXSP+26) * ALFA(23)                          DIS14140
        ALFA(MXSP+26) = M(MXSP+26) * GAMMA(MXSP+26)                     DIS14150
      END IF                                                            DIS14160
                                                                        DIS14170
C ---------------------------------------------------------------------|DIS14180
C     Lead species                                                      |DIS14190
C ---------------                                                      |DIS14200
                                                                        DIS14210
      IF (EXELT(17) .GT. CPUMIN) THEN                                   DIS14220
        M(148) = ALFA(  5)    / (KT1(121) * GAMMA(148))                 DIS14230
        M(149) = ALFA(  5)**2 / (KT1(122) * GAMMA(149))                 DIS14240
        M(150) = ALFA(  5)**3 / (KT1(123) * GAMMA(150))                 DIS14250
        M(151) = 0.0D00                                                 DIS14260
        IF (DABS(KT1(124)) .GT. 1.0D-30)                                DIS14270
     .     M(151) = ALFA(  5)**4 / (KT1(124) * GAMMA(151))              DIS14280
        M(152) = ALFA(  6)    / (KT1(125) * GAMMA(152))                 DIS14290
        M(238) = ALFA( 48)    / (KT1(218) * GAMMA(238))                 DIS14300
        M(239) = ALFA( 48)**2 / (KT1(219) * GAMMA(239))                 DIS14310
        M(240) = ALFA( 48)**3 / (KT1(220) * GAMMA(240))                 DIS14320
        M(262) = ALFA(246)    / (KT1(238) * GAMMA(262))                 DIS14330
        M(278) = ALFA(265)    / (KT1(253) * GAMMA(278))                 DIS14340
        M(286) = ALFA(101)**2 / (KT1(258) * GAMMA(286))                 DIS14350
        M(287) = ALFA(101)**3 / (KT1(259) * GAMMA(287))                 DIS14360
        M(288) = ALFA( 98)    / (KT1(260) * GAMMA(288))                 DIS14370
        M(289) = ALFA(  9)    / (KT1(261) * GAMMA(289))                 DIS14380
        M(MXSP+13) = ALFA(MXSP+ 1) / (KT1(MXAQK+12) * GAMMA(MXSP+13))   DIS14390
        M(MXSP+28) = ALFA(MXSP+16) / (KT1(MXAQK+26) * GAMMA(MXSP+28))   DIS14400
                                                                        DIS14410
        M(25)    = EXELT(17) / (1.0D0 + GAMMA(25) * (M(148) + M(149) +  DIS14420
     .             M(150) + M(151) + M(152) + M(238) + M(239) + M(240) +DIS14430
     .             M(262) + M(278) + M(286) + M(287) + M(288) + M(289) +DIS14440
     .             M(MXSP+13) + M(MXSP+28)))                           DIS14450
        ALFA(25) = M(25) * GAMMA(25)                                    DIS14460
                                                                        DIS14470
                                                                        DIS14480
        DO 330 I = 148, 152                                             DIS14490
          M(I)     = M(I) * ALFA(25)                                    DIS14500
          ALFA(I) = M(I) * GAMMA(I)                                     DIS14510
  330   CONTINUE                                                        DIS14520
                                                                        DIS14530
        DO 340 I = 238, 240                                             DIS14540
          M(I)     = M(I) * ALFA(25)                                    DIS14550
          ALFA(I) = M(I) * GAMMA(I)                                     DIS14560
  340   CONTINUE                                                        DIS14570
                                                                        DIS14580
        M(262)         = M(262)       * ALFA(25)                        DIS14590
        ALFA(262)      = M(262)       * GAMMA(262)                      DIS14600
                                                                        DIS14610
        M(278)         = M(278)       * ALFA(25)                        DIS14620
        ALFA(278)      = M(278)       * GAMMA(278)                      DIS14630
                                                                        DIS14640
        DO 350 I = 286, 289                                             DIS14650
          M(I)     = M(I) * ALFA(25)                                    DIS14660
          ALFA(I) = M(I) * GAMMA(I)                                     DIS14670
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  350   CONTINUE                                                          DIS14680
                                                                          DIS14690
        M(MXSP+13)     = M(MXSP+13) * ALFA(25)                            DIS14700
        ALFA(MXSP+13) = M(MXSP+13) * GAMMA(MXSP+13)                       DIS14710
                                                                          DIS14720
        M(MXSP+28)     = M(MXSP+28) * ALFA(25)                            DIS14730
        ALFA(MXSP+28) = M(MXSP+28) * GAMMA(MXSP+28)                       DIS14740
      END IF                                                              DIS14750
                                                                          DIS14760
C -------------------------------------------------------------------    |DIS14770
C     Strontium species                                                   |DIS14780
C --------------------                                                   |DIS14790
                                                                          DIS14800
  360 CONTINUE                                                            DIS14810
      IF (EXELT(18) .GT. CPUMIN) THEN                                     DIS14820
        M(154) = ALFA(  9) / (KT1(127) * GAMMA(154))                      DIS14830
        M(155) = ALFA( 98) / (KT1(128) * GAMMA(155))                      DIS14840
        M(156) = ALFA(  7) / (KT1(129) * GAMMA(156))                      DIS14850
        M(157) = ALFA(  6) / (KT1(130) * GAMMA(157))                      DIS14860
        M(241) = ALFA( 48) / (KT1(221) * GAMMA(241))                      DIS14870
        M(263) = ALFA(246) / (KT1(239) * GAMMA(263))                      DIS14880
        M(279) = ALFA(265) / (KT1(254) * GAMMA(279))                      DIS14890
        M(MXSP+14) = ALFA(MXSP+ 1) / (KT1(MXAQK+13) * GAMMA(MXSP+14))     DIS14900
        M(MXSP+29) = ALFA(MXSP+16) / (KT1(MXAQK+27) * GAMMA(MXSP+29))     DIS14910
                                                                          DIS14920
        M(26)     = EXELT(18) / (1.0D0 + GAMMA(26) * (M(154) + M(155) +   DIS14930
     .              M(156) + M(157) + M(241) + M(263) + M(279) +          DIS14940
     .              M(MXSP+14) + M(MXSP+29)))                             DIS14950
        ALFA(26) = M(26) * GAMMA(26)                                      DIS14960
                                                                          DIS14970
        DO 370 I = 154, 157                                               DIS14980
          M(I)     = M(I) * ALFA(26)                                      DIS14990
          ALFA(I) = M(I) * GAMMA(I)                                       DIS15000
  370   CONTINUE                                                          DIS15010
                                                                          DIS15020
        M(241)          = M(241)       * ALFA(26)                         DIS15030
        ALFA(241)       = M(241)       * GAMMA(241)                       DIS15040
                                                                          DIS15050
        M(263)          = M(263)       * ALFA(26)                         DIS15060
        ALFA(263)       = M(263)       * GAMMA(263)                       DIS15070
                                                                          DIS15080
        M(279)          = M(279)       * ALFA(26)                         DIS15090
        ALFA(279)       = M(279)       * GAMMA(279)                       DIS15100
                                                                          DIS15110
        M(MXSP+14)     = M(MXSP+14) * ALFA(26)                            DIS15120
        ALFA(MXSP+14) = M(MXSP+14) * GAMMA(MXSP+14)                       DIS15130
                                                                          DIS15140
        M(MXSP+29)     = M(MXSP+29) * ALFA(26)                            DIS15150
        ALFA(MXSP+29) = M(MXSP+29) * GAMMA(MXSP+29)                       DIS15160
                                                                          DIS15170
        IF (IPIT.EQ.1 .AND. PG(26).GT.CPUMIN                              DIS15180
     .                .AND. GAMMA(26).LE.10.0) THEN                       DIS15190
          IF (DABS(PALFA(26)-ALFA(26)) .GT. 1.0D-2*PALFA(26)) THEN        DIS15200
            IF (PALFA(26) .GT. ALFA(26)) THEN                             DIS15210
              INC=0.1                                                     DIS15220
            ELSE                                                          DIS15230
              INC=-0.01                                                   DIS15240
            END IF                                                        DIS15250
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            GAMMA(26)=GAMMA(26)*(1.0+INC)                                    DIS15260
            GO TO 360                                                        DIS15270
          END IF                                                             DIS15280
        END IF                                                               DIS15290
                                                                             DIS15300
        IF (IPIT.EQ.1 .AND. GAMMA(26).GT. 10.0)  GAMMA(26) = 10.0            DIS15310
        IF (IPIT.GT.1 .AND. GAMMA(26).LT.PG(26)) GAMMA(26) = PG(26)          DIS15320
      END IF                                                                 DIS15330
                                                                             DIS15340
C -------------------------------------------------------------------------|DIS15350
C     Zinc species                                                           |DIS15360
C ---------------                                                            |DIS15370
                                                                             DIS15380
      IF (EXELT(19) .GT. CPUMIN) THEN                                        DIS15390
        M(158) = ALFA(  5)    / (KT1(131) * GAMMA(158))                      DIS15400
        M(159) = ALFA(  5)**2 / (KT1(132) * GAMMA(159))                      DIS15410
        M(160) = ALFA(  5)**3 / (KT1(133) * GAMMA(160))                      DIS15420
        M(161) = 0.0D00                                                      DIS15430
        IF (DABS(KT1(134)) .GT. 1.0D-30)                                     DIS15440
     .       M(161) = ALFA(  5)**4 / (KT1(134) * GAMMA(161))                 DIS15450
        M(162) = ALFA(  6)    / (KT1(135) * GAMMA(162))                      DIS15460
        M(244) = ALFA( 48)    / (KT1(222) * GAMMA(244))                      DIS15470
        M(245) = ALFA( 48)**2 / (KT1(126) * GAMMA(245))                      DIS15480
        M(264) = ALFA(246)    / (KT1(240) * GAMMA(264))                      DIS15490
        M(280) = ALFA(265)    / (KT1(255) * GAMMA(280))                      DIS15500
        M(290) = ALFA(101)**2 / (KT1(262) * GAMMA(290))                      DIS15510
        M(291) = ALFA(101)**3 / (KT1(263) * GAMMA(291))                      DIS15520
        M(292) = ALFA(  7)    / (KT1(264) * GAMMA(292))                      DIS15530
        M(293) = ALFA(  9)    / (KT1(265) * GAMMA(293))                      DIS15540
        M(294) = ALFA(  9)**2 / (KT1(266) * GAMMA(294))                      DIS15550
        M(295) = ALFA(101) * ALFA(  9)  / (KT1(267) * GAMMA(295))            DIS15560
        M(MXSP+15) = ALFA(MXSP+ 1) / (KT1(MXAQK+14) * GAMMA(MXSP+15))        DIS15570
        M(MXSP+30) = ALFA(MXSP+16) / (KT1(MXAQK+28) * GAMMA(MXSP+30))        DIS15580
                                                                             DIS15590
        M(27)    = EXELT(19) / (1.0D0 + GAMMA(27) * (M(158) + M(159) +       DIS15600
     .             M(160) + M(161) + M(162) + M(244) + M(245) + M(264) +DIS15610
     .             M(280) + M(290) + M(291) + M(292) + M(293) + M(294) +DIS15620
     .             M(295) + M(MXSP+15) + M(MXSP+30)))                        DIS15630
        ALFA(27) = M(27) * GAMMA(27)                                         DIS15640
                                                                             DIS15650
        DO 380 I = 158, 162                                                  DIS15660
          M(I)    = M(I) * ALFA(27)                                          DIS15670
          ALFA(I) = M(I) * GAMMA(I)                                          DIS15680
  380   CONTINUE                                                             DIS15690
                                                                             DIS15700
        M(244)          = M(244)      * ALFA(27)                             DIS15710
        ALFA(244)       = M(244)      * GAMMA(244)                           DIS15720
                                                                             DIS15730
        M(245)    = M(245) * ALFA(27)                                        DIS15740
        ALFA(245) = M(245) * GAMMA(245)                                      DIS15750
                                                                             DIS15760
        M(264)          = M(264)      * ALFA(27)                             DIS15770
        ALFA(264)       = M(264)      * GAMMA(264)                           DIS15780
                                                                             DIS15790
        M(280)          = M(280)      * ALFA(27)                             DIS15800
        ALFA(280)       = M(280)      * GAMMA(280)                           DIS15810
                                                                             DIS15820
        DO 390 I = 290, 295                                                  DIS15830
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        M(I)     = M(I) * ALFA(27)                                      DIS15840
        ALFA(I) = M(I) * GAMMA(I)                                       DIS15850
  390  CONTINUE                                                         DIS15860
                                                                        DIS15870
       M(MXSP+15)     = M(MXSP+15) * ALFA(27)                          DIS15880
       ALFA(MXSP+15) = M(MXSP+15) * GAMMA(MXSP+15)                     DIS15890
                                                                        DIS15900
       M(MXSP+30)     = M(MXSP+30) * ALFA(27)                          DIS15910
       ALFA(MXSP+30) = M(MXSP+30) * GAMMA(MXSP+30)                     DIS15920
      END IF                                                            DIS15930
                                                                        DIS15940
C ----------------------------------------------------------------------|DIS15950
C     Arsenic species                                                   |DIS15960
C ------------------                                                    |DIS15970
                                                                        DIS15980
      IF (EXELT(20) .GT. CPUMIN) THEN                                   DIS15990
        M(49) = ALFA(8)  / KT1(67) * GAMMA(49)                          DIS16000
                                                                        DIS16010
C ----------------------------------------------------------------------|DIS16020
C     The following statement prevents a divide by zero error if the    |DIS16030
C     concentration or fe+2 is zero                                     |DIS16040
C ----------------------------------------------------------------------|DIS16050
                                                                        DIS16060
        IF (DABS(ALFA(18)) .GT. 1.0D-30) M(50) = (ALFA(19) /            DIS16070
     .    ALFA(18))**2 * ALFA(10) / KT1(136) * ALFA(8)**4 * GAMMA(50)   DIS16080
                                                                        DIS16090
        M(92) = KT1(8)   / ALFA(8)    * GAMMA(92)                       DIS16100
        M(93) = ALFA(8)    / (KT1(68) * GAMMA(93))                      DIS16110
        M(94) = ALFA(8)**2 / (KT1(69) * GAMMA(94))                      DIS16120
        M(95) = ALFA(8)**3 / (KT1(70) * GAMMA(95))                      DIS16130
                                                                        DIS16140
        DO 400 I = 93, 95                                               DIS16150
          M(I) = M(I) * M(50) * GAMMA(50)                               DIS16160
  400   CONTINUE                                                        DIS16170
                                                                        DIS16180
        M(28)    = EXELT(20) / (1.0D0 + GAMMA(28) * (M(49) + M(50) +    DIS16190
     .             M(92) + M(93) + M(94) + M(95)))                     DIS16200
        ALFA(28) = M(28) * GAMMA(28)                                    DIS16210
                                                                        DIS16220
        DO 410 I = 49, 50                                               DIS16230
          M(I)    = M(I) * ALFA(28)                                     DIS16240
          ALFA(I) = M(I) * GAMMA(I)                                     DIS16250
  410   CONTINUE                                                        DIS16260
                                                                        DIS16270
        DO 420 I = 92, 95                                               DIS16280
          M(I)    = M(I) * ALFA(28)                                     DIS16290
          ALFA(I) = M(I) * GAMMA(I)                                     DIS16300
  420   CONTINUE                                                        DIS16310
      END IF                                                            DIS16320
                                                                        DIS16330
C ----------------------------------------------------------------------|DIS16340
C     Uranium species                                                   |DIS16350
C ------------------                                                    |DIS16360
                                                                        DIS16370
      IF (EXELT(27) .GT. CPUMIN) THEN                                   DIS16380
        M(189) = ALFA(9)     / (KT1(167) * GAMMA(189))                  DIS16390
        M(190) = ALFA(9)**2  / (KT1(168) * GAMMA(190))                  DIS16400
        M(191) = M(169) * GAMMA(169) * ALFA(9)**2 /                     DIS16410
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     .              (KT1(169) * GAMMA(191))                                  DIS16420
        M(192) = 0.0D00                                                      DIS16430
        IF (DABS(KT1(170)) .GT. CPUMIN)                                      DIS16440
     .     M(192) = M(169)**2 * GAMMA(169)**2 * ALFA(10)**5 /                DIS16450
     .                (ALFA(8)**5 * GAMMA(192)  * KT1(170))                 DIS16460
        M(193) = 0.0D00                                                      DIS16470
        IF (DABS(KT1(171)) .GT. CPUMIN)                                      DIS16480
     .     M(193) = M(169)**2 * GAMMA(169)**2 * ALFA(10)**7 /                DIS16490
     .              (ALFA(8)**7 * GAMMA(193)  * KT1(171))                   DIS16500
        M(194) = ALFA(6)     / (KT1(172) * GAMMA(194))                       DIS16510
        M(195) = ALFA(6)**2  / (KT1(173) * GAMMA(195))                       DIS16520
        M(196) = ALFA(30)    / (KT1(174) * GAMMA(196))                       DIS16530
        M(197) = ALFA(30)**2 / (KT1(175) * GAMMA(197))                       DIS16540
        M(198) = ALFA(30)**3 / (KT1(176) * GAMMA(198))                       DIS16550
        M(199) = 0.0                                                         DIS16560
        IF (DABS(KT1(177)) .GT. 1.0D-30)                                     DIS16570
     .     M(199) = ALFA(30)**4 / (KT1(177) * GAMMA(199))                    DIS16580
        M(200) = ALFA(5)     / (KT1(178) * GAMMA(200))                       DIS16590
        M(201) = ALFA(11)    / (KT1(179) * GAMMA(201) * ALFA(8))             DIS16600
        M(202) = ALFA(99)    / (KT1(180) * GAMMA(202))                       DIS16610
        M(203) = ALFA(99)**2 / (KT1(181) * GAMMA(203))                       DIS16620
        M(204) = ALFA(99) * ALFA(8) / (KT1(182) * GAMMA(204))                DIS16630
        M(205) = ALFA(99)**2 * ALFA(8)**2 / (KT1(183) * GAMMA(205))          DIS16640
        M(206) = ALFA(99)**3 * ALFA(8)**3 / (KT1(184) * GAMMA(206))          DIS16650
        M(207) = ALFA(98)    / (KT1(185) * GAMMA(207))                       DIS16660
        M(208) = ALFA(98)**2 / (KT1(186) * GAMMA(208))                       DIS16670
        M(209) = ALFA(98)**3 / (KT1(187) * GAMMA(209))                       DIS16680
        M(242) = ALFA(48)    / (KT1(203) * GAMMA(242))                       DIS16690
        M(243) = ALFA(48)**2 / (KT1(204) * GAMMA(243))                       DIS16700
                                                                             DIS16710
C ------------------------------------------------------------------------|DIS16720
C     If uo2 is to be calculated from eh then flags(5) = 1, if from      |DIS16730
C     uo+2 + fe+2 = uo2+ + fe+3 then flags(5) = 0.                       |DIS16740
C ------------------------------------------------------------------------|DIS16750
                                                                             DIS16760
        IF (EHM .LT. 9.0 .AND. FLAGS(5) .EQ. 1) THEN                         DIS16770
          C1     = 10.0**((-EHM * F - LOGKT1(143)) / (2.303 * R * T))        DIS16780
          M(168) = C1 / (GAMMA(169))                                         DIS16790
        ELSE IF (EXELT(25) .LT. CPUMIN)  THEN                                DIS16800
          M(168) = 0.0                                                       DIS16810
        ELSE IF (EXELT(13) .LT. CPUMIN) THEN                                 DIS16820
          M(168) = 0.0                                                       DIS16830
        ELSE IF (FLAGS(5) .EQ. 0) THEN                                       DIS16840
          M(168) = ALFA(18) / (KT1(205) * ALFA(19) * GAMMA(168))             DIS16850
        END IF                                                               DIS16860
                                                                             DIS16870
C ------------------------------------------------------------------------|DIS16880
C     If u+4 is to be calculated from eh then flag(5) = 1, if from       |DIS16890
C     uo2+ + fe+2 + 4h+ = u+4 + fe+3 +2 h2o then flag(5) = 0.            |DIS16900
C ------------------------------------------------------------------------|DIS16910
                                                                             DIS16920
        IF (EHM .LT. 9D0 .AND. FLAGS(5) .EQ. 1) THEN                         DIS16930
          C1     = 1.0D1**((-EHM * F - (LOGKT1(142))) /                      DIS16940
     .             (2.303 * R * T)) + DLOG10(ALFA(10)**2 / ALFA(8)**4)       DIS16950
          M(167) = C1 / GAMMA(168)                                           DIS16960
        ELSE IF (EXELT(25) .LT. CPUMIN .OR. EXELT(13) .LT. CPUMIN) THEN      DIS16970
          M(167) = 0.0D0                                                     DIS16980
        ELSE IF (FLAGS(5) .EQ. 0) THEN                                       DIS16990
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      M(167) =            ALFA(18) * ALFA(8)**4 /                    DIS17000
     .          (KT1(206) * ALFA(19) * GAMMA(167) * ALFA(10)**2)     DIS17010
      END IF                                                         DIS17020
                                                                     DIS17030
      M(167) = M(167) * M(168) * GAMMA(168)                          DIS17040
      M(170) = ALFA(9)      / (KT1(148) * GAMMA(170))                DIS17050
      M(171) = ALFA(9)**2   / (KT1(149) * GAMMA(171))                DIS17060
      M(172) = ALFA(10)**3  / (KT1(150) * GAMMA(172) * ALFA(8)**3)   DIS17070
      M(173) = 0.0D00                                                DIS17080
      IF (DABS(KT1(151)) .GT. 1.0D-30)                               DIS17090
     .  M(173) = ALFA(10)**4  / (KT1(151) * GAMMA(173) * ALFA(8)**4) DIS17100
      M(174) = 0.0D00                                                DIS17110
      IF (DABS(KT1(152)) .GT. 1.0D-30)                               DIS17120
     .  M(174) = ALFA(10)**5  / (KT1(152) * GAMMA(174) * ALFA(8)**5) DIS17130
      M(175) = ALFA(30)     / (KT1(153) * GAMMA(175))                DIS17140
      M(176) = ALFA(30)**2  / (KT1(154) * GAMMA(176))                DIS17150
      M(177) = 0.0D00                                                DIS17160
      IF (DABS(KT1(155)) .GT. 1.0D-30)                               DIS17170
     .  M(177) = ALFA(30)**3  / (KT1(155) * GAMMA(177))              DIS17180
      M(178) = 0.0D00                                                DIS17190
      IF (DABS(KT1(156)) .GT. 1.0D-30)                               DIS17200
     .  M(178) = ALFA(30)**4  / (KT1(156) * GAMMA(178))              DIS17210
      M(179) = 0.0D00                                                DIS17220
      IF (DABS(KT1(157)) .GT. 1.0D-30)                               DIS17230
     .  M(179) = ALFA(30)**5  / (KT1(157) * GAMMA(179))              DIS17240
      M(180) = 0.0D00                                                DIS17250
      IF (DABS(KT1(158)) .GT. 1.0D-30)                               DIS17260
     .  M(180) = ALFA(30)**6  / (KT1(158) * GAMMA(180))              DIS17270
      M(181) = ALFA(5)      / (KT1(159) * GAMMA(181))                DIS17280
      M(182) = ALFA(99)     / (KT1(160) * GAMMA(182))                DIS17290
      M(183) = ALFA(99)**2  / (KT1(161) * GAMMA(183))                DIS17300
      M(184) = ALFA(100)**3 / (KT1(162) * GAMMA(184) * ALFA(8)**3)   DIS17310
      M(185) = 0.0D00                                                DIS17320
      IF (DABS(KT1(185)) .GT. 1.0D-30)                               DIS17330
     .  M(185) = ALFA(100)**4 / (KT1(163) * GAMMA(185) * ALFA(8)**4) DIS17340
      M(186) = ALFA(6)      / (KT1(164) * GAMMA(186))                DIS17350
      M(187) = ALFA(6)**2   / (KT1(165) * GAMMA(187))                DIS17360
                                                                     DIS17370
      IF (ALFA(167) .GT. 0.0D0) THEN                                 DIS17380
        M(188) =  ALFA(10)**12 * ALFA(9)**3  *                       DIS17390
     .     1.0D1**(DLOG10(ALFA(167)) * 5) / (KT1(166) * GAMMA(188) * DIS17400
     .     1.0D1**(DLOG10(ALFA(8)) * 12))                            DIS17410
      END IF                                                         DIS17420
                                                                     DIS17430
      DO 430 I = 170, 188                                            DIS17440
        M(I) = M(I) * M(167) * GAMMA(167)                            DIS17450
  430 CONTINUE                                                       DIS17460
                                                                     DIS17470
      M(169) = M(167) + M(168) +     M(170) +     M(171) +     M(172) DIS17480
     .                + M(173) +     M(174) +     M(175) +     M(176) DIS17490
     .                + M(177) +     M(178) +     M(179) +     M(180) DIS17500
     .                + M(181) +     M(182) +     M(183) +     M(184) DIS17510
     .                + M(185) +     M(186) +     M(187) + 6.0*M(188) DIS17520
     .                + M(189)                                        DIS17530
      M(169) = M(169) + M(190) + 2.0*M(191) + 3.0*M(192) + 3.0*M(193) DIS17540
     .                + M(194) +     M(195) +     M(196) +     M(197) DIS17550
     .                + M(198) +     M(199) +     M(200) +     M(201) DIS17560
     .                + M(202) +     M(203) +     M(204) +     M(205) DIS17570
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     .                  + M(206) +     M(207) +     M(208) +     M(209) DIS17580
     .                  + M(242) +     M(243)                         DIS17590
        M(169)    = EXELT(27) / (1.0D0 + GAMMA(169) * M(169))         DIS17600
        ALFA(169) = M(169) * GAMMA(169)                               DIS17610
                                                                      DIS17620
        M(167)    = M(167) * ALFA(169)                                DIS17630
        ALFA(167) = M(167) * GAMMA(167)                               DIS17640
        M(168)    = M(168) * ALFA(169)                                DIS17650
        ALFA(168) = M(168) * GAMMA(168)                               DIS17660
                                                                      DIS17670
        DO 440 I = 170, 209                                           DIS17680
          M(I)    = M(I) * ALFA(169)                                  DIS17690
          ALFA(I) = M(I) * GAMMA(I)                                   DIS17700
  440   CONTINUE                                                      DIS17710
                                                                      DIS17720
        M(242)    = M(242) * ALFA(169)                                DIS17730
        ALFA(242) = M(242) * GAMMA(242)                               DIS17740
        M(243)    = M(243) * ALFA(169)                                DIS17750
        ALFA(243) = M(243) * GAMMA(243)                               DIS17760
      END IF                                                          DIS17770
                                                                      DIS17780
C ---------------------------------------------------------------------|DIS17790
C     Vanadium species                                                |DIS17800
C ---------------------                                               |DIS17810
                                                                      DIS17820
      IF (EXELT(28) .GT. CPUMIN) THEN                                 DIS17830
        M(213) = ALFA(8)      / (KT1(188) * GAMMA(213))               DIS17840
        M(214) = ALFA(8)**2   / (KT1(189) * GAMMA(214))               DIS17850
        M(215) = ALFA(8)**3   / (KT1(190) * GAMMA(215))               DIS17860
        M(216) = ((ALFA(8)**2 / KT1(191)) / GAMMA(216)) * ALFA(8)**2  DIS17870
        M(217) = ALFA(3) * ALFA(8) / (KT1(192) * GAMMA(217))          DIS17880
        M(218) = ALFA(30)     / (KT1(193) * GAMMA(218))               DIS17890
        M(219) = ALFA(30)**2  / (KT1(194) * GAMMA(218))               DIS17900
                                                                      DIS17910
C ---------------------------------------------------------------------|DIS17920
C     If vo+2 is to be calculated from eh then flags(6) = 1, if       |DIS17930
C     from vo4 -3 + 6h+ + fe+2 = vo+2 + 3h2o + fe+3 then flags(6) = 0. |DIS17940
C ---------------------------------------------------------------------|DIS17950
                                                                      DIS17960
        IF (EHM .LT. 9.0 .AND. FLAGS(6) .EQ. 1) THEN                  DIS17970
          C1     = 10.0**((EHM * F - LOGKT1(145) + DLOG10(ALFA(10))**3) -DIS17980
     .             6.0 * DLOG10(ALFA(8))) / (2.303 * R * T))         DIS17990
          M(211) = C1 / GAMMA(210)                                    DIS18000
        ELSE IF (EXELT(25).LT.CPUMIN .OR. EXELT(13).LT.CPUMIN) THEN   DIS18010
          M(211)  =  0.0D0                                            DIS18020
        ELSE IF (FLAGS(6) .EQ. 0 .AND. ALFA(18) .GT. CPUMIN) THEN     DIS18030
          M(211) = 10.0**(DLOG10(ALFA(8)) * 6.0 + DLOG10(ALFA(18) /   DIS18040
     .             ALFA(19))) / (KT1(208) * GAMMA(167) * ALFA(10)**3)  DIS18050
        ELSE                                                          DIS18060
          M(211)  = 0.0                                               DIS18070
        END IF                                                        DIS18080
                                                                      DIS18090
        M(223) = ALFA(9)     / (KT1(198) * GAMMA(223))                DIS18100
        M(224) = ALFA(6)     / (KT1(199) * GAMMA(224))                DIS18110
        M(225) = ALFA(5)     / (KT1(200) * GAMMA(225))                DIS18120
        M(226) = ALFA(30)    / (KT1(201) * GAMMA(226))                DIS18130
        M(227) = ALFA(30)**2 / (KT1(202) * GAMMA(227))                DIS18140
                                                                      DIS18150
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      DO 450 I = 223, 227                                                DIS18160
        M(I) = M(I) * GAMMA(211) * M(211)                                DIS18170
  450 CONTINUE                                                           DIS18180
                                                                         DIS18190
C -------------------------------------------------------------------|DIS18200
C     If v+3 is to be calculated from eh then flag(6) = 1, if from     |DIS18210
C     vo+2 + 2h+ + fe+2 = v+3 + h2o + fe+3 then flag(6) = 0.           |DIS18220
C -------------------------------------------------------------------|DIS18230
                                                                         DIS18240
      IF (EHM .LT. 9.0 .AND. FLAGS(6) .EQ. 1) THEN                       DIS18250
        C1 = 10.0**((EHM * F * LOGKT1(144) + DLOG10(ALFA(10)) -          DIS18260
     .        2.0 * DLOG10(ALFA(8))) / (2.303 * R * T))                  DIS18270
        M(212) = C1 / GAMMA(211)                                         DIS18280
      ELSE IF (EXELT(25) .LT. CPUMIN)  THEN                              DIS18290
        M(211) = 0.0                                                     DIS18300
      ELSE IF (EXELT(13) .LT. CPUMIN) THEN                               DIS18310
        M(220) = 0.0                                                     DIS18320
      ELSE IF (FLAGS(6) .EQ. 0) THEN                                     DIS18330
        M(212) = ALFA(18)   * ALFA(8)**2 / (KT1(207) * ALFA(19) *        DIS18340
     .           GAMMA(167) * ALFA(10))                                  DIS18350
      END IF                                                             DIS18360
                                                                         DIS18370
      M(220) = ALFA(9)    / (KT1(195) * GAMMA(220))                      DIS18380
      M(221) = ALFA(9)**2 / (KT1(196) * GAMMA(221))                      DIS18390
      M(222) = ALFA(9)**2 / (KT1(197) * GAMMA(222))                      DIS18400
                                                                         DIS18410
      DO 460 I = 220, 222                                                DIS18420
        M(I) = M(I) * M(212) * GAMMA(212)                                DIS18430
  460 CONTINUE                                                           DIS18440
                                                                         DIS18450
      C1 = 0.0D0                                                         DIS18460
                                                                         DIS18470
      DO 470 I = 211, 227                                                DIS18480
        C1 = C1 + M(I)                                                   DIS18490
  470 CONTINUE                                                           DIS18500
                                                                         DIS18510
      M(210)    = EXELT(28) / (1.0 + GAMMA(210) * C1)                    DIS18520
      ALFA(210) = M(210) * GAMMA(210)                                    DIS18530
                                                                         DIS18540
      DO 480 I = 211, 227                                                DIS18550
        M(I)    = M(I) * ALFA(210)                                       DIS18560
        ALFA(I) = M(I) * GAMMA(I)                                        DIS18570
  480 CONTINUE                                                           DIS18580
    END IF                                                               DIS18590
                                                                         DIS18600
C -------------------------------------------------------------------|DIS18610
C     Summation of anion species                                       |DIS18620
C -------------------------------------------------------------------|DIS18630
                                                                         DIS18640
    S(1) =     M(7)   + 2.0*M(98)  + 2.0*M(51)  +     M(52)  +         DIS18650
     .      2.0*M(55)  +     M(56)  + 2.0*M(114) + 2.0*M(120) +         DIS18660
     .          M(121) +     M(132) + 2.0*M(138) +     M(139) +         DIS18670
     .      2.0*M(140) + 2.0*M(155) +     M(156) + 2.0*M(207) +         DIS18680
     .      4.0*M(208) + 6.0*M(209) + 2.0*M(288) +     M(292) +         DIS18690
     .          M(MXSP+34)          + 2.0*M(MXSP+39)                    DIS18700
                                                                         DIS18710
    S(2) =     M(6)   +     M(41)  + 2.0*M(42)  +     M(47)  +         DIS18720
     .          M(54)  +     M(61)  +     M(70)  +     M(78)  +         DIS18730
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.           M(83)  + 2.0*M(84)  +     M(103) +     M(109) +        DIS18740
.           M(115) +     M(116) +     M(119) +     M(124) +        DIS18750
.           M(133) +     M(141) +     M(142) +     M(152) +        DIS18760
.           M(157) +     M(162) +     M(186) + 2.0*M(187) +        DIS18770
.           M(194) + 2.0*M(195) +     M(224) +     M(MXSP+33)      DIS18780
                                                                   DIS18790
 S(3) =     M(30)  +     M(34)  + 2.0*M(35)  + 3.0*M(36)  +        DIS18800
.       4.0*M(37)  +     M(96)  +     M(122) +     M(144) +        DIS18810
.       5.0*M(163) + 6.0*M(164) +     M(175) + 2.0*M(176) +        DIS18820
.       3.0*M(177) + 4.0*M(178) + 5.0*M(179) + 6.0*M(180) +        DIS18830
.           M(196) + 2.0*M(197) + 3.0*M(198) + 4.0*M(199) +        DIS18840
.           M(218) + 2.0*M(219) +     M(226) + 2.0*M(227) +        DIS18850
.           M(283) + 6.0*M(284) +     M(MXSP+37)                   DIS18860
                                                                   DIS18870
 S(4) =     M(29)  +     M(58)  +     M(59)  +     M(60)  +        DIS18880
.           M(73)  +     M(74)  +     M(99)  +     M(100) +        DIS18890
.           M(117) +     M(125) +     M(126) +     M(127) +        DIS18900
.           M(134) +     M(143) +     M(182) + 2.0*M(183) +        DIS18910
.       3.0*M(184) + 4.0*M(185) +     M(202) + 2.0*M(203) +        DIS18920
.           M(204) + 2.0*M(205) + 3.0*M(206) +     M(MXSP+36)      DIS18930
                                                                   DIS18940
 S(5) =     M(5)   +     M(43)  + 2.0*M(44)  + 3.0*M(45)  +        DIS18950
.       4.0*M(46)  +     M(62)  + 2.0*M(63)  + 3.0*M(64)  +        DIS18960
.           M(65)  + 2.0*M(66)  + 3.0*M(67)  + 4.0*M(68)  +        DIS18970
.           M(71)  + 2.0*M(72)  +     M(79)  + 2.0*M(80)  +        DIS18980
.       3.0*M(81)  + 4.0*M(82)  +     M(105) + 2.0*M(106) +        DIS18990
.       3.0*M(107) + 4.0*M(108) +     M(113) +     M(128)          DIS19000
 S(5) = S(5)       +                                               DIS19010
.       2.0*M(129) + 3.0*M(130) + 4.0*M(131) +     M(137) +        DIS19020
.           M(148) + 2.0*M(149) + 3.0*M(150) + 4.0*M(151) +        DIS19030
.           M(153) +     M(158) + 2.0*M(159) + 3.0*M(160) +        DIS19040
.       4.0*M(161) +     M(181) +     M(200) +     M(225) +        DIS19050
.           M(281) + 2.0*M(282) +     M(MXSP+32)                   DIS19060
                                                                   DIS19070
 S(6) =     M(48)  +     M(228) +     M(229) +     M(230) +        DIS19080
.           M(231) +     M(232) +     M(233) + 2.0*M(234) +        DIS19090
.           M(235) +     M(236) +     M(237) +     M(238) +        DIS19100
.       2.0*M(239) + 3.0*M(240) +     M(241) +     M(242) +        DIS19110
.       2.0*M(243) +     M(244) + 2.0*M(245) +     M(MXSP+38)      DIS19120
                                                                   DIS19130
 S(7) =     M(33)  +     M(101) +     M(102) + 4.0*M(110) +        DIS19140
.       3.0*M(111) +     M(145) + 2.0*M(286) + 3.0*M(287) +        DIS19150
.       2.0*M(290) + 3.0*M(291) +     M(295)                       DIS19160
                                                                   DIS19170
 S(8) =     M(246) +     M(247) +     M(248) +     M(249) +        DIS19180
.       2.0*M(250) +     M(251) +     M(252) +     M(253) +        DIS19190
.           M(254) +     M(255) +     M(256) +     M(257) +        DIS19200
.       2.0*M(258) + 3.0*M(259) +     M(260) +     M(261) +        DIS19210
.           M(262) +     M(263) +     M(264) +     M(MXSP+41)      DIS19220
                                                                   DIS19230
 S(9) =     M(265) +     M(266) +     M(267) +     M(268) +        DIS19240
.       2.0*M(269) +     M(270) +     M(271) +     M(272) +        DIS19250
.           M(273) +     M(274) +     M(275) +     M(276) +        DIS19260
.           M(277) +     M(278) +     M(279) +     M(280) +        DIS19270
.           M(MXSP+42)                                           DIS19280
                                                                   DIS19290
 S(10) = M(MXSP+ 1) + M(MXSP+ 2) + M(MXSP+ 3) + M(MXSP+ 4) +      DIS19300
.        M(MXSP+ 5) + M(MXSP+ 6) + M(MXSP+ 7) + M(MXSP+ 8) +      DIS19310
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     .        M(MXSP+ 9) + M(MXSP+10) + M(MXSP+11) + M(MXSP+12) +        DIS19320
     .        M(MXSP+13) + M(MXSP+14) + M(MXSP+15) + M(MXSP+43)          DIS19330
                                                                         DIS19340
       S(11) = M(MXSP+16) + M(MXSP+17) + M(MXSP+18) + M(MXSP+19) +       DIS19350
     .         M(MXSP+20) + M(MXSP+21) + M(MXSP+22) + M(MXSP+23) +       DIS19360
     .         M(MXSP+24) + M(MXSP+25) + M(MXSP+26) + M(MXSP+27) +       DIS19370
     .         M(MXSP+28) + M(MXSP+29) + M(MXSP+30) + M(MXSP+44)         DIS19380
                                                                         DIS19390
      SCO2 =     M(7)   +     M(51)  +     M(52)  +     M(55)  +        DIS19400
     .           M(56)  +     M(97)  +     M(98)  +     M(114) +        DIS19410
     .           M(120) +     M(121) +     M(132) +     M(138) +        DIS19420
     .           M(139) +     M(140) +     M(155) +     M(156) +        DIS19430
     .           M(207) + 2.0*M(208) + 3.0*M(209) +     M(288) +        DIS19440
     .           M(292) +     M(MXSP+34) +               M(MXSP+39)      DIS19450
                                                                         DIS19460
      IF (ALK .EQ. 1) THEN                                               DIS19470
        ANALCO = EXELT(29)                                               DIS19480
      ELSE IF (ALK .EQ. 0) THEN                                          DIS19490
        ANALCO = EXELT(29)  -     M(9)   -     M(28)  - 3.0*M(29)  -     DIS19500
     .               M(38)  - 2.0*M(39)  - 4.0*M(40)  -     M(48)  -     DIS19510
     .           3.0*M(50)  -     M(53)  -     M(57)  -     M(69)  -     DIS19520
     .               M(75)  - 2.0*M(76)  -     M(77)  -     M(85)  -     DIS19530
     .           2.0*M(86)  - 3.0*M(87)  - 4.0*M(88)  -     M(89)  -     DIS19540
     .           2.0*M(90)  -     M(91)  - 2.0*M(92)  - 2.0*M(93)  -     DIS19550
     .               M(94)  - 2.0*M(99)  -     M(100) -     M(101)       DIS19560
        ANALCO = ANALCO     -                                            DIS19570
     .           2.0*M(102) -     M(103) -     M(118) -     M(123) -     DIS19580
     .               M(135) -     M(147) -     M(154) -     M(165) -     DIS19590
     .           2.0*M(166) -     M(170) - 2.0*M(171) - 3.0*M(172) -     DIS19600
     .           4.0*M(173) - 5.0*M(174) - 2.0*M(182) - 4.0*M(183) -     DIS19610
     .           6.0*M(184) - 8.0*M(185) -15.0*M(188) -     M(189) -     DIS19620
     .           2.0*M(190) - 2.0*M(191) - 5.0*M(192) - 7.0*M(193)       DIS19630
        ANALCO = ANALCO     -                                            DIS19640
     .               M(201) - 2.0*M(202) - 4.0*M(203) -     M(204) -     DIS19650
     .           2.0*M(205) - 3.0*M(206) - 4.0*M(212) - 3.0*M(213) -     DIS19660
     .           2.0*M(214) -     M(215) - 3.0*M(217) -     M(220) -     DIS19670
     .           2.0*M(221) - 3.0*M(222) -     M(223) -     M(234) -     DIS19680
     .               M(239) - 2.0*M(240) -     M(243) -     M(245) -     DIS19690
     .               M(246) -     M(250) -     M(258) - 2.0*M(259)       DIS19700
        ANALCO = ANALCO     -                                            DIS19710
     .           2.0*M(265) -     M(266) -     M(269) -     M(289) -     DIS19720
     .               M(293) - 2.0*M(294) -     M(295)                    DIS19730
        ANALCO = ANALCO     -     M(MXSP+34) -     M(MXSP+35) -          DIS19740
     .           3.0*M(MXSP+36) - M(MXSP+38) - 2.0*M(MXSP+39) -          DIS19750
     .           2.0*M(MXSP+41) - M(MXSP+40) - 2.0*M(MXSP+42)            DIS19760
        DO 490 I = 229, 245                                              DIS19770
          ANALCO = ANALCO - M(I)                                         DIS19780
  490   CONTINUE                                                         DIS19790
                                                                         DIS19800
        DO 500 I = 249, 264                                              DIS19810
          ANALCO = ANALCO - M(I)                                         DIS19820
  500   CONTINUE                                                         DIS19830
                                                                         DIS19840
        DO 510 I = 268, 280                                              DIS19850
          ANALCO = ANALCO - M(I)                                         DIS19860
  510   CONTINUE                                                         DIS19870
      ELSE                                                               DIS19880
        S(1) = SCO2                                                      DIS19890
```

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        IF (ANMTIC .GT. 0.0D0) THEN                                          DIS19900
          ANALCO = ANMTIC                                                    DIS19910
        ELSE                                                                 DIS19920
          ANALCO = ANALM(7) + ANALM(98)                                      DIS19930
        END IF                                                               DIS19940
      END IF                                                                 DIS19950
                                                                             DIS19960
      IF ((DABS(HITEMP-TEMP)) .GT. 1.0D-10) CO2F = SCO2                      DIS19970
                                                                             DIS19980
      IF (ITIC .EQ. 2) THEN                                                  DIS19990
        S(1)     = SCO2                                                      DIS20000
        ANALCO   = CO2F + DCO2                                               DIS20010
      END IF                                                                 DIS20020
                                                                             DIS20030
C -------------------------------------------------------------------------| DIS20040
C     Iteration test                                                       | DIS20050
C -------------------------------------------------------------------------| DIS20060
                                                                             DIS20070
      DONE = .TRUE.                                                          DIS20080
                                                                             DIS20090
      IF (ANALCO .GT. CPUMIN) THEN                                           DIS20100
        X = (S(1) - ANALCO) / ANALCO                                         DIS20110
        CROSS = .FALSE.                                                      DIS20120
        IF ((X * DIFF(1)) .LT. 0.0)  CROSS = .TRUE.                          DIS20130
        DIFF(1) = X                                                          DIS20140
        IF (DABS(DIFF(1)) .GE. CONV1) DONE = .FALSE.                         DIS20150
                                                                             DIS20160
        IF (DONE) THEN                                                       DIS20170
            FACTOR(1) = 1.0                                                  DIS20180
        ELSE IF (ITER .GT. 7) THEN                                           DIS20190
          X = ANALCO / S(1)                                                  DIS20200
          CALL AITLIM (FACTOR(1), X, CROSS)                                  DIS20210
        END IF                                                               DIS20220
        X = FACTOR(1)                                                        DIS20230
                                                                             DIS20240
        IF (S(1) .GT. CPUMIN) THEN                                           DIS20250
          TITR(1) = TITR(1) - (X * (1.0 - (ANALCO / S(1))) * TITR(1))        DIS20260
        ELSE                                                                 DIS20270
          TITR(1) = ANALCO                                                   DIS20280
        END IF                                                               DIS20290
      END IF                                                                 DIS20300
                                                                             DIS20310
      IF (EXELT(6) .GE. CPUMIN) THEN                                         DIS20320
        X = (S(2) - EXELT(6)) / EXELT(6)                                     DIS20330
        CROSS = .FALSE.                                                      DIS20340
        IF ((X * DIFF(2)) .LT. 0.0)  CROSS = .TRUE.                          DIS20350
        DIFF(2) = X                                                          DIS20360
        IF (DABS(DIFF(2)) .GE. CONV1) DONE = .FALSE.                         DIS20370
                                                                             DIS20380
        IF (DONE) THEN                                                       DIS20390
            FACTOR(2) = 1.0                                                  DIS20400
        ELSE IF (ITER .GT. 7) THEN                                           DIS20410
          X = EXELT(6) / S(2)                                                DIS20420
          CALL AITLIM (FACTOR(2), X, CROSS)                                  DIS20430
        END IF                                                               DIS20440
        X = FACTOR(2)                                                        DIS20450
        IF (S(2) .GT. CPUMIN) THEN                                           DIS20460
          TITR(2) = TITR(2) - (X * (1.0 - (EXELT(6) / S(2))) * TITR(2))      DIS20470
```

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  ELSE                                                                  DIS20480
    TITR(2) = EXELT(6)                                                  DIS20490
  END IF                                                                DIS20500
END IF                                                                  DIS20510
                                                                        DIS20520
IF (EXELT(22) .GE. CPUMIN) THEN                                         DIS20530
  X = (S(3) - EXELT(22)) / EXELT(22)                                    DIS20540
  CROSS = .FALSE.                                                       DIS20550
  IF ((X * DIFF(3)) .LT. 0.0)  CROSS = .TRUE.                           DIS20560
  DIFF(3) = X                                                           DIS20570
  IF (DABS(DIFF(3)) .GE. CONV1) DONE = .FALSE.                          DIS20580
  IF (DONE) THEN                                                        DIS20590
      FACTOR(3) = 1.0                                                   DIS20600
  ELSE IF (ITER .GT. 7) THEN                                            DIS20610
    X = EXELT(22) / S(3)                                                DIS20620
    CALL AITLIM (FACTOR(3), X, CROSS)                                   DIS20630
  END IF                                                                DIS20640
  X = FACTOR(3)                                                         DIS20650
  IF (S(3) .GT. CPUMIN) THEN                                            DIS20660
    TITR(3) = TITR(3) - (X * (1.0 - (EXELT(22) / S(3))) * TITR(3))      DIS20670
  ELSE                                                                  DIS20680
    TITR(3) = EXELT(22)                                                 DIS20690
  END IF                                                                DIS20700
END IF                                                                  DIS20710
                                                                        DIS20720
IF (EXELT(21) .GE. CPUMIN) THEN                                         DIS20730
  X = (S(4) - EXELT(21)) / EXELT(21)                                    DIS20740
  CROSS = .FALSE.                                                       DIS20750
  IF ((X * DIFF(4)) .LT. 0.0)  CROSS = .TRUE.                           DIS20760
  DIFF(4) = X                                                           DIS20770
  IF (DABS(DIFF(4)) .GE. CONV1) DONE = .FALSE.                          DIS20780
  IF (DONE) THEN                                                        DIS20790
      FACTOR(4) = 1.0                                                   DIS20800
  ELSE IF (ITER .GT. 7) THEN                                            DIS20810
    X = EXELT(21) / S(4)                                                DIS20820
    CALL AITLIM (FACTOR(4), X, CROSS)                                   DIS20830
  END IF                                                                DIS20840
  X = FACTOR(4)                                                         DIS20850
  IF (S(4) .GT. CPUMIN) THEN                                            DIS20860
    TITR(4) = TITR(4) - (X * (1.0 - (EXELT(21) / S(4))) * TITR(4))      DIS20870
  ELSE                                                                  DIS20880
    TITR(4) = EXELT(21)                                                 DIS20890
  END IF                                                                DIS20900
END IF                                                                  DIS20910
                                                                        DIS20920
IF (EXELT(5) .GE. CPUMIN) THEN                                          DIS20930
  X = (S(5) - EXELT(5)) / EXELT(5)                                      DIS20940
  CROSS = .FALSE.                                                       DIS20950
  IF ((X * DIFF(5)) .LT. 0.0)  CROSS = .TRUE.                           DIS20960
  DIFF(5) = X                                                           DIS20970
  IF (DABS(DIFF(5)) .GE. CONV1) DONE = .FALSE.                          DIS20980
  IF (DONE) THEN                                                        DIS20990
    FACTOR(5) = 1.0                                                     DIS21000
  ELSE IF (ITER .GT. 7) THEN                                            DIS21010
    X = EXELT(5) / S(5)                                                 DIS21020
    CALL AITLIM (FACTOR(5), X, CROSS)                                   DIS21030
  END IF                                                                DIS21040
  X = FACTOR(5)                                                         DIS21050
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  IF (S(5) .GT. CPUMIN) THEN                                          DIS21060
    TITR(5) = TITR(5) - (X * (1.0 - (EXELT(5) / S(5))) * TITR(5))     DIS21070
  ELSE                                                                DIS21080
    TITR(5) = EXELT(5)                                                DIS21090
  END IF                                                              DIS21100
END IF                                                                DIS21110
                                                                      DIS21120
IF (EXELT(26) .GE. CPUMIN) THEN                                       DIS21130
  X = (S(6) - EXELT(26)) / EXELT(26)                                  DIS21140
  CROSS = .FALSE.                                                     DIS21150
  IF ((X * DIFF(6)) .LT. 0.0)  CROSS = .TRUE.                         DIS21160
  DIFF(6) = X                                                         DIS21170
  IF (DABS(DIFF(6)) .GE. CONV1) DONE = .FALSE.                        DIS21180
  IF (DONE) THEN                                                      DIS21190
    FACTOR(6) = 1.0                                                   DIS21200
  ELSE IF (ITER .GT. 7) THEN                                          DIS21210
    X = EXELT(26) / S(6)                                              DIS21220
    CALL AITLIM (FACTOR(6), X, CROSS)                                 DIS21230
  END IF                                                              DIS21240
  X = FACTOR(6)                                                       DIS21250
  IF (S(6) .GT. CPUMIN) THEN                                          DIS21260
    TITR(6) = TITR(6) - (X * (1.0 - (EXELT(26) / S(6))) * TITR(6))DIS21270
  ELSE                                                                DIS21280
    TITR(6) = EXELT(26)                                               DIS21290
  END IF                                                              DIS21300
END IF                                                                DIS21310
                                                                      DIS21320
IF (EXELT(25) .GT. CPUMIN) THEN                                       DIS21330
  X = (S(7) - EXELT(25)) / EXELT(25)                                  DIS21340
  CROSS = .FALSE.                                                     DIS21350
  IF ((X * DIFF(7)) .LT. 0.0)  CROSS = .TRUE.                         DIS21360
  DIFF(7) = X                                                         DIS21370
  IF (DABS(DIFF(7)) .GE. CONV1) DONE = .FALSE.                        DIS21380
  IF (DONE) THEN                                                      DIS21390
    FACTOR(7) = 1.0                                                   DIS21400
  ELSE IF (ITER .GT. 7) THEN                                          DIS21410
    X = EXELT(25) / S(7)                                              DIS21420
    CALL AITLIM (FACTOR(7), X, CROSS)                                 DIS21430
  END IF                                                              DIS21440
  X = FACTOR(7)                                                       DIS21450
  IF (S(7) .GT. CPUMIN) THEN                                          DIS21460
    TITR(7) = TITR(7) - (X * (1.0 - (EXELT(25) / S(7))) * TITR(7))DIS21470
  ELSE                                                                DIS21480
    TITR(7) = EXELT(25)                                               DIS21490
  END IF                                                              DIS21500
END IF                                                                DIS21510
                                                                      DIS21520
IF (EXELT(30) .GT. CPUMIN) THEN                                       DIS21530
  X = (S(8) - EXELT(30)) / EXELT(30)                                  DIS21540
  CROSS = .FALSE.                                                     DIS21550
  IF ((X * DIFF(8)) .LT. 0.0)  CROSS = .TRUE.                         DIS21560
  DIFF(8) = X                                                         DIS21570
  IF (DABS(DIFF(8)) .GE. CONV1) DONE = .FALSE.                        DIS21580
  IF (DONE) THEN                                                      DIS21590
    FACTOR(8) = 1.0                                                   DIS21600
  ELSE IF (ITER .GT. 7) THEN                                          DIS21610
    X = EXELT(30) / S(8)                                              DIS21620
    CALL AITLIM (FACTOR(8), X, CROSS)                                 DIS21630
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  END IF                                                                DIS21640
  X = FACTOR(8)                                                         DIS21650
  IF (S(8) .GT. CPUMIN) THEN                                            DIS21660
    TITR(8) = TITR(8) - (X * (1.0 - (EXELT(30) / S(8))) * TITR(8))DIS21670
  ELSE                                                                  DIS21680
    TITR(8) = EXELT(30)                                                 DIS21690
  END IF                                                                DIS21700
END IF                                                                  DIS21710
                                                                        DIS21720
IF (EXELT(31) .GT. CPUMIN) THEN                                         DIS21730
  DIFF(9) = (S(9) - EXELT(31)) / EXELT(31)                              DIS21740
  X = (S(9) - EXELT(31)) / EXELT(31)                                    DIS21750
  CROSS = .FALSE.                                                       DIS21760
  IF ((X * DIFF(9)) .LT. 0.0)  CROSS = .TRUE.                           DIS21770
  DIFF(9) = X                                                           DIS21780
  IF (DABS(DIFF(9)) .GE. CONV1) DONE = .FALSE.                          DIS21790
  IF (DONE) THEN                                                        DIS21800
    FACTOR(9) = 1.0                                                     DIS21810
  ELSE IF (ITER .GT. 7) THEN                                            DIS21820
    X = EXELT(31) / S(9)                                                DIS21830
    CALL AITLIM (FACTOR(9), X, CROSS)                                   DIS21840
  END IF                                                                DIS21850
  X = FACTOR(9)                                                         DIS21860
  IF (S(9) .GT. CPUMIN) THEN                                            DIS21870
    TITR(9) = TITR(9) - (X * (1.0 - (EXELT(31) / S(9))) * TITR(9))DIS21880
  ELSE                                                                  DIS21890
    TITR(9) = EXELT(31)                                                 DIS21900
  END IF                                                                DIS21910
END IF                                                                  DIS21920
                                                                        DIS21930
IF (EXELT(33) .GT. CPUMIN) THEN                                         DIS21940
  X = (S(10) - EXELT(33)) / EXELT(33)                                   DIS21950
  CROSS = .FALSE.                                                       DIS21960
  IF ((X * DIFF(10)) .LT. 0.0)  CROSS = .TRUE.                          DIS21970
  DIFF(10) = X                                                          DIS21980
  IF (DABS(DIFF(10)) .GE. CONV1) DONE = .FALSE.                         DIS21990
  IF (DONE) THEN                                                        DIS22000
    FACTOR(10) = 1.0                                                    DIS22010
  ELSE IF (ITER .GT. 7) THEN                                            DIS22020
    X = EXELT(33) / S(10)                                               DIS22030
    CALL AITLIM (FACTOR(10), X, CROSS)                                  DIS22040
  END IF                                                                DIS22050
  X = FACTOR(10)                                                        DIS22060
  IF (S(10) .GT. CPUMIN) THEN                                           DIS22070
    TITR(10) = TITR(10) - (X * (1.0 - (EXELT(33) / S(10))) *            DIS22080
               TITR(10))                                                DIS22090
  ELSE                                                                  DIS22100
    TITR(10) = EXELT(33)                                                DIS22110
  END IF                                                                DIS22120
END IF                                                                  DIS22130
                                                                        DIS22140
IF (EXELT(34) .GT. CPUMIN) THEN                                         DIS22150
  X = (S(11) - EXELT(34)) / EXELT(34)                                   DIS22160
  CROSS = .FALSE.                                                       DIS22170
  IF ((X * DIFF(11)) .LT. 0.0)  CROSS = .TRUE.                          DIS22180
  DIFF(11) = X                                                          DIS22190
  IF (DABS(DIFF(11)) .GE. CONV1) DONE = .FALSE.                         DIS22200
  IF (DONE) THEN                                                        DIS22210
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          FACTOR(11) = 1.0                                                  DIS22220
        ELSE IF (ITER .GT. 7) THEN                                          DIS22230
          X = EXELT(34) / S(11)                                             DIS22240
          CALL AITLIM (FACTOR(11), X, CROSS)                                DIS22250
        END IF                                                              DIS22260
        X = FACTOR(11)                                                      DIS22270
        IF (S(11) .GT. CPUMIN) THEN                                         DIS22280
          TITR(11) = TITR(11) - (X * (1.0 - (EXELT(34) / S(11))) *          DIS22290
     .               TITR(11))                                              DIS22300
        ELSE                                                                DIS22310
          TITR(11) = EXELT(34)                                              DIS22320
        END IF                                                              DIS22330
      END IF                                                                DIS22340
                                                                            DIS22350
      IF (ITER .GE. 100) DONE = .TRUE.                                      DIS22360
                                                                            DIS22370
      IF (IPRIN1 .NE. 0) THEN                                               DIS22380
        IF (ITER .EQ. 1 .OR. DONE .OR. MOD(ITER,10) .EQ. 0) THEN            DIS22390
          IF (IPGLN .GT. 57) THEN                                           DIS22400
            CALL PAGE                                                       DIS22410
            WRITE (UNO, 1001) TITLE, TITMIX                                 DIS22420
            WRITE (UNO, 1002) TEMP                                          DIS22430
            WRITE (UNO, 1003)                                               DIS22440
            WRITE (UNO, 1004) CR                                            DIS22450
            IPGLN = IPGLN + 9                                               DIS22460
          END IF                                                            DIS22470
          WRITE (UNO,1005) ITER, (DIFF(I),I=1,11)                           DIS22480
          IPGLN = IPGLN + 1                                                 DIS22490
        END IF                                                              DIS22500
      END IF                                                                DIS22510
                                                                            DIS22520
C -----------------------------------------------------------------------|  DIS22530
C     GO BACK OR QUIT                                                     |  DIS22540
C -----------------------------------------------------------------------|  DIS22550
                                                                            DIS22560
      IF (.NOT. DONE) GO TO 30                                              DIS22570
                                                                            DIS22580
      IF (ITER .GE. 100) THEN                                               DIS22590
        IF (IPGLN .GT. 59) THEN                                             DIS22600
          CALL PAGE                                                         DIS22610
          WRITE (UNO, 1001) TITLE, TITMIX                                   DIS22620
          WRITE (UNO, 1002) TEMP                                            DIS22630
          IPGLN = IPGLN + 5                                                 DIS22640
        END IF                                                              DIS22650
        WRITE (UNO,1006)                                                    DIS22660
        IPGLN = IPGLN + 2                                                   DIS22670
      END IF                                                                DIS22680
                                                                            DIS22690
      IF (IPRIN1 .NE. 0) THEN                                               DIS22700
        IF (IPGLN .GT. 57) THEN                                             DIS22710
          CALL PAGE                                                         DIS22720
          WRITE (UNO, 1001) TITLE, TITMIX                                   DIS22730
          WRITE (UNO, 1002) TEMP                                            DIS22740
          IPGLN = IPGLN + 5                                                 DIS22750
        END IF                                                              DIS22760
        WRITE (UNO,1007) ITER, PH                                           DIS22770
        IPGLN = IPGLN + 2                                                   DIS22780
      END IF                                                                DIS22790
```

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                                                                      DIS22800
      HTOT  = M(7)   +     M(8)   + 4.0*M(11)  + 2.0*M(28)  +         DIS22810
     .    2.0*M(33)  + 3.0*M(49)  +     M(52)  +     M(56)  +         DIS22820
     .        M(59)  + 2.0*M(60)  +     M(73)  + 3.0*M(74)  +         DIS22830
     .    2.0*M(90)  + 3.0*M(91)  +     M(92)  +     M(93)  +         DIS22840
     .    2.0*M(94)  + 3.0*M(95)  +     M(96)  + 2.0*M(97)  +         DIS22850
     .        M(99)  + 2.0*M(100) +     M(101) +     M(103) +         DIS22860
     .        M(104) + 4.0*M(110) + 3.0*M(111) +     M(115) +         DIS22870
     .        M(117) +     M(121) +     M(126) + 2.0*M(127) +         DIS22880
     .        M(132) +     M(134) +     M(139) +     M(143)           DIS22890
      HTOT  = HTOT   +                                                DIS22900
     .        M(145) +                 M(156) +     M(182) +         DIS22910
     .    2.0*M(183) + 3.0*M(184) + 4.0*M(185) +     M(202) +         DIS22920
     .    2.0*M(203) + 2.0*M(204) + 4.0*M(205) + 6.0*M(206) +         DIS22930
     .        M(213) + 2.0*M(214) + 3.0*M(215) + 4.0*M(216) +         DIS22940
     .        M(217) +     M(228) +     M(247) + 2.0*M(248) +         DIS22950
     .        M(266) + 2.0*M(267) + 2.0*M(286) + 3.0*M(287) +         DIS22960
     .    2.0*M(290) + 3.0*M(291) +     M(292) +     M(295) +         DIS22970
     .        M(MXSP+34)          +     M(MXSP+40)                    DIS22980
                                                                      DIS22990
      OHTOT = M(9)   + 3.0*M(31)  +     M(38)  + 2.0*M(39)  +         DIS23000
     .    4.0*M(40)  +     M(53)  +     M(57)  +     M(69)  +         DIS23010
     .        M(75)  + 2.0*M(76)  +     M(77)  +     M(85)  +         DIS23020
     .    2.0*M(86)  + 3.0*M(87)  + 4.0*M(88)  + 4.0*M(89)  +         DIS23030
     .        M(118) +     M(123) +     M(135) +     M(147) +         DIS23040
     .        M(154) +     M(165) + 2.0*M(166) +     M(170)           DIS23050
      OHTOT = OHTOT  +                                                DIS23060
     .    2.0*M(171) + 3.0*M(172) + 4.0*M(173) + 5.0*M(174) +         DIS23070
     .   15.0*M(188) +     M(189) + 2.0*M(190) + 2.0*M(191) +         DIS23080
     .    5.0*M(192) + 7.0*M(193) +     M(220) + 2.0*M(221) +         DIS23090
     .    3.0*M(222) +     M(223) +     M(289) +     M(293) +         DIS23100
     .    2.0*M(294) +     M(295) +     M(MXSP+35)                    DIS23110
                                                                      DIS23120
      IF (PALFA(6) .GT. CPUMIN .AND. DABS(PALFA(6)-ALFA(6))           DIS23130
     .    .GT. 1.0D-2*PALFA(6) .AND. IPIT .EQ. 1) THEN                DIS23140
        ALFA(6) = PALFA(6)                                            DIS23150
      END IF                                                          DIS23160
      IF (PALFA(1) .GT. CPUMIN .AND. DABS(PALFA(1)-ALFA(1))           DIS23170
     .    .GT. 1.0D-2*PALFA(1) .AND. IPIT .EQ. 1) THEN                DIS23180
        ALFA(1) = PALFA(1)                                            DIS23190
      END IF                                                          DIS23200
                                                                      DIS23210
      RETURN                                                          DIS23220
                                                                      DIS23230
 1000 FORMAT (/, 2X,'SOLMINEQ.87 (VERSION:  ',A14,                    DIS23240
     .            ') - SOLUTION-MINERAL-EQUILIBRIUM COMPUTATIONS',    DIS23250
     .       /,A1,2X,77('_'),///)                                     DIS23260
 1001 FORMAT (' SAMPLE IDENT:- ',A80,/,20X,A40)                       DIS23270
 1002 FORMAT (//,6X,'ITERATIVE CONVERGENCE TEST AT TEMPERATURE =',F8.2) DIS23280
 1003 FORMAT (//, 1X, 'ITER', 1X,  'CARBONATE', 3X,    'SULFATE', 4X, DIS23290
     .           'FLUORIDE', 2X,  'PHOSPHATE', 3X,   'CHLORIDE', 3X, DIS23300
     .            'ACETATE', 4X,    'SULFIDE', 4X,    'OXYLATE', 3X, DIS23310
     .          'SUCCINATE', 2X, 'USR-DEF #1', 1X, 'USR-DEF #2')     DIS23320
 1004 FORMAT  (A1, '____', 1X, 11('__________', 1X))                  DIS23330
 1005 FORMAT  (1X, I3, 2X, 1P, 11(E10.3, 1X))                        DIS23340
 1006 FORMAT ('  *** NO CONVERGENCE IN 100 ITERATIONS DURING SPECIES', DIS23350
     .        ' DISTRIBUTION ***',/,13X,'RESULTS MAY BE IN ERROR')    DIS23360
 1007 FORMAT (/,6X, 'Total number of iterations = ',I3,               DIS23370
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     .              ' at pH = ',F5.2)                                    DIS23380
 1008 FORMAT (/,6X,' *** ACT. OF SO4 FROM PITZER ***',E12.5)             DIS23390
 1009 FORMAT (/,6X,' *** ACT. OF Ca FROM PITZER ***',E12.5)              DIS23400
                                                                         DIS23410
      END                                                                DIS23420


      SUBROUTINE DPVT (TC, TISA, PBAR, VDEN)                            DPV 0010
C ======================================================================|DPV 0020
C     Routine dpvt calculates the vapor pressure and vapor density      |DPV 0030
C     given tc and the ionic strength of the solution.                  |DPV 0040
C ----------------------------------------------------------------------|DPV 0050
C     ALPHA     DBL   Coefficient of thermal expansion                  |DPV 0060
C     AW        DBL   Activity of water                                 |DPV 0070
C     BETAG     DBL   Coefficient of compressibility                    |DPV 0080
C     GG        DBL   Intermediate storage variable                     |DPV 0090
C     GL0       DBL   Initial gibbs free energy per mole                |DPV 0100
C     GX        DBL   Gibbs free energy per mole                        |DPV 0110
C     I         INT   Loop variable                                     |DPV 0120
C     P0        DBL   Saturation pressure                               |DPV 0130
C     PBAR      DBL   Pressure in bars                                  |DPV 0140
C     PHI       DBL   Osmotic coefficient                               |DPV 0150
C     R         DBL   Gas constant                                      |DPV 0160
C     RQ        DBL   Gas constant in cubic centimeters                 |DPV 0170
C     T         DBL   Temperature in kelvin                             |DPV 0180
C     TC        DBL   Temperature in celcius                            |DPV 0190
C     TISA      DBL   Sum of Molality * charge / 2                      |DPV 0200
C     VDEN      DBL   Vapor density                                     |DPV 0210
C     XG        DBL   Density                                           |DPV 0220
C     XS        DBL   Intermediate storage variable                     |DPV 0230
C     YP        DBL   Low temperature fit constants                     |DPV 0240
C     ZP        DBL   High temperature fit constants                    |DPV 0250
C ----------------------------------------------------------------------|DPV 0260
                                                                         DPV 0270
      INTEGER I                                                          DPV 0280
                                                                         DPV 0290
      DOUBLE PRECISION ALPHA, AW, BETAG, GG, GL0, GX                     DPV 0300
      DOUBLE PRECISION P0, PBAR, PHI, R, RQ                              DPV 0310
      DOUBLE PRECISION T, TC, TISA, VDEN                                 DPV 0320
      DOUBLE PRECISION XG, XS, YP(57), ZP(57)                            DPV 0330
                                                                         DPV 0340
      EXTERNAL NACALC, PSAT, WAPVT                                       DPV 0350
                                                                         DPV 0360
      INTRINSIC DABS, DEXP, DLOG                                         DPV 0370
                                                                         DPV 0380
      DATA YP /-71659.702,          2.3483335,       -8.3668484D-5,      DPV 0390
     .          2.4018168D-9,  624.88205,          -5.3697119D-4,      DPV 0400
     .          3.5126966D-7,    0.,             -110.74702,           DPV 0410
     .          0.038900801,     2.6973456D-6,     -6.2746876D-10,      DPV 0420
     .         -1.5267612D-5,    0.,              516.99706,           DPV 0430
     .         -5.9960300D6,  -656.81518,          24.879183,          DPV 0440
     .         -2.1552731D-5,    5.0166855D-8,      0.,                DPV 0450
     .         -4.4640952,       0.011087099,      -6.4479761D-8,      DPV 0460
     .         -2.3234032D-10,   0.,               -5.2194871D-6,      DPV 0470
     .          2.4445210D-10,   2.8527066D-13,    -1.5696231,         DPV 0480
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     .              2.2337864D-3,   -6.3933891D-7,     4.5270573D-11,   DPV 0490
     .              5.4151933,       0.,               0.,              DPV 0500
     .              0.,            119.31966,         -0.48309327,       DPV 0510
     .              1.4068095D-3,   -4.2345814,       -6.1084589,        DPV 0520
     .              0.40743803,     -6.8152430D-6,    -0.075354649,      DPV 0530
     .              1.2609014D-4,    6.2480692D-8,     1.8994373D-8,     DPV 0540
     .             -1.0731284D-10,   0.32136572,      -2.5382945D-4,     DPV 0550
     .              0.,              0.,               1.,               DPV 0560
     .              1.,              1.,               1./               DPV 0570
      DATA ZP /-71637.375,            2.2209012,       -7.7991396D-5,     DPV 0580
     .             -4.8099272D-9,   624.68121,         6.0159787D-4,      DPV 0590
     .              3.4069074D-7,    2.1962044D-11, -110.74702,          DPV 0600
     .              0.039494473,    -6.5313475D-7,    -6.4781894D-10,    DPV 0610
     .             -1.5842012D-5,    3.2452006D-9,   516.99706,          DPV 0620
     .             -5.9960301D6,  -656.81518,          24.86913,         DPV 0630
     .              5.3812753D-5,   -5.5887470D-8,     6.5893263D-12,    DPV 0640
     .             -4.4640952,       0.011109914,    -2.6573399D-7,     DPV 0650
     .              1.7460070D-10,   1.0462619D-14,   -5.3070129D-6,     DPV 0660
     .              8.6340233D-10,  -4.1785962D-13,   -1.579366,         DPV 0670
     .              2.2022821D-3,   -1.3105503D-7,    -6.3813683D-11,    DPV 0680
     .              9.706578,       -2.6860396D-2,     1.5344744D-5,     DPV 0690
     .             -3.2153983D-9,   119.31966,        -0.48309327,       DPV 0700
     .              1.4068095D-3,   -4.2345814,       -6.1084589,        DPV 0710
     .              0.40217793,      2.2902837D-5,    -0.075354649,      DPV 0720
     .              1.5317673D-4,   -9.0550901D-8,    -1.5386008D-8,     DPV 0730
     .              8.6926600D-11,   0.35310414,      -4.3314252D-4,     DPV 0740
     .             -0.091871455,     5.1904777D-4,     1.,               DPV 0750
     .              1.,              1.,               1./               DPV 0760
                                                                         DPV 0770
C ========================================================================|DPV 0780
                                                                         DPV 0790
C ------------------------------------------------------------------------|DPV 0800
C     Nacalc calculates the osmotic coefficients of the nacl solution    |DPV 0810
C     and the free energy of pure water at the saturation pressure of    |DPV 0820
C     pure water and temperature.                                        |DPV 0830
C ------------------------------------------------------------------------|DPV 0840
                                                                         DPV 0850
      IF (TC .LT. 65.1) THEN                                             DPV 0860
        CALL NACALC (TC, TISA, PBAR, PHI, YP, GL0)                       DPV 0870
      ELSE                                                               DPV 0880
        CALL NACALC (TC, TISA, PBAR, PHI, ZP, GL0)                       DPV 0890
      END IF                                                             DPV 0900
                                                                         DPV 0910
C ------------------------------------------------------------------------|DPV 0920
C     Calculate water activity from phi.                                 |DPV 0930
C ------------------------------------------------------------------------|DPV 0940
                                                                         DPV 0950
      AW = DEXP(-3.60304D-2 * PHI * TISA)                                DPV 0960
                                                                         DPV 0970
      CALL PSAT (TC, P0)                                                 DPV 0980
                                                                         DPV 0990
      R  =  8.31424                                                      DPV 1000
      RQ = 83.14699                                                      DPV 1010
      T  = TC + 273.15                                                   DPV 1020
                                                                         DPV 1030
C ------------------------------------------------------------------------|DPV 1040
C     Calculate an initial guess for the density of the vapor from the   |DPV 1050
C     ideal gas law.                                                     |DPV 1060
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C -----------------------------------------------------------------|DPV 1070
                                                                    DPV 1080
      XG = 18.0153 * P0 / (RQ * T)                                  DPV 1090
                                                                    DPV 1100
C -----------------------------------------------------------------|DPV 1110
C     Calculate the free energy of the salt solution from the free  |DPV 1120
C     energy of pure liquid water and the activity of water in      |DPV 1130
C     solution.                                                     |DPV 1140
C -----------------------------------------------------------------|DPV 1150
                                                                    DPV 1160
      GG = GL0 + (R * T) * DLOG(AW)                                 DPV 1170
                                                                    DPV 1180
C -----------------------------------------------------------------|DPV 1190
C     Use wapvt to calculate the vapor pressure and vapor density at|DPV 1200
C     tc.  wapvt is used iteratively along with a free energy       |DPV 1210
C     adjustment of the vapor density until the vapor density       |DPV 1220
C     converges.  this requires that the free energy of the liquid and|DPV 1230
C     vapor are the same and that the equilibrium vapor pressure and|DPV 1240
C     density have been determined.                                 |DPV 1250
C -----------------------------------------------------------------|DPV 1260
                                                                    DPV 1270
      DO 10 I = 1, 100                                              DPV 1280
        CALL WAPVT (TC, XG, PBAR, BETAG, GX, ALPHA)                 DPV 1290
        XS = XG                                                     DPV 1300
        XG = XG * DEXP((GG - GX) / (R * T))                         DPV 1310
        IF (DABS((XG-XS)/XS) .LT. 1.0D-8) GO TO 20                  DPV 1320
   10 CONTINUE                                                      DPV 1330
                                                                    DPV 1340
   20 CONTINUE                                                      DPV 1350
      VDEN = XG                                                     DPV 1360
                                                                    DPV 1370
      RETURN                                                        DPV 1380
      END                                                           DPV 1390
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      SUBROUTINE GASES (TC, PTOTAL, MNACLD, PH2O, FCCSAT, IGAS, IMAX,   GAS 0010
     .                  IPRIN2)                                        GAS 0020
C ================================================================|GAS 0030
C     Partitions gases between the oil, water, and gas phases       |GAS 0040
C -----------------------------------------------------------------|GAS 0050
C     A          DBL   Temperary working variable                  |GAS 0060
C     ANALM      DBL   Analyzed molality of species i              |GAS 0070
C     B          DBL   Temperary working variable                  |GAS 0080
C     C          DBL   Temperary working variable                  |GAS 0090
C     CH4DIF     DBL   Difference in total CH4 ... zero is root    |GAS 0100
C     CH4TRY     DBL   Next value of CH4 to try                    |GAS 0110
C     CO2DIF     DBL   Difference in total CO2 ... zero is root    |GAS 0120
C     CO2TRY     DBL   Next value of CO2 to try                    |GAS 0130
C     CPUMIN     DBL   Smallest positive real value program uses   |GAS 0140
C     D          DBL   Temperary working variable                  |GAS 0150
C     DCH4       DBL   Concentration of CH4 lost before pH measurement|GAS 0160
C     DCO2       DBL   Concentration of CO2 lost before pH measurement|GAS 0170
C     DH2S       DBL   Concentration of H2S lost before pH measurement|GAS 0180
C     DONE       LOG   Done?                                       |GAS 0190
C     E          DBL   Temperary working variable                  |GAS 0200
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C     EXELT     DBL   Total amount of components                          |GAS 0210
C     FCCSAT    DBL   Zero Test value                                    |GAS 0220
C     G         DBL   Temperary working variable                         |GAS 0230
C     H2SDIF    DBL   Difference in total H2S ... zero is root           |GAS 0240
C     H2STRY    DBL   Next value of H2S to try                           |GAS 0250
C     HTOT      DBL   Current sum of all H+ in solution                  |GAS 0260
C     HTOTI     DBL   Target sum of all H+ in solution                   |GAS 0270
C     I         INT   Loop counter                                        GAS 0280
C     IGAS      INT   Loop variable for gas option                       |GAS 0290
C     IMAX      INT   Max number of iterations for various options       |GAS 0300
C     IPAGE     INT   Current page number of output file                 |GAS 0310
C     IPGLN     INT   Current line number of the output file             |GAS 0320
C     IPHASE    INT   Switch used for GAS options                        |GAS 0330
C     IPRIN2    INT   Print switch                                       |GAS 0340
C     J         DBL   Temperary working variable                         |GAS 0350
C     JCO3      INT   Switch to control printing of some headings        |GAS 0360
C     KCH4OL    DBL   Henry's law coefficient for CH4 in oil             |GAS 0370
C     KCH4W     DBL   Henry's law coefficient for CH4 in water           |GAS 0380
C     KCO2OL    DBL   Henry's law coefficient for CO2 in oil             |GAS 0390
C     KCO2W     DBL   Henry's law coefficient for CO2 in water           |GAS 0400
C     KH2SOL    DBL   Henry's law coefficient for H2S in oil             |GAS 0410
C     KH2SW     DBL   Henry's law coefficient for H2S in water           |GAS 0420
C     KHCH4     DBL   Function to Calculate the Henry's law K for CH4    |GAS 0430
C     KHCO2     DBL   Function to Calculate the Henry's law K for CO2    |GAS 0440
C     KHH2S     DBL   Function to Calculate the Henry's law K for H2S    |GAS 0450
C     M         DBL   Calculated molality of aqueous species             |GAS 0460
C     MNACLD    DBL   Sum of Molality * charge / 2                       |GAS 0470
C     NMAX      INT   General array dimension to allow easy expansion    |GAS 0480
C     OHTOT     DBL   Total OH in system                                 |GAS 0490
C     OHTOTI    DBL   initial total OH in system                         |GAS 0500
C     ORGCH4    DBL   Initial amount of CH4 in system                    |GAS 0510
C     ORGCO2    DBL   Initial amount of CO2 in system                    |GAS 0520
C     ORGH2S    DBL   Initial amount of H2S in system                    |GAS 0530
C     ORGT1     DBL   Original TOTEL(1)                                  |GAS 0540
C     PCH4W     DBL   Partial Pressure of Methane                        |GAS 0550
C     PCO2W     DBL   Partial Pressure of Carbon Dioxide                 |GAS 0560
C     PH2O      DBL   Partial Pressure of Water                          |GAS 0570
C     PH2SW     DBL   Partial Pressure of Hydrogen Sulphide              |GAS 0580
C     PTOTAL    DBL   Total pressure on the system                       |GAS 0590
C     ROOT      DBL   Root of the equation                               |GAS 0600
C     SCO2      DBL   Sum of CO2 species                                 |GAS 0610
C     STEP      DBL   Step adjustment for the moles of each gas          |GAS 0620
C     TC        DBL   Temperature in deg C                               |GAS 0630
C     TCH4M     DBL   Moles CH4 distributed between oil, water, vapor    |GAS 0640
C     TCH4O     DBL   Moles CH4 in oil                                   |GAS 0650
C     TCH4V     DBL   Moles CH4 in vapor                                 |GAS 0660
C     TCH4W     DBL   Moles CH4 in water                                 |GAS 0670
C     TCO2M     DBL   Moles CO2 distributed between oil, water, vapor    |GAS 0680
C     TCO2O     DBL   Moles CO2 in oil                                   |GAS 0690
C     TCO2V     DBL   Moles CO2 in vapor                                 |GAS 0700
C     TCO2W     DBL   Moles CO2 in water                                 |GAS 0710
C     TEST      DBL   Insure sum of partitioned moles equal total moles  |GAS 0720
C     TH2SM     DBL   Moles H2S distributed between oil, water, vapor    |GAS 0730
C     TH2SO     DBL   Moles H2S in oil                                   |GAS 0740
C     TH2SV     DBL   Moles H2S in vapor                                 |GAS 0750
C     TH2SW     DBL   Moles H2S in water                                 |GAS 0760
C     TITR      DBL   Iteration array in DISTRB, used for guesses        |GAS 0770
C     TK        DBL   Temperature in deg K                               |GAS 0780
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C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                    |GAS 0790
C     UNO       INT   File unit assigned for output file                  |GAS 0800
C     WROIL     DBL   Oil to water weight ratio                           |GAS 0810
C -------------------------------------------------------------------------|GAS 0820
                                                                           GAS 0830
      INTEGER NMAX, UNO                                                    GAS 0840
      DOUBLE PRECISION CPUMIN                                              GAS 0850
      PARAMETER (NMAX = 340, UNO = 6, CPUMIN = 1.0D-35)                    GAS 0860
                                                                           GAS 0870
      INTEGER I, IGAS, IMAX, IOPT, IPAGE, IPGLN, IPHASE, IPRIN2            GAS 0880
      INTEGER PHHIT, PPHHIT, JCO3                                          GAS 0890
                                                                           GAS 0900
      LOGICAL DONE                                                         GAS 0910
                                                                           GAS 0920
      DOUBLE PRECISION A, ALFA(NMAX), ANALM(NMAX), B                       GAS 0930
      DOUBLE PRECISION C, CH4DIF(3), CH4TRY(3), CO2F                       GAS 0940
      DOUBLE PRECISION CO2DIF(3), CO2TRY(3), CUNITS(NMAX)                  GAS 0950
      DOUBLE PRECISION D, DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3            GAS 0960
      DOUBLE PRECISION DCH4, DDCH4, E, EXELT(35), FCCSAT, FIXIT, G         GAS 0970
      DOUBLE PRECISION H2SDIF(3), H2STRY(3), HTOT, HTOTI, J                GAS 0980
      DOUBLE PRECISION KHCH4, KHCO2, KHH2S, KCH4OL, KCO2OL, KH2SOL         GAS 0990
      DOUBLE PRECISION KCH4W, KCO2W, KH2SW                                 GAS 1000
      DOUBLE PRECISION M(NMAX), MNACLD, OHTOT, OHTOTI                      GAS 1010
      DOUBLE PRECISION ORGCH4, ORGCO2, ORGH2S, ORGT1                       GAS 1020
      DOUBLE PRECISION PCH4W, PCO2W, PH2SW, PH, PH2O, DSEP, PTOTAL         GAS 1030
      DOUBLE PRECISION ROOT, SCO2, STEP(4)                                 GAS 1040
      DOUBLE PRECISION TC, TCH4M, TCO2M, TH2SM                             GAS 1050
      DOUBLE PRECISION TCO2O, TCO2V, TCO2W                                 GAS 1060
      DOUBLE PRECISION TCH4O, TCH4V, TCH4W                                 GAS 1070
      DOUBLE PRECISION TH2SO, TH2SV, TH2SW                                 GAS 1080
      DOUBLE PRECISION TEST, TITR(11), TK, TOTEL(5), WROIL                 GAS 1090
                                                                           GAS 1100
      EXTERNAL KHCH4, KHCO2, KHH2S, POLY, PAGE                             GAS 1110
                                                                           GAS 1120
      INTRINSIC DABS, DLOG10, DSIGN                                        GAS 1130
                                                                           GAS 1140
      COMMON /DIST  / TCO2M,  TCH4M, TH2SM, WROIL, KCH4OL, KCO2OL,         GAS 1150
     .                KH2SOL, IPHASE, DSEP                                GAS 1160
      COMMON /EXTOT / EXELT, TOTEL, TITR                                   GAS 1170
      COMMON /FORM  / IPAGE, IPGLN                                         GAS 1180
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,               GAS 1190
     .                DCH4, DDCH4, IOPT, FIXIT                            GAS 1200
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                           GAS 1210
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                                  GAS 1220
      COMMON /ZPH   / PHHIT, PPHHIT, JCO3, SCO2, HTOT, OHTOT               GAS 1230
                                                                           GAS 1240
      SAVE ORGT1, STEP, CO2DIF, CO2TRY, H2SDIF, H2STRY, CH4DIF, CH4TRY     GAS 1250
      SAVE TCO2O, TCO2V, TCO2W, ORGCO2, PCO2W, KCO2W                       GAS 1260
      SAVE TCH4O, TCH4V, TCH4W, ORGCH4, PCH4W, KCH4W                       GAS 1270
      SAVE TH2SO, TH2SV, TH2SW, ORGH2S, PH2SW, KH2SW                       GAS 1280
                                                                           GAS 1290
C =========================================================================|GAS 1300
                                                                           GAS 1310
      TK    = TC + 273.15D00                                               GAS 1320
                                                                           GAS 1330
      KCO2W = KHCO2 (TK, MNACLD)                                           GAS 1340
      KH2SW = KHH2S (TK, MNACLD)                                           GAS 1350
                                                                           GAS 1360
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      IF (IGAS .EQ. 1) THEN                                                GAS 1370
        HTOTI  = HTOT                                                      GAS 1380
        OHTOTI = OHTOT                                                     GAS 1390
        ORGH2S = ANALM(33)                                                 GAS 1400
        ORGCH4 = ANALM(285)                                                GAS 1410
        ORGCO2 = SCO2                                                      GAS 1420
        ORGT1  = TOTEL(1)                                                  GAS 1430
        TCO2M  = TCO2M + SCO2                                              GAS 1440
        TCH4M  = TCH4M + ANALM(285)                                        GAS 1450
        TH2SM  = TH2SM + ANALM(33)                                         GAS 1460
        TCO2W  = ORGCO2                                                    GAS 1470
        TCH4W  = ORGCH4                                                    GAS 1480
        TH2SW  = ORGH2S                                                    GAS 1490
        PCH4W  = 1.0                                                       GAS 1500
        IF (TCH4M .GT. CPUMIN) THEN                                        GAS 1510
          DO 10 I = 1, 5                                                   GAS 1520
            KCH4W = KHCH4 (TK, MNACLD, PCH4W)                              GAS 1530
            PCH4W = TCH4M / ((WROIL / KCH4OL) + (1.0 / KCH4W))             GAS 1540
            IF (PCH4W .GT. PTOTAL) PCH4W = PTOTAL                          GAS 1550
            IF (PCH4W .LT. 1.0)    PCH4W = 1.0                             GAS 1560
10        CONTINUE                                                         GAS 1570
        ELSE                                                               GAS 1580
          KCH4W = 1.0D00                                                   GAS 1590
          PCH4W = 0.0D00                                                   GAS 1600
        END IF                                                             GAS 1610
        IF (TCO2M .LT. CPUMIN) KCO2W = 1.0D00                              GAS 1620
        IF (TH2SM .LT. CPUMIN) KH2SW = 1.0D00                              GAS 1630
        TCH4O  = WROIL * (PCH4W / KCH4OL)                                  GAS 1640
        TCH4W  = TCH4M - TCH4O                                             GAS 1650
        IF (TCH4W .LE. CPUMIN .AND. TCH4M .GT. CPUMIN) THEN                GAS 1660
          TCH4W = TCH4M / 2.0D00                                           GAS 1670
          TCH4O = TCH4W                                                    GAS 1680
        ELSE IF (TCH4W .LE. CPUMIN .AND. TCH4M .LE. CPUMIN) THEN           GAS 1690
          TCH4W = 0.0                                                      GAS 1700
          TCH4O = 0.0                                                      GAS 1710
        END IF                                                             GAS 1720
        M(285) = TCH4W                                                     GAS 1730
        DO 20 I = 1, 4                                                     GAS 1740
          STEP(I) = 0.0                                                    GAS 1750
20      CONTINUE                                                           GAS 1760
      END IF                                                               GAS 1770
                                                                           GAS 1780
      PCO2W  = KCO2W * M(97)                                               GAS 1790
      PCH4W  = KCH4W * M(285)                                              GAS 1800
      PH2SW  = KH2SW * M(33)                                               GAS 1810
                                                                           GAS 1820
      IF ((PH2O + PCO2W + PCH4W + PH2SW) .LT. PTOTAL) THEN                 GAS 1830
        IPHASE = 2                                                         GAS 1840
        TCO2O  = WROIL * (PCO2W / KCO2OL)                                  GAS 1850
        TCH4O  = WROIL * (PCH4W / KCH4OL)                                  GAS 1860
        TH2SO  = WROIL * (PH2SW / KH2SOL)                                  GAS 1870
        TCO2V  = 0.0D00                                                    GAS 1880
        TCH4V  = 0.0D00                                                    GAS 1890
        TH2SV  = 0.0D00                                                    GAS 1900
      ELSE                                                                 GAS 1910
        IPHASE = 3                                                         GAS 1920
        A = TCO2M - SCO2 + M(97)                                           GAS 1930
        B = TCH4M                                                          GAS 1940
```

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      C = TH2SM - ANALM(33) + M(33)                                          GAS 1950
      E = PTOTAL - PH2O                                                      GAS 1960
      D = E * ((WROIL/KCO2OL) + (1.0D00/KCO2W))                              GAS 1970
      G = E * ((WROIL/KCH4OL) + (1.0D00/KCH4W))                              GAS 1980
      J = E * ((WROIL/KH2SOL) + (1.0D00/KH2SW))                              GAS 1990
      CALL POLY( A, B, C, E, D, G, J, ROOT)                                  GAS 2000
      D = D / E                                                              GAS 2010
      G = G / E                                                              GAS 2020
      J = J / E                                                              GAS 2030
      PCO2W = A / (D + ROOT)                                                 GAS 2040
      PCH4W = B / (G + ROOT)                                                 GAS 2050
      PH2SW = C / (J + ROOT)                                                 GAS 2060
                                                                             GAS 2070
      TCO2O  = WROIL * (PCO2W / KCO2OL)                                      GAS 2080
      TCH4O  = WROIL * (PCH4W / KCH4OL)                                      GAS 2090
      TH2SO  = WROIL * (PH2SW / KH2SOL)                                      GAS 2100
                                                                             GAS 2110
      TCO2V  = PCO2W * ROOT                                                  GAS 2120
      TCH4V  = PCH4W * ROOT                                                  GAS 2130
      TH2SV  = PH2SW * ROOT                                                  GAS 2140
                                                                             GAS 2150
      A = PCO2W / KCO2W                                                      GAS 2160
      B = PCH4W / KCH4W                                                      GAS 2170
      C = PH2SW / KH2SW                                                      GAS 2180
                                                                             GAS 2190
      IF (A .GT. CPUMIN) THEN                                                GAS 2200
        TCO2O  = TCO2O * M(97)  / A                                          GAS 2210
        TCO2V  = TCO2V * M(97)  / A                                          GAS 2220
      END IF                                                                 GAS 2230
                                                                             GAS 2240
      IF (B .GT. CPUMIN) THEN                                                GAS 2250
        TCH4O  = TCH4O * M(285) / B                                          GAS 2260
        TCH4V  = TCH4V * M(285) / B                                          GAS 2270
      END IF                                                                 GAS 2280
                                                                             GAS 2290
      IF (C .GT. CPUMIN) THEN                                                GAS 2300
        TH2SO  = TH2SO * M(33)  / C                                          GAS 2310
        TH2SV  = TH2SV * M(33)  / C                                          GAS 2320
      END IF                                                                 GAS 2330
    END IF                                                                   GAS 2340
                                                                             GAS 2350
    DONE = .TRUE.                                                            GAS 2360
                                                                             GAS 2370
    IF (TCO2M .GT. CPUMIN) THEN                                              GAS 2380
      TEST = (TCO2O + TCO2V + SCO2) / TCO2M                                  GAS 2390
      IF (TEST .LT. CPUMIN) TEST = CPUMIN                                    GAS 2400
      IF (IGAS .GT. 3 .AND. DABS(DLOG10(TEST)) .GT. FCCSAT) THEN             GAS 2410
        DO 30 I = 1, 2                                                       GAS 2420
          CO2TRY(I) = CO2TRY(I+1)                                            GAS 2430
          CO2DIF(I) = CO2DIF(I+1)                                            GAS 2440
30      CONTINUE                                                             GAS 2450
      END IF                                                                 GAS 2460
      TEST = TEST - 1.0D00                                                   GAS 2470
      I = IGAS                                                               GAS 2480
      IF (IGAS .GT. 3) I = 3                                                 GAS 2490
      CO2TRY(I) = TCO2W                                                      GAS 2500
      CO2DIF(I) = TEST                                                       GAS 2510
      IF (IGAS .EQ. 1) THEN                                                  GAS 2520
```

```
        IF (TEST .GT. -0.98) THEN                                       GAS 2530
          STEP(1) = TCO2W * ((1.0 / (TEST + 1.0)) - 1.0)                GAS 2540
        ELSE                                                            GAS 2550
          STEP(1) = TCO2M / 3.0                                         GAS 2560
        END IF                                                          GAS 2570
        IF (DABS(STEP(1)) .LT. CPUMIN) STEP(1) = TCO2M * 1.0D-04        GAS 2580
      ELSE                                                              GAS 2590
        IF ((CO2DIF(I) * CO2DIF(I-1)) .LE. 0.0) THEN                    GAS 2600
          STEP(1) = STEP(1) * (-0.40)                                   GAS 2610
        END IF                                                          GAS 2620
        IF ((TCO2W + STEP(1)) .LT. 0.0) STEP(1) = TCO2W * (-0.90)       GAS 2630
        IF ((TCO2W + STEP(1)) .GT. TCO2M)                               GAS 2640
     .    STEP(1) = (TCO2M - TCO2W) * 0.90                              GAS 2650
      END IF                                                            GAS 2660
      STEP(1) = (-1.0) * DSIGN(STEP(1), TEST)                           GAS 2670
      TEST = TEST + 1.0D00                                              GAS 2680
      IF (DABS(DLOG10(TEST)) .GT. FCCSAT) THEN                          GAS 2690
        DONE  = .FALSE.                                                 GAS 2700
        TCO2W = TCO2W + STEP(1)                                         GAS 2710
      END IF                                                            GAS 2720
    END IF                                                              GAS 2730
                                                                        GAS 2740
    IF (TH2SM .GT. CPUMIN) THEN                                         GAS 2750
      TEST = (TH2SO + TH2SV + ANALM(33)) / TH2SM                        GAS 2760
      IF (TEST .LT. CPUMIN) TEST = CPUMIN                               GAS 2770
                                                                        GAS 2780
      IF (IGAS .GT. 3 .AND. DABS(DLOG10(TEST)) .GT. FCCSAT) THEN        GAS 2790
        DO 40 I = 1, 2                                                  GAS 2800
          H2STRY(I) = H2STRY(I+1)                                       GAS 2810
          H2SDIF(I) = H2SDIF(I+1)                                       GAS 2820
40      CONTINUE                                                        GAS 2830
      END IF                                                            GAS 2840
                                                                        GAS 2850
      TEST = TEST - 1.0D00                                              GAS 2860
      I = IGAS                                                          GAS 2870
      IF (IGAS .GT. 3) I = 3                                            GAS 2880
      H2STRY(I) = TH2SW                                                 GAS 2890
      H2SDIF(I) = TEST                                                  GAS 2900
                                                                        GAS 2910
      IF (IGAS .EQ. 1) THEN                                             GAS 2920
        IF (TEST .GT. -0.98) THEN                                       GAS 2930
          STEP(2) = TH2SW * ((1.0 / (TEST + 1.0)) - 1.0)                GAS 2940
        ELSE                                                            GAS 2950
          STEP(2) = TH2SM / 3.0                                         GAS 2960
        END IF                                                          GAS 2970
        IF (DABS(STEP(2)) .LT. CPUMIN) STEP(2) = TH2SM * 1.0D-04        GAS 2980
      ELSE                                                              GAS 2990
        IF ((H2SDIF(I) * H2SDIF(I-1)) .LE. 0.0) THEN                    GAS 3000
          STEP(2) = STEP(2) * (-0.40)                                   GAS 3010
        END IF                                                          GAS 3020
        IF ((TH2SW + STEP(2)) .LT. 0.0) STEP(2) = TH2SW * (-0.90)       GAS 3030
        IF ((TH2SW + STEP(2)) .GT. TH2SM)                               GAS 3040
     .    STEP(2) = (TH2SM - TH2SW) * 0.90                              GAS 3050
      END IF                                                            GAS 3060
                                                                        GAS 3070
      STEP(2) = (-1.0) * DSIGN(STEP(2), TEST)                           GAS 3080
      TEST = TEST + 1.0D00                                              GAS 3090
                                                                        GAS 3100
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      IF (DABS(DLOG10(TEST)) .GT. FCCSAT) THEN                          GAS 3110
        DONE  = .FALSE.                                                 GAS 3120
        TH2SW = TH2SW + STEP(2)                                         GAS 3130
      END IF                                                            GAS 3140
    END IF                                                              GAS 3150
                                                                        GAS 3160
    IF (TCH4M .GT. CPUMIN) THEN                                         GAS 3170
      TEST = (TCH4O + TCH4V + ANALM(285)) / TCH4M                       GAS 3180
      IF (TEST .LT. CPUMIN) TEST = CPUMIN                               GAS 3190
                                                                        GAS 3200
      IF (IGAS .GT. 3 .AND. DABS(DLOG10(TEST)) .GT. FCCSAT) THEN        GAS 3210
        DO 50 I = 1, 2                                                  GAS 3220
          CH4TRY(I) = CH4TRY(I+1)                                       GAS 3230
          CH4DIF(I) = CH4DIF(I+1)                                       GAS 3240
50      CONTINUE                                                        GAS 3250
      END IF                                                            GAS 3260
                                                                        GAS 3270
      TEST = TEST - 1.0D00                                              GAS 3280
      I = IGAS                                                          GAS 3290
      IF (IGAS .GT. 3) I = 3                                            GAS 3300
      CH4TRY(I) = TCH4W                                                 GAS 3310
      CH4DIF(I) = TEST                                                  GAS 3320
                                                                        GAS 3330
      IF (IGAS .EQ. 1) THEN                                             GAS 3340
        IF (TEST .GT. -0.98) THEN                                       GAS 3350
          STEP(3) = TCH4W * ((1.0 / (TEST + 1.0)) - 1.0)                GAS 3360
        ELSE                                                            GAS 3370
          STEP(3) = TCH4M / 3.0                                         GAS 3380
        END IF                                                          GAS 3390
        IF (DABS(STEP(3)) .LT. CPUMIN) STEP(3) = TCH4M * 1.0D-04        GAS 3400
      ELSE                                                              GAS 3410
        IF ((CH4DIF(I) * CH4DIF(I-1)) .LE. 0.0) THEN                    GAS 3420
          STEP(3) = STEP(3) * (-0.40)                                   GAS 3430
        END IF                                                          GAS 3440
        IF ((TCH4W + STEP(3)) .LT. 0.0) STEP(3) = TCH4W * (-0.90)       GAS 3450
        IF ((TCH4W + STEP(3)) .GT. TCH4M)                               GAS 3460
          STEP(3) = (TCH4M - TCH4W) * 0.90                              GAS 3470
      END IF                                                            GAS 3480
      STEP(3) = (-1.0) * DSIGN(STEP(3), TEST)                           GAS 3490
      TEST = TEST + 1.0D00                                              GAS 3500
      IF (DABS(DLOG10(TEST)) .GT. FCCSAT) THEN                          GAS 3510
        DONE  = .FALSE.                                                 GAS 3520
        TCH4W = TCH4W + STEP(3)                                         GAS 3530
      END IF                                                            GAS 3540
    END IF                                                              GAS 3550
                                                                        GAS 3560
    IF (DONE .OR. IGAS .EQ. IMAX) THEN                                  GAS 3570
      IPHASE = 0                                                        GAS 3580
      CALL PAGE                                                         GAS 3590
      IPGLN = IPGLN + 6                                                 GAS 3600
      WRITE (UNO,1000)                                                  GAS 3610
      IPGLN = IPGLN + 3                                                 GAS 3620
      WRITE (UNO, 1010) SCO2,  TCO2O, TCO2V, TCO2M, PCO2W               GAS 3630
      WRITE (UNO, 1020) TCH4W, TCH4O, TCH4V, TCH4M, PCH4W               GAS 3640
      WRITE (UNO, 1030) TH2SW, TH2SO, TH2SV, TH2SM, PH2SW               GAS 3650
      IPGLN = IPGLN + 9                                                 GAS 3660
      WRITE (UNO, 1040) KCO2W, KCO2OL, KCH4W, KCH4OL, KH2SW, KH2SOL     GAS 3670
      IPGLN = IPGLN + 3                                                 GAS 3680
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      WRITE (UNO, 1050) WROIL, FCCSAT                                    GAS 3690
      DCO2 = 0.0                                                         GAS 3700
      DH2S = 0.0                                                         GAS 3710
      DCH4 = 0.0                                                         GAS 3720
    ELSE                                                                 GAS 3730
      TOTEL(3) = TCO2W                                                   GAS 3740
      HTOTI    = ORGT1                                                   GAS 3750
                                                                         GAS 3760
      DCO2 = TCO2W - ORGCO2                                              GAS 3770
      EXELT(29)  = TCO2W                                                 GAS 3780
      TITR(1)    = TCO2W                                                 GAS 3790
      ANALM(7)   = TCO2W                                                 GAS 3800
      ANALM(98)  = 0.0                                                   GAS 3810
                                                                         GAS 3820
      DH2S = TH2SW - ORGH2S                                              GAS 3830
      EXELT(25)  = TH2SW                                                 GAS 3840
      TITR(7)    = TH2SW                                                 GAS 3850
      ANALM(33)  = TH2SW                                                 GAS 3860
                                                                         GAS 3870
      DCH4 = TCH4W - ORGCH4                                              GAS 3880
      ANALM(285) = TCH4W                                                 GAS 3890
      M(285)     = TCH4W                                                 GAS 3900
                                                                         GAS 3910
      IF (IPRIN2 .EQ. 0) RETURN                                          GAS 3920
      IF (IGAS .EQ. 1 .OR. IPGLN .GT. 45) CALL PAGE                      GAS 3930
      IPGLN = IPGLN + 7                                                  GAS 3940
      WRITE (UNO, 1060)                                                  GAS 3950
      IPGLN = IPGLN + 4                                                  GAS 3960
      I = IGAS                                                           GAS 3970
      IF (IGAS .GT. 3) I = 3                                             GAS 3980
      WRITE (UNO, 1010) CO2TRY(I), TCO2O, TCO2V, TCO2M, PCO2W, TCO2W     GAS 3990
      WRITE (UNO, 1020) CH4TRY(I), TCH4O, TCH4V, TCH4M, PCH4W, TCH4W     GAS 4000
      WRITE (UNO, 1030) H2STRY(I), TH2SO, TH2SV, TH2SM, PH2SW, TH2SW     GAS 4010
    END IF                                                               GAS 4020
    RETURN                                                               GAS 4030
                                                                         GAS 4040
1000 FORMAT( //,' ************ COMPOSITION OF CO-EXISTING GAS,'          GAS 4050
   .           ,' OIL, AND WATER ********* ',                           GAS 4060
   .         //,19X,'Total Moles in',12X,'Sum in Water,',3X             GAS 4070
   .           ,'Pressure',/,10X,'Water',8X,'Oil',10X,'Gas'             GAS 4080
   .           ,7X,'Oil and Gas',5X,'(bars)',/,5X,65('='))              GAS 4090
1010 FORMAT(' CO2  ',6(E12.5,1X))                                        GAS 4100
1020 FORMAT(' CH4  ',6(E12.5,1X))                                        GAS 4110
1030 FORMAT(' H2S  ',6(E12.5,1X))                                        GAS 4120
1040 FORMAT(///,'         HENRY LAW CONSTANTS used for',                 GAS 4130
   .           ' Calculations',//,                                       GAS 4140
   .           ' K(CO2/H2O) = ',E12.5,7X,'K(CO2/OIL) =',E12.5,/,         GAS 4150
   .           ' K(CH4/H2O) = ',E12.5,7X,'K(CH4/OIL) =',E12.5,/,         GAS 4160
   .           ' K(H2S/H2O) = ',E12.5,7X,'K(H2S/OIL) =',E12.5,/)         GAS 4170
1050 FORMAT(/,  ' Oil to Water ratio  (WROIL) = ',E12.5,                 GAS 4180
   .       /,  ' Convergence Factor (FCCSAT) = ',E12.5)                  GAS 4190
1060 FORMAT( //,' ********** COMPOSITION OF CO-EXISTING GAS,',          GAS 4200
   .           ' OIL, AND WATER ********** ',                           GAS 4210
   .          /,' **************CALCULATED PRE-STEP VALUES',           GAS 4220
   .           ' ****************************',                        GAS 4230
   .         //,19X,'Total Moles in',12X,'Sum in Water,',3X,           GAS 4240
   .           'Pressure',3X,'Next Guess for',                           GAS 4250
   .          /,10X,'Water',8X,'Oil',10X,'Gas',                        GAS 4260
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     .          7X,'Oil and Gas',5X,'(bars)',4X,'Moles in Water',      GAS 4270
     .        /,5X,65('='))                                            GAS 4280
      END                                                              GAS 4290



      INTEGER FUNCTION GETUNT (NAME)                                   GET 0010
C ===================================================================|GET 0020
C     This function determines if a file is opened and return the unit |GET 0030
C     it is opened under.  If the file is not opened it will open the  |GET 0040
C     the file and return the unit it was opened under                 |GET 0050
C -------------------------------------------------------------------|GET 0060
C     BASE      INT   Starting choice for file unit                    |GET 0070
C     NAME      CHA   Name of file                                     |GET 0080
C     OPEN      LOG   Determines if file opened under name             |GET 0090
C     UNTNUM    INT   File unit number                                 |GET 0100
C     YES       LOG   Determines if file opened under unit             |GET 0110
C -------------------------------------------------------------------|GET 0120
      INTEGER BASE, UNTNUM                                             GET 0130
      LOGICAL OPEN, YES                                                GET 0140
      CHARACTER * 80 NAME                                              GET 0150
                                                                       GET 0160
C ===================================================================|GET 0170
                                                                       GET 0180
      BASE = 40                                                        GET 0190
      INQUIRE (FILE = NAME, NUMBER = UNTNUM, OPENED = OPEN)            GET 0200
                                                                       GET 0210
      IF (.NOT. OPEN) THEN                                             GET 0220
   10   INQUIRE (UNIT = BASE, OPENED = YES)                           GET 0230
        IF (YES) THEN                                                  GET 0240
          BASE = BASE + 1                                              GET 0250
          GO TO 10                                                     GET 0260
        END IF                                                         GET 0270
        OPEN (BASE, FILE = NAME, STATUS = 'UNKNOWN')                   GET 0280
        GETUNT = BASE                                                  GET 0290
      ELSE                                                             GET 0300
        GETUNT = UNTNUM                                                GET 0310
      END IF                                                           GET 0320
                                                                       GET 0330
      RETURN                                                           GET 0340
      END                                                              GET 0350



      SUBROUTINE GUESS (XX, FXX, NEWX, NPTS)                           GUE 0010
C ===================================================================|GUE 0020
C     Calculate the value of X where FUN(X) = 0                        |GUE 0030
C                                                                      |GUE 0040
C     Input values ... X   - NPTS values of X                          |GUE 0050
C                                                                      |GUE 0060
C                    FX    - NPTS values of FUN(X).  MUST be ordered   |GUE 0070
C                            from lowest to highest.                   |GUE 0080
C                    NPTS  - number of X, FUN(X) pairs                |GUE 0090
C                                                                      |GUE 0100
```

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C     Returned values ...                                                |GUE 0110
C                     NEWX - "Guessed" value of X where FUN(X) is zero   |GUE 0120
C                                                                        |GUE 0130
C     Uses method of Lagrangian interpolation.  Note that we solve       |GUE 0140
C     using FX as the x variable, and X as the Y variable, and then      |GUE 0150
C     interpolate for a value of FX = 0.0                                |GUE 0160
C ---------------------------------------------------------------------- |GUE 0170
C     A          DBL     Intermediate calculation                        |GUE 0180
C     B          DBL     Intermediate calculation                        |GUE 0190
C     FX         DBL     Local storage of FXX                            |GUE 0200
C     FXX        DBL     Values of the function of X                     |GUE 0210
C     I          INT     Loop variable                                   |GUE 0220
C     IHIGH      INT     Pointer to value just above root                |GUE 0230
C     ILOW       INT     Pointer to value just below the root            |GUE 0240
C     J          INT     Loop variable                                   |GUE 0250
C     JHIGH      INT     Pointer to value just above the root            |GUE 0260
C     JLOW       INT     Pointer to value just below the root            |GUE 0270
C     NEWX       DBL     New value of x where f(x) = 0                   |GUE 0280
C     NPTS       INT     Number of points                                |GUE 0290
C     START      INT     Restricts the range of points looked at         |GUE 0300
C     STOP       INT     Restricts the range of points looked at         |GUE 0310
C     X          DBL     Local storage of XX                             |GUE 0320
C     XX         DBL     Ordinate values                                 |GUE 0330
C ---------------------------------------------------------------------- |GUE 0340
                                                                          GUE 0350
      INTEGER NPTS, I, J, START, STOP, IHIGH, JHIGH, ILOW, JLOW           GUE 0360
                                                                          GUE 0370
      DOUBLE PRECISION XX(*), FXX(*), NEWX, A, B                          GUE 0380
      DOUBLE PRECISION X(30), FX(30)                                      GUE 0390
                                                                          GUE 0400
      INTRINSIC DABS                                                      GUE 0410
                                                                          GUE 0420
C ======================================================================= |GUE 0430
                                                                          GUE 0440
      START = 1                                                           GUE 0450
      STOP  = NPTS                                                        GUE 0460
                                                                          GUE 0470
      DO 10 I = START, STOP                                               GUE 0480
        X(I)  = XX(I)                                                     GUE 0490
        FX(I) = FXX(I)                                                    GUE 0500
   10 CONTINUE                                                            GUE 0510
                                                                          GUE 0520
   50 CONTINUE                                                            GUE 0530
      NEWX = 0.0                                                          GUE 0540
      DO 200 I = START, STOP                                              GUE 0550
        A = 1.0D00                                                        GUE 0560
        B = 1.0D00                                                        GUE 0570
        DO 100 J = START, STOP                                            GUE 0580
          IF (J .NE. I) THEN                                              GUE 0590
            A = A * (FX(I) - FX(J))                                       GUE 0600
            B = B * (-1.0D00) * FX(J)                                     GUE 0610
          END IF                                                          GUE 0620
  100   CONTINUE                                                          GUE 0630
        NEWX = NEWX + (X(I) * B / A)                                      GUE 0640
  200 CONTINUE                                                            GUE 0650
                                                                          GUE 0660
C ---------------------------------------------------------------------- |GUE 0670
C     Check for a "fish hook" function...ie: new value of X must be       |GUE 0680
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C     between previous bounding values.  If not, recalculate using      |GUE 0690
C     one less order polynomial than present try.                        |GUE 0700
C ------------------------------------------------------------------------|GUE 0710
                                                                          GUE 0720
      IHIGH = STOP                                                        GUE 0730
      ILOW  = START                                                       GUE 0740
      JHIGH = STOP                                                        GUE 0750
      JLOW  = START                                                       GUE 0760
                                                                          GUE 0770
      DO 300 I = START+1, STOP                                            GUE 0780
        IF (FX(I) .LT. 0.0) THEN                                          GUE 0790
          IF (DABS(X(IHIGH) - X(ILOW)) .GT. DABS(X(IHIGH) - X(I)))        GUE 0800
     .      ILOW = I                                                       GUE 0810
          IF (DABS(X(JHIGH) - X(JLOW)) .LT. DABS(X(JHIGH) - X(I)))        GUE 0820
     .      JLOW = I                                                       GUE 0830
        ELSE                                                              GUE 0840
          IF (DABS(X(IHIGH) - X(ILOW)) .GT. DABS(X(I) - X(ILOW)))         GUE 0850
     .      IHIGH = I                                                      GUE 0860
          IF (DABS(X(JHIGH) - X(JLOW)) .LT. DABS(X(I) - X(JLOW)))         GUE 0870
     .      JHIGH = I                                                      GUE 0880
        END IF                                                            GUE 0890
  300 CONTINUE                                                            GUE 0900
                                                                          GUE 0910
      IF ((NEWX .LT. X(ILOW) .AND. NEWX .LT. X(IHIGH))  .OR.              GUE 0920
     .    (NEWX .GT. X(ILOW) .AND. NEWX .GT. X(IHIGH))) THEN              GUE 0930
        IF (DABS(X(JHIGH)-X(IHIGH)).GT.DABS(X(JLOW)-X(ILOW))) THEN        GUE 0940
          J = JHIGH                                                       GUE 0950
        ELSE                                                              GUE 0960
          J = JLOW                                                        GUE 0970
        END IF                                                            GUE 0980
        IF (J .LT. STOP) THEN                                             GUE 0990
          DO 400 I = J, (STOP-1)                                          GUE 1000
            X(I)  = X(I+1)                                                GUE 1010
            FX(I) = FX(I+1)                                               GUE 1020
  400     CONTINUE                                                        GUE 1030
        END IF                                                            GUE 1040
        STOP = STOP - 1                                                   GUE 1050
        GO TO 50                                                          GUE 1060
      END IF                                                              GUE 1070
                                                                          GUE 1080
      RETURN                                                              GUE 1090
      END                                                                 GUE 1100
```

```
      SUBROUTINE INPUT (UNI, TEMP, HITEMP, DNS, PHHIT, IEXCH, ICO2,      INP 0010
     .                  MIXFLG)                                           INP 0020
C ========================================================================|INP 0030
C     This routine reads in one set of data at a time.                    |INP 0040
C ------------------------------------------------------------------------|INP 0050
C     ACTUAL     INT   Calculated index value                             |INP 0060
C     ADEX       INT   Flag for surface chemistry option                  |INP 0070
C     ALK        INT   Flag for distribution of carbonate species         |INP 0080
C     AMOL       DBL   Molality of aqueous/mineral species added          |INP 0090
C     ANALM      DBL   Analyzed molality of species i                     |INP 0100
C     ANS        CHA   Determines if ion exchange or adsorption           |INP 0110
```

```
C     ANS1      INT   Number of complexes for added anion #1          |INP 0120
C     ANS2      INT   Number of complexes for added anion #2          |INP 0130
C     AVOG      DBL   Avogadro's number                               |INP 0140
C     CEC       DBL   Cation exchange capacity                        |INP 0150
C     COEF      DBL   Stoichiometric coefficient and ID number        |INP 0160
C     CONV1     DBL   Tolerance factor for convergence of anions      |INP 0170
C     CONV2     DBL   Tolerance factor for hydronium mass-balance     |INP 0180
C     CPUMIN    DBL   Smallest positive real value program uses       |INP 0190
C     CUNITS    DBL   Analytical input concentration                  |INP 0200
C     DCH4      DBL   Concentration of CH4 lost up annulas            |INP 0210
C     DDCH4     DBL   Concentration of CH4 lost before pH measurement |INP 0220
C     DCO2      DBL   Concentration of CO2 lost up annulas            |INP 0230
C     DDCO2     DBL   Concentration of CO2 lost before pH measurement |INP 0240
C     DH2S      DBL   Concentration of H2S lost up annulas            |INP 0250
C     DDH2S     DBL   Concentration of H2S lost before pH measurement |INP 0260
C     DNH3      DBL   Concentration of NH3 lost up annulas            |INP 0270
C     DDNH3     DBL   Concentration of NH3 lost before pH measurement |INP 0280
C     DENS      DBL   Density                                         |INP 0290
C     DFRAC1    DBL   Smallest fraction of soln 1 mixed with soln 2   |INP 0300
C     DHA       DBL   Ion size parameter                              |INP 0310
C     DINC      DBL   Increment of solution 1 to be added             |INP 0320
C     DNA       DBL   Temporary ion size parameter for added ions     |INP 0330
C     DNS       CHA   Determines if density should be calculated      |INP 0340
C     DP        DBL   Dissolution/precipitation switch                |INP 0350
C     DSEP      DBL   Density of oil at 15 degree C                   |INP 0360
C     EHM       DBL   Measured Eh in volts                            |INP 0370
C     EHMC      DBL   Measured Eh using the Calomel electrode         |INP 0380
C     EMFZSC    DBL   Measured Eh using the Zobell's solution         |INP 0390
C     FBOIL     DBL   Fraction of solution boiled-off as steam        |INP 0400
C     FCCSAT    DBL   Tolerance factor for pH and CO2 options         |INP 0410
C     FIXIT     DBL   Fixing value in the CO2 option                  |INP 0420
C     FLAGS     INT   Selection flags for calculation of redox equil. |INP 0430
C     GEOTH     INT   Flag to select geothermometer                   |INP 0440
C     GFW       DBL   Gram formula weight of aqueous species          |INP 0450
C     HIGHKT    DBL   K(T) at temp 2 for added options                |INP 0460
C     HITEMP    DBL   In-situ temperature                             |INP 0470
C     I         INT   Loop counting variable                          |INP 0480
C     IBMIX     INT   Switch for mixing option                        |INP 0490
C     ICCSAT    INT   Switch for pH option                            |INP 0500
C     ICO2      INT   Switch for CO2 option                           |INP 0510
C     IDDP      INT   Id number of the mineral to be dissolved/ppt    |INP 0520
C     IDMIX     INT   Id number of the aqueous species to be added    |INP 0530
C     IDN       INT   Id numbers of the ISCOMP components adsorption  |INP 0540
C     IDSAT     INT   Id number of the mineral to be equilibrated     |INP 0550
C     IEXCH     INT   Switch for exchange option                      |INP 0560
C     ILP       INT   Index list of the analytical species            |INP 0570
C     ILQ       INT   Index list of the complexing cations            |INP 0580
C     ILR       INT   Index list of the complexing anions             |INP 0590
C     IMCO3     INT   Selects CO2 option                              |INP 0600
C     INDEX     INT   Reference index for added ions                  |INP 0610
C     INFORM    INT   Flag to print all the log K values in data base |INP 0620
C     INMIX     INT   Total number of mixtures of two solution mixed  |INP 0630
C     INSP      INT   Total number of surface sites for adsorption    |INP 0640
C     IOPT      INT   Switch for co2/h option                         |INP 0650
C     IPAGE     INT   Current page number of output file              |INP 0660
C     IPGLN     INT   Current line number of the output file          |INP 0670
C     IPHASE    INT   Switch for oil/water/gas calculations           |INP 0680
C     IPIT      INT   Flag to use pitzer activity coefficients        |INP 0690
```

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C     IPRIN1    INT   Flag for printing iteration of anions                |INP 0700
C     IPRIN2    INT   Flag for printing hydronium balance                  |INP 0710
C     IRXDP     INT   Id number of the aqueous species to be added         |INP 0720
C     ISCHG     INT   Charge of each surface site for adsorption           |INP 0730
C     ISCOMP    INT   Total number of components in dissociation           |INP 0740
C     ITIC      INT   Hitemp distribution of carbonate species             |INP 0750
C     ITMIX     INT   Switch for the mineral saturation option             |INP 0760
C     ITT       INT   Number of aqueous species to add/sub with water      |INP 0770
C     J         INT   Loop counting variable                               |INP 0780
C     KCH4OL    DBL   Henry's law coefficient for CH4 in oil               |INP 0790
C     KCO2OL    DBL   Henry's law coefficient for CO2 in oil               |INP 0800
C     KH2SOL    DBL   Henry's law coefficient for H2S in oil               |INP 0810
C     KRXN      DBL   K for dissociation reaction of surface species       |INP 0820
C     LINE      INT   Line count used for error location                   |INP 0830
C     LOWKT     DBL   Log K(T) at temp 1 for added options                 |INP 0840
C     MBASE     DBL   Equivalence Mole Fraction (initial) on surface       |INP 0850
C     MINCO     DBL   Stoichiometric coefficient for added minerals        |INP 0860
C     MININD    INT   Index number of the added mineral                    |INP 0870
C     MINLOG    DBL   Log K values for added minerals                      |INP 0880
C     MXMNK     INT   Total number of mineral log k values                 |INP 0890
C     MXSP      INT   Total number of aqueous species                      |INP 0900
C     NAME      CHA   Name of each complex formed by association           |INP 0910
C     NDUM      INT   Id of mineral/aqueous complex with K(T) changed      |INP 0920
C     NMAX      INT   General array dimension to allow easy expansion      |INP 0930
C     NOSE      INT   Number of species in the equation                    |INP 0940
C     NUFLAG    INT   Sets the activity coefficients of neutral species    |INP 0950
C     NUMCOM    INT   Number of complex the ion is associated with         |INP 0960
C     NUMINS    INT   Number of minerals added                             |INP 0970
C     ODUM      CHA   Switch to indicate a mineral/aqueous complex         |INP 0980
C     OK        INT   Error flag for Lagrange interpolation routine        |INP 0990
C     OUTIN     CHA   Name of restart file name                            |INP 1000
C     PAGE1     CHA   Names of aqueous species                             |INP 1010
C     PAGE3     CHA   Names of solubility constants                        |INP 1020
C     PH        DBL   Measured pH of the solution                          |INP 1030
C     PHHIT     INT   Hitemp pH switch                                     |INP 1040
C     PRESS     DBL   Total pressure                                       |INP 1050
C     RATIO     INT   Flag for printing activity ratios of elements        |INP 1060
C     RXDP      DBL   Molal amount of the aqueous species added            |INP 1070
C     SAREA     DBL   Total surface area per kilogram of solvent           |INP 1080
C     SPN       CHA   Name of each surface species adsorption              |INP 1090
C     TAREA     DBL   Site density per unit area adsorption                |INP 1100
C     TCH4M     DBL   Moles CH4 distributed between oil, water, vapor      |INP 1110
C     TCO2M     DBL   Moles CO2 distributed between oil, water, vapor      |INP 1120
C     TEMP      DBL   Temperature of the solution when pH was measured     |INP 1130
C     TH2SM     DBL   Moles H2S distributed between oil, water, vapor      |INP 1140
C     TIC       DBL   Concentration of total inorganic carbon              |INP 1150
C     TITLE     CHA   Name of the sample                                   |INP 1160
C     TOF       CHA   Places a form feed in output file                    |INP 1170
C     UNI       INT   File unit assigned for input file                    |INP 1180
C     UNITS     CHA   Units of concentration                               |INP 1190
C     UNO       INT   File unit assigned for output file                   |INP 1200
C     WROIL     DBL   Oil to water weight ratio                            |INP 1210
C     XD        DBL   Holds Log K's for additional anions & cations        |INP 1220
C     XDUM      DBL   New log K(T) value                                   |INP 1230
C     Z         INT   Charge of aqueous species                            |INP 1240
C ---------------------------------------------------------------------    |INP 1250
                                                                           INP 1260
      INTEGER NMAX, UNO                                                    INP 1270
```

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      DOUBLE PRECISION AVOG, CPUMIN                                          INP 1280
                                                                             INP 1290
      PARAMETER (NMAX = 340, UNO = 6)                                        INP 1300
      PARAMETER (AVOG = 6.022D+23, CPUMIN = 1.0D-35)                         INP 1310
                                                                             INP 1320
      INTEGER ACTUAL, ALK, ANS1, ANS2, FLAGS(6), GEOTH                       INP 1330
      INTEGER I, IBMIX, ICCSAT, ICO2, IDDP, IDMIX(50)                        INP 1340
      INTEGER IDN(10,10), IDSAT, IEXCH, ISCHG(10), ILP(33)                   INP 1350
      INTEGER ILQ(15), ILR(13), IMCO3, IMIX, INDEX, INFORM, INMIX, INSP      INP 1360
      INTEGER IOPT, IPAGE, IPGLN, IPHASE, IPIT, IPRIN1, IPRIN2               INP 1370
      INTEGER IRXDP(10), ISCOMP(10), ITIC, ITMIX, ITT                        INP 1380
      INTEGER J, LINE, MININD(8,5), MIXFLG, MXMNK, MXSP, NDUM(12), NOSE      INP 1390
      INTEGER NUFLAG, NUMCOM, NUMINS, OK, PHHIT, RATIO, UNI, Z(NMAX)         INP 1400
                                                                             INP 1410
      CHARACTER *  1 ADEX, CR, DNS, ODUM(12), TOF                            INP 1420
      CHARACTER *  5 UNITS                                                   INP 1430
      CHARACTER *  8 NAME, PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)             INP 1440
      CHARACTER * 10 SPN(10)                                                 INP 1450
      CHARACTER * 40 TITMIX                                                  INP 1460
      CHARACTER * 80 DUMMY, MIXFLE, OUTIN, TITLE                             INP 1470
                                                                             INP 1480
      DOUBLE PRECISION ALFA(NMAX), AMOL(50), ANALM(NMAX)                     INP 1490
      DOUBLE PRECISION CEC, COEF(10,10), CONV1, CONV2, CUNITS(NMAX)          INP 1500
      DOUBLE PRECISION DCH4, DCO2, DDCH4, DDCO2, DDH2S, DDNH3, DEBYE         INP 1510
      DOUBLE PRECISION DENS, DFRAC1, DH2S, DINC, DHA(NMAX), DNA, DNH3        INP 1520
      DOUBLE PRECISION DP, EHM, EHMC, EMFZSC, FBOIL, FCCSAT, FIXIT           INP 1530
      DOUBLE PRECISION GFW(NMAX), HIGHKT, HITEMP, KCH4OL, KCO2OL             INP 1540
      DOUBLE PRECISION KH2SOL, KRXN(10), LOWKT                               INP 1550
      DOUBLE PRECISION M(NMAX), MBASE(10), MINCO(9,5)                        INP 1560
      DOUBLE PRECISION MINLOG(2,5), PH, PRESS, DSEP, RXDP(10)                INP 1570
      DOUBLE PRECISION SAREA, TAREA, TCH4M, TCO2M, TEMP                      INP 1580
      DOUBLE PRECISION TH2SM, TIC, WROIL, X, XD(2,45), XDUM(12)              INP 1590
                                                                             INP 1600
      EXTERNAL DEBYE, PAGE                                                   INP 1610
                                                                             INP 1620
      INTRINSIC DABS, IABS                                                   INP 1630
                                                                             INP 1640
      COMMON /AL    / NDUM, XDUM                                             INP 1650
      COMMON /AMM   / IDMIX, AMOL, ITMIX, INMIX, DFRAC1, DINC, FBOIL         INP 1660
      COMMON /BASIC / DENS, PRESS, EHM, EHMC, EMFZSC, TIC, FCCSAT, XD,       INP 1670
     .                NUMCOM, NUMINS, MINLOG, MINCO, MININD, CONV1,          INP 1680
     .                CONV2                                                  INP 1690
      COMMON /CH    / ODUM                                                   INP 1700
      COMMON /DIST  / TCO2M,  TCH4M, TH2SM, WROIL, KCH4OL, KCO2OL,           INP 1710
     .                KH2SOL, IPHASE, DSEP                                   INP 1720
      COMMON /EXCHAN/ COEF, MBASE, KRXN, CEC, TAREA,                         INP 1730
     .                SAREA, IDN, ISCHG, ISCOMP, INSP                        INP 1740
      COMMON /FLAGCM/ ALK, ITIC, ICCSAT, IMCO3, ITT, ANS1, ANS2,             INP 1750
     .                NUFLAG, IPIT, FLAGS, INFORM, RATIO, GEOTH,             INP 1760
     .                IPRIN1, IPRIN2                                         INP 1770
      COMMON /FMFD  / TOF, CR, TITMIX                                        INP 1780
      COMMON /FORM  / IPAGE, IPGLN                                           INP 1790
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,                 INP 1800
     .                DCH4, DDCH4, IOPT, FIXIT                               INP 1810
      COMMON /IMM   / IBMIX, IMIX                                            INP 1820
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                             INP 1830
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                    INP 1840
      COMMON /NAMES2/ SPN                                                    INP 1850
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      COMMON /NAMES3/ MIXFLE, OUTIN, TITLE, UNITS, ADEX                  INP 1860
      COMMON /SAT   / IDDP, IDSAT, DP, RXDP, IRXDP                       INP 1870
      COMMON /TABCOM/ MXSP, MXMNK, GFW, Z, DHA                           INP 1880
                                                                         INP 1890
      DATA ILP /3, 4, 22, 1, 2, 18, 14, 12, 5, 6, 33, 7, 98, 30, 29,     INP 1900
     .          136, 32, 31, 26, 15, 25, 27, 16, 23, 21, 13, 28, 169,   INP 1910
     .          210, 48, 246, 265, 285/                                 INP 1920
      DATA ILQ /8, 8, 8, 14, 15, 1, 16, 18, 4, 2, 23, 3, 25, 26, 27/     INP 1930
      DATA ILR /5, 6, 7, 9, 29, 30, 48, 98, 101, 246, 265, 0, 0/         INP 1940
                                                                         INP 1950
C ========================================================================|INP 1960
                                                                         INP 1970
C -------------------------------------------------------------------------|INP 1980
C     Get basic input data                                               |INP 1990
C -------------------------------------------------------------------------|INP 2000
                                                                         INP 2010
      LINE = 1                                                           INP 2020
      READ (UNI, 9000, END = 160) TITLE                                  INP 2030
                                                                         INP 2040
      CALL PAGE                                                          INP 2050
      WRITE (UNO, 9010) TITLE                                            INP 2060
      IPGLN = IPGLN + 1                                                  INP 2070
                                                                         INP 2080
      LINE = LINE + 1                                                    INP 2090
      READ (UNI, 9020, ERR = 150) TEMP, HITEMP, DENS, PRESS              INP 2100
                                                                         INP 2110
      LINE = LINE + 1                                                    INP 2120
      READ (UNI, 9020, ERR = 150) PH, EHM, EHMC, EMFZSC, UNITS           INP 2130
                                                                         INP 2140
C -------------------------------------------------------------------------|INP 2150
C     Check to make sure the units are correct                           |INP 2160
C -------------------------------------------------------------------------|INP 2170
                                                                         INP 2180
      OK = 0                                                             INP 2190
                                                                         INP 2200
      DO 1 I=1,5                                                         INP 2210
          IF (UNITS(I:I).EQ.'m') UNITS(I:I)='M'                          INP 2220
          IF (UNITS(I:I).EQ.'g') UNITS(I:I)='G'                          INP 2230
          IF (UNITS(I:I).EQ.'l') UNITS(I:I)='L'                          INP 2240
          IF (UNITS(I:I).EQ.'p') UNITS(I:I)='P'                          INP 2250
          IF (UNITS(I:I).EQ.'o') UNITS(I:I)='O'                          INP 2260
          IF (UNITS(I:I).EQ.'e') UNITS(I:I)='E'                          INP 2270
          IF (UNITS(I:I).EQ.'q') UNITS(I:I)='Q'                          INP 2280
          IF (UNITS(I:I).EQ.'k') UNITS(I:I)='K'                          INP 2290
    1 CONTINUE                                                           INP 2300
                                                                         INP 2310
      IF (UNITS .EQ. 'MG/L ') THEN                                       INP 2320
        OK = 1                                                           INP 2330
      ELSE IF (UNITS .EQ. 'PPM  ') THEN                                  INP 2340
        OK = 1                                                           INP 2350
      ELSE IF (UNITS .EQ. 'MOL/L') THEN                                  INP 2360
        OK = 1                                                           INP 2370
      ELSE IF (UNITS .EQ. 'MOL/K') THEN                                  INP 2380
        OK = 1                                                           INP 2390
      ELSE IF (UNITS .EQ. 'MEQ/L') THEN                                  INP 2400
        OK = 1                                                           INP 2410
      ELSE                                                               INP 2420
        OK = 0                                                           INP 2430
```

```
      END IF                                                            INP 2440
                                                                        INP 2450
      IF (OK .NE. 1) THEN                                               INP 2460
        WRITE (UNO, 9160) TOF                                           INP 2470
        WRITE (UNO, '(A,A5,A)') 'Must use proper units. "',             INP 2480
     .                   UNITS, '" are not recognized.'                 INP 2490
        STOP                                                            INP 2500
      END IF                                                            INP 2510
                                                                        INP 2520
      WRITE (UNO, 9030) '  TEMP', '  HITEMP', '  DENS', '  PRESS'      INP 2530
      WRITE (UNO, 9040)    TEMP,     HITEMP,     DENS,     PRESS       INP 2540
      WRITE (UNO, 9030) '  PH', '  EHM', '  EHMC', '  EMFZSC'          INP 2550
      WRITE (UNO, 9050)    PH,     EHM,     EHMC,     EMFZSC           INP 2560
      WRITE (UNO, 9060) UNITS                                           INP 2570
      IPGLN = IPGLN + 5                                                 INP 2580
                                                                        INP 2590
C -----------------------------------------------------------------------|INP 2600
C     Get concentration of species                                       |INP 2610
C -----------------------------------------------------------------------|INP 2620
                                                                        INP 2630
      LINE = LINE + 1                                                   INP 2640
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 1, 7)            INP 2650
      WRITE (UNO, 9080) 'Na      ', 'K       ', 'Li      ', 'Ca      ', INP 2660
     .                  'Mg      ', 'Fe      ', 'Al      '             INP 2670
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 1, 7)                      INP 2680
      IPGLN = IPGLN + 2                                                 INP 2690
                                                                        INP 2700
      LINE = LINE + 1                                                   INP 2710
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 8, 13), TIC      INP 2720
      WRITE (UNO, 9080) 'SiO2    ', 'Cl      ', 'SO4     ', 'H2S     ', INP 2730
     .                  'HCO3    ', 'CO3     ', 'TIC     '             INP 2740
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 8, 13),  TIC               INP 2750
      IPGLN = IPGLN + 2                                                 INP 2760
                                                                        INP 2770
      LINE = LINE + 1                                                   INP 2780
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 14, 20)          INP 2790
      WRITE (UNO, 9080) 'F       ', 'PO4     ', 'NO3     ', 'NH3     ', INP 2800
     .                  'B       ', 'Sr      ', 'Ba      '             INP 2810
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 14, 20)                    INP 2820
      IPGLN = IPGLN + 2                                                 INP 2830
                                                                        INP 2840
      LINE = LINE + 1                                                   INP 2850
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 21, 26)          INP 2860
      WRITE (UNO, 9080) 'Pb      ', 'Zn      ', 'Cu      ', 'Mn      ', INP 2870
     .                  'Hg      ', 'Ag      '                         INP 2880
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 21, 26)                    INP 2890
      IPGLN = IPGLN + 2                                                 INP 2900
                                                                        INP 2910
      LINE = LINE + 1                                                   INP 2920
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 27, 29)          INP 2930
      WRITE (UNO, 9080) 'As      ', 'U       ', 'V       '             INP 2940
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 27, 29)                    INP 2950
      IPGLN = IPGLN + 2                                                 INP 2960
                                                                        INP 2970
      LINE = LINE + 1                                                   INP 2980
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 30, 33)          INP 2990
      WRITE (UNO, 9080) 'Acetate ', 'Oxalate ', 'Succinate', 'CH4'      INP 3000
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 30, 33)                    INP 3010
```

```
      IPGLN = IPGLN + 2                                                    INP 3020
                                                                           INP 3030
C -----------------------------------------------------------------------|INP 3040
C     Adjust B and As to the forms the program uses                      |INP 3050
C -----------------------------------------------------------------------|INP 3060
                                                                           INP 3070
      IF (UNITS .EQ. 'PPM ' .OR. UNITS .EQ. 'MG/L ') THEN                  INP 3080
        CUNITS(31)  = CUNITS(31)  * 5.720                                  INP 3090
        CUNITS(28)  = CUNITS(28)  * 1.668                                  INP 3100
        CUNITS(169) = CUNITS(169) * 1.134                                  INP 3110
        CUNITS(210) = CUNITS(210) * 1.942                                  INP 3120
      END IF                                                               INP 3130
                                                                           INP 3140
C -----------------------------------------------------------------------|INP 3150
C     Carbon, High temperature carbon option                             |INP 3160
C -----------------------------------------------------------------------|INP 3170
                                                                           INP 3180
      LINE = LINE + 1                                                      INP 3190
      READ (UNI, 9100, ERR = 150) ALK, ITIC                                INP 3200
      WRITE (UNO, 9130) '  ALK  ', ' ITIC   '                             INP 3210
      WRITE (UNO, 9110) ALK, ITIC                                          INP 3220
      IPGLN = IPGLN + 2                                                    INP 3230
                                                                           INP 3240
C -----------------------------------------------------------------------|INP 3250
C     Gas addition option                                                |INP 3260
C -----------------------------------------------------------------------|INP 3270
      DDCO2 = 0.0                                                          INP 3280
      DCO2  = 0.0                                                          INP 3290
      DDNH3 = 0.0                                                          INP 3300
      DNH3  = 0.0                                                          INP 3310
      DDH2S = 0.0                                                          INP 3320
      DH2S  = 0.0                                                          INP 3330
      DDCH4 = 0.0                                                          INP 3340
      DCH4  = 0.0                                                          INP 3350
                                                                           INP 3360
      LINE = LINE + 1                                                      INP 3370
      READ (UNI, 9070, ERR = 150) DDCO2, DDH2S, DDNH3, DDCH4               INP 3380
      WRITE (UNO, 9080) '  DCO2  ', '  DH2S  ', '  DNH3  ', '  DCH4  '    INP 3390
      WRITE (UNO, 9050) DDCO2, DDH2S, DDNH3, DDCH4                         INP 3400
      IPGLN = IPGLN + 2                                                    INP 3410
                                                                           INP 3420
C -----------------------------------------------------------------------|INP 3430
C     pH and co2 saturation option                                       |INP 3440
C -----------------------------------------------------------------------|INP 3450
                                                                           INP 3460
      LINE = LINE + 1                                                      INP 3470
      READ (UNI, 9100, ERR = 150) ICCSAT, IMCO3, FIXIT, FCCSAT             INP 3480
      WRITE (UNO, 9080) ' ICCSAT ', 'IMCO3   ', 'FIXIT   ', ' FCCSAT '    INP 3490
      WRITE (UNO, 9110) ICCSAT, IMCO3, FIXIT, FCCSAT                       INP 3500
      IPGLN = IPGLN + 2                                                    INP 3510
                                                                           INP 3520
      IF (IMCO3 .EQ. 0) ICO2 = 0                                           INP 3530
      IF (IMCO3 .GT. 0) ICO2 = 1                                           INP 3540
                                                                           INP 3550
      IF (FCCSAT .LT. CPUMIN) FCCSAT = 2.0D-3                              INP 3560
      IF (FCCSAT .GT. 0.1)    FCCSAT = 0.05                                INP 3570
                                                                           INP 3580
C -----------------------------------------------------------------------|INP 3590
```

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C     Gas-water-oil option                                                |INP 3600
C ------------------------------------------------------------------------|INP 3610
                                                                          INP 3620
      LINE = LINE + 1                                                     INP 3630
      READ (UNI, 9070, ERR = 150) TCO2M,  TCH4M,  TH2SM,  WROIL,          INP 3640
     .                            KCO2OL, KCH4OL, KH2SOL, DSEP           INP 3650
      WRITE (UNO, 9080) 'TCO2M   ', 'TCH4M   ', 'TH2SM   ', 'WROIL   ',  INP 3660
     .                  'KCO2OL  ', 'KCH4OL  ', 'KH2SOL  ', 'DSEP    '   INP 3670
      WRITE (UNO, 9050) TCO2M,  TCH4M, TH2SM, WROIL, KCO2OL,              INP 3680
     .                  KCH4OL, KH2SOL, DSEP                            INP 3690
      IPGLN = IPGLN + 2                                                   INP 3700
      IF (DABS(KCO2OL) .LT. CPUMIN) KCO2OL = 1.0                          INP 3710
      IF (DABS(KCH4OL) .LT. CPUMIN) KCH4OL = 1.0                          INP 3720
      IF (DABS(KH2SOL) .LT. CPUMIN) KH2SOL = 1.0                          INP 3730
                                                                          INP 3740
C ------------------------------------------------------------------------|INP 3750
C     Read and write data for ion exchange or adsorption                  |INP 3760
C ------------------------------------------------------------------------|INP 3770
                                                                          INP 3780
      LINE = LINE + 1                                                     INP 3790
      READ (UNI, 9160, ERR = 150) ADEX                                    INP 3800
      WRITE (UNO, '(A, A1)') '  Adsorption/Exchange option (N=no) = ',    INP 3810
     .                       ADEX                                       INP 3820
      IF      (ADEX .EQ. 'a' .OR. ADEX .EQ. 'A') THEN                     INP 3830
        ADEX = 'A'                                                        INP 3840
      ELSE IF (ADEX .EQ. 'e' .OR. ADEX .EQ. 'E') THEN                     INP 3850
        ADEX = 'E'                                                        INP 3860
      ELSE                                                                INP 3870
        ADEX = 'N'                                                        INP 3880
      END IF                                                              INP 3890
      X = 0.0                                                             INP 3900
      IF (ADEX .EQ. 'A') THEN                                             INP 3910
        IEXCH = 1                                                         INP 3920
        WRITE (UNO, 9220) ' Adsorption (Double layer model)'              INP 3930
        WRITE (UNO, 9080) '  CEC   ', ' TAREA  ', ' SAREA  ', '  INSP  'INP 3940
                                                                          INP 3950
        LINE = LINE + 1                                                   INP 3960
        READ (UNI, 9150) CEC, TAREA, SAREA, INSP                          INP 3970
        WRITE (UNO, 9240) CEC, TAREA, SAREA, INSP                         INP 3980
                                                                          INP 3990
        WRITE (UNO, 9090) ' NAME  ', ' CHARGE ',                          INP 4000
     .                    'Fract. Surf. Sites '                          INP 4010
                                                                          INP 4020
        IPGLN = IPGLN + 4                                                 INP 4030
        DO 10 I = 1, INSP                                                 INP 4040
          LINE = LINE + 1                                                 INP 4050
          READ (UNI, 9200, ERR = 150) ISCHG(I), MBASE(I),  SPN(I)         INP 4060
          LINE = LINE + 1                                                 INP 4070
                                                                          INP 4080
          WRITE (UNO, 9250) SPN(I), ISCHG(I), MBASE(I)                    INP 4090
                                                                          INP 4100
          LINE = LINE + 1                                                 INP 4110
          READ (UNI, 9210, ERR = 150) KRXN(I), ISCOMP(I),                 INP 4120
     .         (COEF(I,J), IDN(I,J), J=1,ISCOMP(I))                       INP 4130
                                                                          INP 4140
          X     = X + MBASE(I)                                            INP 4150
          IPGLN = IPGLN + 1                                               INP 4160
          IF (IPGLN .GT. 58) CALL PAGE                                    INP 4170
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10    CONTINUE                                                          INP 4180
                                                                        INP 4190
      IF (DABS(1.0D00 - X) .GT. 0.001) THEN                             INP 4200
        WRITE (UNO, '(A, A, A)')                                        INP 4210
     .       ' ERROR in absorption/ion exchange',                       INP 4220
     .       ' data.  The sum of fraction of',                          INP 4230
     .       ' surface sites is not 1.0'                                INP 4240
        STOP                                                            INP 4250
      END IF                                                            INP 4260
                                                                        INP 4270
      WRITE (UNO, '(11X, A, A)') 'K  =   1. *          ',              INP 4280
     .                           '   * Coef  *  ID    +   ....  '      INP 4290
                                                                        INP 4300
      DO 20 I = 1, INSP                                                 INP 4310
        WRITE (UNO, 9260) KRXN(I), SPN(I), (COEF(I,J), IDN(I,J),        INP 4320
     .         J = 1, ISCOMP(I))                                        INP 4330
        IPGLN = IPGLN + 1                                               INP 4340
        IF (IPGLN .GT. 57) CALL PAGE                                    INP 4350
20    CONTINUE                                                          INP 4360
    ELSE IF (ADEX .EQ. 'E') THEN                                        INP 4370
      IEXCH = 2                                                         INP 4380
      WRITE (UNO, 9220) 'Ion Exchange: '                                INP 4390
      WRITE (UNO, 9080) '  CEC   ', ' TAREA  ', ' SAREA  ', '  INSP  'INP 4400
                                                                        INP 4410
      LINE = LINE + 1                                                   INP 4420
      READ (UNI, 9150)  CEC, TAREA, SAREA, INSP                         INP 4430
      WRITE (UNO, 9240) CEC, TAREA, SAREA, INSP                         INP 4440
                                                                        INP 4450
      WRITE (UNO, 9090) ' NAME  ', ' CHARGE ',                          INP 4460
     .                  'Fract. Surf. Sites '                           INP 4470
                                                                        INP 4480
      IPGLN = IPGLN + 4                                                 INP 4490
      DO 30 I = 1, INSP                                                 INP 4500
        LINE = LINE + 1                                                 INP 4510
        READ (UNI, 9200, ERR = 150) ISCHG(I), MBASE(I),  SPN(I)         INP 4520
        LINE = LINE + 1                                                 INP 4530
                                                                        INP 4540
        WRITE (UNO, 9250) SPN(I), ISCHG(I), MBASE(I)                    INP 4550
                                                                        INP 4560
        X     = X + MBASE(I)                                            INP 4570
        LINE = LINE + 1                                                 INP 4580
        READ (UNI, 9210, ERR = 150) KRXN(I), ISCOMP(I),                 INP 4590
     .       (COEF(I,J), IDN(I,J), J=1,ISCOMP(I))                       INP 4600
                                                                        INP 4610
        IPGLN = IPGLN + 1                                               INP 4620
        IF (IPGLN .GT. 57) CALL PAGE                                    INP 4630
30    CONTINUE                                                          INP 4640
                                                                        INP 4650
      IF (DABS(1.0D00 - X) .GT. 0.001) THEN                             INP 4660
        WRITE (UNO, '(A, A, A)')                                        INP 4670
     .       ' ERROR in absorption/ion exchange',                       INP 4680
     .       ' data.  The sum of fraction of',                          INP 4690
     .       ' surface sites is not 1.0'                                INP 4700
        STOP                                                            INP 4710
      END IF                                                            INP 4720
                                                                        INP 4730
      WRITE (UNO, '(11X, A, A)') 'K  =   1. *          ',              INP 4740
     .                           '   * Coef  *  ID    +   ....  '      INP 4750
```

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                                                                      INP 4760
      DO 40 I = 1, INSP                                               INP 4770
        WRITE (UNO, 9260) KRXN(I), SPN(I), (COEF(I,J), IDN(I,J),      INP 4780
     .                                        J = 1, ISCOMP(I))      INP 4790
        IPGLN = IPGLN + 1                                             INP 4800
        IF (IPGLN .GT. 57) CALL PAGE                                  INP 4810
   40   CONTINUE                                                      INP 4820
                                                                      INP 4830
      END IF                                                          INP 4840
      IF (IEXCH .GT. 0) THEN                                          INP 4850
        IF (CEC .LE. CPUMIN) CEC = TAREA * SAREA * 1000.0 / AVOG      INP 4860
      END IF                                                          INP 4870
                                                                      INP 4880
C -------------------------------------------------------------------|INP 4890
C     Precipitation/mixing/boiling option                             |INP 4900
C -------------------------------------------------------------------|INP 4910
C       IF (MIXFLG .EQ. 0) THEN set all values read equal to zero     |INP 4920
C -------------------------------------------------------------------|INP 4930
                                                                      INP 4940
      IF (IPGLN .GT. 59) CALL PAGE                                    INP 4950
      IDDP  = 0                                                       INP 4960
      IDSAT = 0                                                       INP 4970
                                                                      INP 4980
      LINE = LINE + 1                                                 INP 4990
      READ (UNI, 9100, ERR = 150) IBMIX, ITMIX                        INP 5000
      IF (IPGLN .GT. 59) CALL PAGE                                    INP 5010
      IPGLN = IPGLN + 2                                               INP 5020
      WRITE (UNO, 9130) 'IBMIX', 'ITMIX'                              INP 5030
      WRITE (UNO, 9110)  IBMIX,   ITMIX                               INP 5040
      IF (MIXFLG .NE. 0) THEN                                         INP 5050
        IF (IPGLN .GT. 59) CALL PAGE                                  INP 5060
        IPGLN = IPGLN + 2                                             INP 5070
        IF (IBMIX .EQ. 1) THEN                                        INP 5080
          WRITE (UNO, 9710)                                           INP 5090
        ELSE IF (IBMIX .EQ. 2) THEN                                   INP 5100
          WRITE (UNO, 9720)                                           INP 5110
        ELSE IF (IBMIX .EQ. 3) THEN                                   INP 5120
          WRITE (UNO, 9730)                                           INP 5130
        END IF                                                        INP 5140
      END IF                                                          INP 5150
      IF (IBMIX .EQ. 1) THEN                                          INP 5160
        IF (ITMIX .GT. 0) THEN                                        INP 5170
          LINE = LINE + 1                                             INP 5180
          IF (MIXFLG .EQ. 0) THEN                                     INP 5190
            WRITE (UNO, 9080) '      SPECIES', 'MOLALITY'             INP 5200
            IPGLN = IPGLN + 1                                         INP 5210
            IF (IPGLN .GT. 59) CALL PAGE                              INP 5220
          END IF                                                      INP 5230
          DO 50 I = 1, ITMIX                                          INP 5240
            LINE = LINE + 1                                           INP 5250
            READ (UNI, 9290, ERR = 150) IDMIX(I), AMOL(I)             INP 5260
            IF (MIXFLG .EQ. 0) THEN                                   INP 5270
              WRITE (UNO, 9490)  PAGE1(IDMIX(I)), AMOL(I)             INP 5280
              IPGLN = IPGLN + 1                                       INP 5290
              IF (IPGLN .GT. 59) CALL PAGE                            INP 5300
            ELSE                                                      INP 5310
              IDMIX(I) = 0                                            INP 5320
              AMOL(I)  = 0.0                                          INP 5330
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        END IF                                                              INP 5340
50    CONTINUE                                                              INP 5350
      ELSE IF (ITMIX .EQ. 0) THEN                                           INP 5360
        LINE = LINE + 1                                                     INP 5370
        READ (UNI, 9270, ERR = 150) IDSAT, IDDP, DP                         INP 5380
        IF (MIXFLG .EQ. 0) THEN                                             INP 5390
          WRITE (UNO, 9420) PAGE3(IDSAT), IDSAT                             INP 5400
          IPGLN = IPGLN + 1                                                 INP 5410
          IF (IPGLN .GT. 59) CALL PAGE                                      INP 5420
        END IF                                                              INP 5430
        IF (IDDP .EQ. 0) THEN                                               INP 5440
          LINE = LINE + 1                                                   INP 5450
          READ (UNI, 9280, ERR = 150) ITT                                   INP 5460
          IF (MIXFLG .EQ. 0) THEN                                           INP 5470
            WRITE (UNO, 9440)                                               INP 5480
            IPGLN = IPGLN + 1                                               INP 5490
            IF (IPGLN .GT. 59) CALL PAGE                                    INP 5500
          END IF                                                            INP 5510
          DO 60 I = 1, ITT                                                  INP 5520
            LINE = LINE + 1                                                 INP 5530
            READ (UNI, 9290, ERR = 150) IRXDP(I), RXDP(I)                   INP 5540
            IF (MIXFLG .EQ. 0) THEN                                         INP 5550
              WRITE (UNO, 9460) IRXDP(I), PAGE1(IRXDP(I)), RXDP(I)         INP 5560
              IPGLN = IPGLN + 1                                             INP 5570
              IF (IPGLN .GT. 59) CALL PAGE                                  INP 5580
            END IF                                                          INP 5590
60        CONTINUE                                                          INP 5600
          IF (MIXFLG .EQ. 0) THEN                                           INP 5610
            WRITE (UNO, 9450) DP                                            INP 5620
            IPGLN = IPGLN + 1                                               INP 5630
            IF (IPGLN .GT. 59) CALL PAGE                                    INP 5640
          ELSE                                                              INP 5650
            IDSAT = 0                                                       INP 5660
            IDDP  = 0                                                       INP 5670
            ITT   = 0                                                       INP 5680
            DP    = 0.0                                                     INP 5690
          END IF                                                            INP 5700
        ELSE                                                                INP 5710
          IF (MIXFLG .EQ. 0) THEN                                           INP 5720
            WRITE (UNO, 9430) PAGE3(IDDP), IDDP                             INP 5730
            IPGLN = IPGLN + 1                                               INP 5740
            IF (IPGLN .GT. 59) CALL PAGE                                    INP 5750
          ELSE                                                              INP 5760
            IDDP = 0                                                        INP 5770
          END IF                                                            INP 5780
        END IF                                                              INP 5790
      ELSE IF (ITMIX .LT. 0) THEN                                           INP 5800
        LINE = LINE + 1                                                     INP 5810
        READ (UNI, 9290, ERR = 150) IDDP, AMOL(1)                           INP 5820
        IF (MIXFLG .EQ. 0) THEN                                             INP 5830
          WRITE (UNO, 9140) 'IDDP ', 'AMOL(1) '                             INP 5840
          WRITE (UNO, 9410) IDDP, AMOL(1)                                   INP 5850
          IPGLN = IPGLN + 2                                                 INP 5860
          IF (IPGLN .GT. 59) CALL PAGE                                      INP 5870
        ELSE                                                                INP 5880
          IDDP    = 0                                                       INP 5890
          AMOL(1) = 0.0                                                     INP 5900
        END IF                                                              INP 5910
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        END IF                                                                  INP 5920
        IF (MIXFLG .EQ. 1) MIXFLG = 0                                           INP 5930
      ELSE IF (IBMIX .EQ. 3) THEN                                               INP 5940
        IF (MIXFLG .EQ. 0) THEN                                                 INP 5950
          LINE = LINE + 1                                                       INP 5960
          READ (UNI, 9070, ERR = 150) FBOIL                                     INP 5970
          WRITE (UNO, 9470) FBOIL                                               INP 5980
          IPGLN = IPGLN + 1                                                     INP 5990
          IF (IPGLN .GT. 59) CALL PAGE                                          INP 6000
        ELSE                                                                    INP 6010
          READ (UNI, '(A80)') DUMMY                                             INP 6020
          MIXFLG = 0                                                            INP 6030
        END IF                                                                  INP 6040
                                                                                INP 6050
      ELSE IF (IBMIX .EQ. 2) THEN                                               INP 6060
        IF (MIXFLG .EQ. 0) THEN                                                 INP 6070
          LINE = LINE + 1                                                       INP 6080
          READ (UNI, 9290, ERR = 150) INMIX, DFRAC1, DINC, MIXFLE               INP 6090
          IPGLN = IPGLN + 2                                                     INP 6100
          IF (IPGLN .GT. 59) CALL PAGE                                          INP 6110
          WRITE (UNO, 9480) INMIX, DFRAC1, DINC                                 INP 6120
          IF (MIXFLE .NE. '      ') THEN                                        INP 6130
              WRITE (UNO, 9481) MIXFLE(1:40)                                    INP 6140
          ELSE                                                                  INP 6150
              WRITE (UNO, 9482)                                                 INP 6160
          END IF                                                                INP 6170
          MIXFLG = 1                                                            INP 6180
        ELSE                                                                    INP 6190
          READ (UNI, '(A80)') DUMMY                                             INP 6200
          MIXFLG = 0                                                            INP 6210
        END IF                                                                  INP 6220
      END IF                                                                    INP 6230
                                                                                INP 6240
C -----------------------------------------------------------------------|INP 6250
C     Optional user Read in miscellaneous options                        |INP 6260
C -----------------------------------------------------------------------|INP 6270
                                                                                INP 6280
      LINE = LINE + 1                                                           INP 6290
      READ (UNI, 9180, ERR = 150) (ODUM(I), NDUM(I), XDUM(I), I = 1, 6)         INP 6300
      WRITE (UNO, 9340) TEMP                                                    INP 6310
      WRITE (UNO, 9190) (ODUM(I), NDUM(I), XDUM(I), I = 1, 6)                   INP 6320
      IPGLN = IPGLN + 2                                                         INP 6330
      IF (IPGLN .GT. 59) CALL PAGE                                              INP 6340
                                                                                INP 6350
      LINE = LINE + 1                                                           INP 6360
      READ (UNI, 9180, ERR = 150) (ODUM(I), NDUM(I), XDUM(I), I = 7, 12)INP 6370
      WRITE (UNO, 9340) HITEMP                                                  INP 6380
      WRITE (UNO, 9190) (ODUM(I), NDUM(I), XDUM(I), I = 7, 12)                  INP 6390
      IPGLN = IPGLN + 2                                                         INP 6400
      IF (IPGLN .GT. 59) CALL PAGE                                              INP 6410
                                                                                INP 6420
C -----------------------------------------------------------------------|INP 6430
C     Read user defined anions                                           |INP 6440
C -----------------------------------------------------------------------|INP 6450
                                                                                INP 6460
      LINE = LINE + 1                                                           INP 6470
      READ (UNI, 9300, ERR = 150) ANS1, ANS2                                    INP 6480
      WRITE (UNO, 9130) 'ANS1', 'ANS2'                                          INP 6490
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      WRITE (UNO, 9110) ANS1, ANS2                                      INP 6500
      IPGLN = IPGLN + 2                                                 INP 6510
      IF (IPGLN .GT. 59) CALL PAGE                                      INP 6520
                                                                        INP 6530
      DO 70 I = 1, 45                                                   INP 6540
        XD(1,I) = 0.0D0                                                 INP 6550
        XD(2,I) = 0.0D0                                                 INP 6560
   70 CONTINUE                                                          INP 6570
                                                                        INP 6580
      IF (ANS1 .EQ. 0 .AND. ANS2 .NE. 0) THEN                           INP 6590
        ANS1 = ANS2                                                     INP 6600
        ANS2 = 0                                                        INP 6610
      END IF                                                            INP 6620
                                                                        INP 6630
      IF (ANS1 .GT. 0) THEN                                             INP 6640
        WRITE (UNO, 9500) 'NAME', 'CONC', 'GFW', 'CHARGE', 'DHA'        INP 6650
        LINE = LINE + 1                                                 INP 6660
        READ (UNI, 9360, ERR = 150) CUNITS(MXSP+1), GFW(MXSP+1),        INP 6670
     .                  Z(MXSP+1), DHA(MXSP+1), PAGE1(MXSP+1)          INP 6680
        WRITE (UNO, 9380) PAGE1(MXSP+1), CUNITS(MXSP+1), GFW(MXSP+1),   INP 6690
     .                  Z(MXSP+1), DHA(MXSP+1)                         INP 6700
        IPGLN = IPGLN + 2                                               INP 6710
        IF (IPGLN .GT. 59) CALL PAGE                                    INP 6720
        WRITE (UNO, 9400)                                               INP 6730
        IPGLN = IPGLN + 1                                               INP 6740
                                                                        INP 6750
        DO 80 I = 1, ANS1                                               INP 6760
          LINE = LINE + 1                                               INP 6770
          READ (UNI, 9370, ERR = 150) INDEX, DNA, LOWKT, HIGHKT, NAME   INP 6780
          WRITE (UNO, 9390) NAME, INDEX, LOWKT, HIGHKT, DNA             INP 6790
          IPGLN = IPGLN + 1                                             INP 6800
          IF (IPGLN .GT. 59) CALL PAGE                                  INP 6810
                                                                        INP 6820
          ACTUAL = MXSP + INDEX                                         INP 6830
          PAGE1(ACTUAL) = NAME                                          INP 6840
                                                                        INP 6850
          XD(1,INDEX) = LOWKT                                           INP 6860
          XD(2,INDEX) = HIGHKT                                          INP 6870
                                                                        INP 6880
          GFW(ACTUAL) = GFW(MXSP+1) + GFW(ILQ(INDEX))                   INP 6890
          IF (INDEX .EQ. 3) GFW(ACTUAL) = GFW(ACTUAL) + GFW(ILQ(INDEX)) INP 6900
                                                                        INP 6910
          Z(ACTUAL) = Z(MXSP+1) + Z(ILQ(INDEX))                         INP 6920
          IF (INDEX .EQ. 3) Z(ACTUAL) = Z(ACTUAL) + Z(ILQ(INDEX))       INP 6930
                                                                        INP 6940
          DHA(ACTUAL) = DEBYE (Z(ACTUAL), DNA)                          INP 6950
                                                                        INP 6960
   80   CONTINUE                                                        INP 6970
      END IF                                                            INP 6980
                                                                        INP 6990
      IF (ANS2 .NE. 0) THEN                                             INP 7000
        WRITE (UNO, 9500) 'NAME', 'CONC', 'GFW', 'CHARGE', 'DHA'        INP 7010
        LINE = LINE + 1                                                 INP 7020
        READ (UNI, 9360, ERR = 150) CUNITS(MXSP+16), GFW(MXSP+16),      INP 7030
     .        Z(MXSP+16), DHA(MXSP+16), PAGE1(MXSP+16)                  INP 7040
        WRITE (UNO, 9380) PAGE1(MXSP+16), CUNITS(MXSP+16), GFW(MXSP+16),INP 7050
     .         Z(MXSP+16), DHA(MXSP+16)                                 INP 7060
        IPGLN = IPGLN + 2                                               INP 7070
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        IF (IPGLN .GT. 59) CALL PAGE                                        INP 7080
        WRITE (UNO, 9400)                                                   INP 7090
        IPGLN = IPGLN + 1                                                   INP 7100
        DO 90 I = 1, ANS2                                                   INP 7110
          LINE = LINE + 1                                                   INP 7120
          READ (UNI, 9370, ERR = 150) INDEX, DNA, LOWKT, HIGHKT, NAME       INP 7130
          WRITE (UNO, 9390) NAME, INDEX, LOWKT, HIGHKT, DNA                 INP 7140
          IPGLN = IPGLN + 1                                                 INP 7150
          IF (IPGLN .GT. 59) CALL PAGE                                      INP 7160
                                                                            INP 7170
          ACTUAL = MXSP + INDEX + 15                                        INP 7180
          PAGE1(ACTUAL) = NAME                                              INP 7190
                                                                            INP 7200
          XD(1,INDEX+15) = LOWKT                                            INP 7210
          XD(2,INDEX+15) = HIGHKT                                           INP 7220
                                                                            INP 7230
          GFW(ACTUAL) = GFW(MXSP+16) + GFW(ILQ(INDEX))                      INP 7240
          IF (INDEX .EQ. 3) GFW(ACTUAL) = GFW(ACTUAL) + GFW(ILQ(INDEX))     INP 7250
                                                                            INP 7260
          Z(ACTUAL) = Z(MXSP+16) + Z(ILQ(INDEX))                            INP 7270
          IF (INDEX .EQ. 3) Z(ACTUAL) = Z(ACTUAL) + Z(ILQ(INDEX))           INP 7280
                                                                            INP 7290
          DHA(ACTUAL) = DEBYE (Z(ACTUAL), DNA)                              INP 7300
                                                                            INP 7310
   90   CONTINUE                                                           INP 7320
        END IF                                                              INP 7330
                                                                            INP 7340
C ------------------------------------------------------------------------|INP 7350
C     Read user defined cations                                           |INP 7360
C ------------------------------------------------------------------------|INP 7370
                                                                            INP 7380
        LINE = LINE + 1                                                     INP 7390
        READ (UNI, 9510) NUMCOM, Z(MXSP+31), DHA(MXSP+31), GFW(MXSP+31),    INP 7400
     .       CUNITS(MXSP+31), PAGE1(MXSP+31)                                INP 7410
        IF (NUMCOM .GT. 0) THEN                                             INP 7420
          WRITE (UNO, 9520) 'NAME', 'CHARGE', 'DHA', 'GFW', 'CONC'          INP 7430
          WRITE (UNO, 9530) PAGE1(MXSP+31), Z(MXSP+31), DHA(MXSP+31),       INP 7440
     .          GFW(MXSP+31), CUNITS(MXSP+31)                               INP 7450
          IPGLN = IPGLN + 2                                                 INP 7460
          IF (IPGLN .GT. 59) CALL PAGE                                      INP 7470
          ILR(12) = MXSP + 1                                                INP 7480
          ILR(13) = MXSP + 16                                               INP 7490
                                                                            INP 7500
          DO 100 I = 1, NUMCOM                                              INP 7510
            WRITE (UNO, 9540) '  NAME', 'DHA', 'LOWKT', 'HIGHKT'           INP 7520
            READ (UNI, 9550) INDEX, DNA, LOWKT, HIGHKT, NAME                INP 7530
            WRITE (UNO, 9560) INDEX, NAME, DNA, LOWKT, HIGHKT               INP 7540
            IPGLN = IPGLN + 2                                               INP 7550
            IF (IPGLN .GT. 59) CALL PAGE                                    INP 7560
                                                                            INP 7570
            ACTUAL = MXSP + INDEX + 30                                      INP 7580
                                                                            INP 7590
            PAGE1(ACTUAL) = NAME                                            INP 7600
            Z(ACTUAL)     = Z(MXSP+31) + Z(ILR(INDEX-1))                    INP 7610
                                                                            INP 7620
            DHA(ACTUAL) = DEBYE (Z(ACTUAL), DNA)                            INP 7630
                                                                            INP 7640
            GFW(ACTUAL) = GFW(MXSP+31) + GFW(ILR(INDEX-1))                  INP 7650
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                                                                      INP 7660
        ACTUAL = 30 + INDEX                                           INP 7670
                                                                      INP 7680
        XD(1,ACTUAL) = LOWKT                                          INP 7690
        XD(2,ACTUAL) = HIGHKT                                         INP 7700
  100   CONTINUE                                                      INP 7710
    END IF                                                            INP 7720
                                                                      INP 7730
C ------------------------------------------------------------------|INP 7740
C     Read user defined minerals                                    |INP 7750
C ------------------------------------------------------------------|INP 7760
                                                                      INP 7770
    LINE = LINE + 1                                                   INP 7780
    READ (UNI, 9270, ERR = 150) NUMINS                                INP 7790
    IPGLN = IPGLN + 1                                                 INP 7800
    IF (IPGLN .GT. 59) CALL PAGE                                      INP 7810
    WRITE (UNO, *) '  Number of Additional Minerals = ', NUMINS       INP 7820
                                                                      INP 7830
    DO 120 I = 1, 5                                                   INP 7840
       MINLOG(1,I) = 999.9                                            INP 7850
       MINLOG(2,I) = 999.9                                            INP 7860
       DO 110 J = 1, 9                                                INP 7870
         MINCO(J,I) = 0.0                                             INP 7880
         IF (J .LE. 8) MININD(J,I) = 0                                INP 7890
  110  CONTINUE                                                       INP 7900
  120 CONTINUE                                                       INP 7910
                                                                      INP 7920
    DO 140 I = 1, NUMINS                                              INP 7930
      LINE = LINE + 1                                                 INP 7940
      READ (UNI, 9570, ERR = 150) MINLOG(1,I), MINLOG(2,I),           INP 7950
     .                            MINCO(9,I), PAGE3(MXMNK+I)         INP 7960
      LINE = LINE + 1                                                 INP 7970
      READ (UNI, 9210, ERR = 150) (MINCO(J,I), MININD(J,I), J = 1, 8) INP 7980
                                                                      INP 7990
      IPGLN = IPGLN + 3                                               INP 8000
      IF (IPGLN .GT. 59) CALL PAGE                                    INP 8010
                                                                      INP 8020
      NOSE = 0                                                        INP 8030
      DO 130 J = 1, 8                                                 INP 8040
        IF (MINCO(J,I) .GT. 0) NOSE = NOSE + 1                        INP 8050
  130   CONTINUE                                                      INP 8060
                                                                      INP 8070
      WRITE (UNO, 9580) PAGE3(MXMNK+I), 'Log K at T1 = ',             INP 8080
     .             MINLOG(1,I), 'Log K at T2 = ', MINLOG(2,I)       INP 8090
      WRITE (UNO, 9590) (MINCO(J,I), '*', PAGE1(MININD(J,I)), ' + ',  INP 8100
     .                   J = 1, NOSE), MINCO(9,I)                   INP 8110
  140 CONTINUE                                                       INP 8120
                                                                      INP 8130
C ------------------------------------------------------------------|INP 8140
C     Assign flags and convergence factors                          |INP 8150
C ------------------------------------------------------------------|INP 8160
                                                                      INP 8170
    LINE = LINE + 1                                                   INP 8180
    READ (UNI, 9300, ERR = 150) NUFLAG, IPIT, (FLAGS(I), I = 1, 6)    INP 8190
    WRITE (UNO, 9310) NUFLAG, IPIT                                    INP 8200
    WRITE (UNO, 9320) 'Fe', 'Cu', 'Hg', 'Mn', ' U', ' V',             INP 8210
     .                (FLAGS(I), I = 1, 6)                           INP 8220
    IPGLN = IPGLN + 2                                                 INP 8230
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      IF (IPGLN .GT. 59) CALL PAGE                                          INP 8240
                                                                            INP 8250
      LINE = LINE + 1                                                       INP 8260
      READ (UNI, 9600, ERR = 150) INFORM, RATIO, GEOTH, IPRIN1, IPRIN2,     INP 8270
     .                            OUTIN                                    INP 8280
                                                                            INP 8290
      LINE = LINE + 1                                                       INP 8300
      READ (UNI, 9070, ERR = 150) CONV1, CONV2                              INP 8310
                                                                            INP 8320
      IF (CONV2 .LT. 1.0D-08 .OR. CONV2 .GT. 1.0D-2) CONV2 = 0.5D-04        INP 8330
      IF (CONV1 .LT. 1.0D-08 .OR. CONV1 .GT. 1.0D-2) CONV1 = 0.5D-04        INP 8340
                                                                            INP 8350
      WRITE (UNO, 9350)                                                     INP 8360
      WRITE (UNO, 9080) ' INFORM ', '  RATIO ', '  GEOTH ',                INP 8370
     .                  ' IPRIN1 ', ' IPRIN2 '                             INP 8380
      WRITE (UNO, 9120) INFORM, RATIO, GEOTH, IPRIN1, IPRIN2                INP 8390
      IF (OUTIN .NE. '    ') THEN                                           INP 8400
          WRITE( UNO, 9610) OUTIN                                           INP 8410
          IPGLN = IPGLN + 1                                                 INP 8420
      END IF                                                                INP 8430
      WRITE (UNO, 9330) CONV1, CONV2                                        INP 8440
      IPGLN = IPGLN + 4                                                     INP 8450
                                                                            INP 8460
C -------------------------------------------------------------------------|INP 8470
C     Set defaults                                                         |INP 8480
C -------------------------------------------------------------------------|INP 8490
                                                                            INP 8500
      IF (DENS .LT. CPUMIN) THEN                                            INP 8510
        DNS  = 'U'                                                          INP 8520
        DENS = 1.0D0                                                        INP 8530
      ELSE                                                                  INP 8540
        DNS = 'Y'                                                           INP 8550
      END IF                                                                INP 8560
                                                                            INP 8570
      IF (DABS(HITEMP-TEMP) .LE. CPUMIN) HITEMP = 0.0D00                    INP 8580
      IF (HITEMP .GT. CPUMIN) PHHIT = 1                                     INP 8590
                                                                            INP 8600
C -------------------------------------------------------------------------|INP 8610
C     If the gas or co2 option is to be used, initialize this              |INP 8620
C     option so that it is performed after the hi-temperature              |INP 8630
C     option, if requested, is performed.                                  |INP 8640
C -------------------------------------------------------------------------|INP 8650
                                                                            INP 8660
      IOPT  = 0                                                             INP 8670
                                                                            INP 8680
      IF (DABS(DDCO2) .GT. CPUMIN .OR. DABS(DDNH3) .GT. CPUMIN .OR.         INP 8690
     .    DABS(DDH2S) .GT. CPUMIN .OR. DABS(DDCH4) .GT. CPUMIN)             INP 8700
     .    IOPT = 2                                                          INP 8710
                                                                            INP 8720
      IF (ICO2 .GT. 0 .AND. IMCO3 .GT. 0) THEN                              INP 8730
        IOPT = 1                                                            INP 8740
      ELSE                                                                  INP 8750
        ICO2 = 0                                                            INP 8760
      END IF                                                                INP 8770
                                                                            INP 8780
      IF (TCO2M .GT. CPUMIN .OR. TCH4M .GT. CPUMIN                          INP 8790
     .                      .OR. TH2SM .GT. CPUMIN) IPHASE = 2              INP 8800
                                                                            INP 8810
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      IPGLN = 60                                                          INP 8820
                                                                          INP 8830
      RETURN                                                              INP 8840
                                                                          INP 8850
C -----------------------------------------------------------------------|INP 8860
C     Error Messages                                                     |INP 8870
C -----------------------------------------------------------------------|INP 8880
                                                                          INP 8890
  150 CONTINUE                                                            INP 8900
      WRITE (UNO, 9160) TOF                                               INP 8910
      WRITE (UNO, 9170) LINE                                              INP 8920
      STOP                                                                INP 8930
                                                                          INP 8940
                                                                          INP 8950
C -----------------------------------------------------------------------|INP 8960
C     Out of data                                                        |INP 8970
C     If there are no more data sets in file assigned to unit 5, stop.   |INP 8980
C -----------------------------------------------------------------------|INP 8990
                                                                          INP 9000
  160 CLOSE (UNI)                                                         INP 9010
      CLOSE (UNO)                                                         INP 9020
      STOP                                                                INP 9030
                                                                          INP 9040
C -----------------------------------------------------------------------|INP 9050
C     Format statements                                                  |INP 9060
C -----------------------------------------------------------------------|INP 9070
                                                                          INP 9080
 9000 FORMAT (A80)                                                        INP 9090
 9010 FORMAT ('  ****** INPUT DATA ECHO ****** ',//,'  TITLE : ',A80)     INP 9100
 9020 FORMAT (4E10.4, A5)                                                 INP 9110
 9030 FORMAT (2X, 6(A10, 2X))                                             INP 9120
 9040 FORMAT (2X, 5(E10.4, 2X), A5)                                       INP 9130
 9050 FORMAT (2X,10(E10.4, 2X))                                           INP 9140
 9060 FORMAT ('  CONCENTRATION UNITS :', 2X, A5)                         INP 9150
 9070 FORMAT (8E10.4)                                                     INP 9160
 9080 FORMAT (2X, 10(2X, A, 2X))                                          INP 9170
 9090 FORMAT (2X, 10(2X, A))                                              INP 9180
 9100 FORMAT (2I2, 2E10.4)                                                INP 9190
 9110 FORMAT (2X,2(3X,I3,4X),E12.5,2X,F12.4)                              INP 9200
 9120 FORMAT (2X,  6(5X, I2, 5X))                                         INP 9210
 9130 FORMAT (5X, A8, 2X, A8)                                             INP 9220
 9140 FORMAT (A8, 2X, A8)                                                 INP 9230
 9150 FORMAT (3E10.4, I3)                                                 INP 9240
 9160 FORMAT (A1)                                                         INP 9250
 9170 FORMAT (5X,'ERROR IN READING REQUIRED INPUT LINE NO. ', I2,         INP 9260
     .        /,'   Program Stop')                                       INP 9270
 9180 FORMAT (6(A1, I4, E10.4))                                           INP 9280
 9190 FORMAT (6(1X, A1, 1X, I4, 1X, E10.4,3X))                            INP 9290
 9200 FORMAT (I4, E10.4, A10)                                             INP 9300
 9210 FORMAT (11(E10.4, I3))                                              INP 9310
 9220 FORMAT ('  Surface Chemistry input for ',A)                         INP 9320
 9230 FORMAT (2X, 3(E12.4, 2X), 3X, I3)                                   INP 9330
 9240 FORMAT (2X, 3(E10.4, 2X), 3X, I3)                                   INP 9340
 9250 FORMAT (2X, A10, 6X, I3, 4X, E10.4)                                 INP 9350
 9260 FORMAT (4X, F10.4, 3X, A, 4(5(5X, E12.5, 2X, I3), /))               INP 9360
 9270 FORMAT (2I4,E10.4)                                                  INP 9370
 9280 FORMAT (I4,F12.0)                                                   INP 9380
 9290 FORMAT (I4, 2E10.4, A80)                                            INP 9390
```

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9300 FORMAT (8I2, A80)                                                  INP 9400
9310 FORMAT ('  FLAG FOR ACTIVITY COEFF OF NEUTRAL SPECIES:    ',I2,/,  INP 9410
     .       '  FLAG FOR ACTIVITY COEFF BY PITZERS EQUATIONS: ',I2)    INP 9420
9320 FORMAT ('  FLAGS FOR CALCULATING REDOX SPECIES: ',/,               INP 9430
     .          6(2X, A2),/,                                          INP 9440
     .          6(2X, I2))                                            INP 9450
9330 FORMAT ('  TOLERANCE FACTORS:', 2X, 'CONV1 = ', E12.4, 2X,        INP 9460
     .       'CONV2 = ', E12.4)                                       INP 9470
9340 FORMAT ('  LOG KT TO BE CHANGED AT TEMP = ', F6.2)                 INP 9480
9350 FORMAT ('  PRINTING OPTIONS:')                                     INP 9490
9360 FORMAT (2E10.4, I2, E10.4, A8)                                     INP 9500
9370 FORMAT (I2, 3E10.4, A8)                                            INP 9510
9380 FORMAT (1X, A8, 4X, E10.4, 2X, E10.4, 6X, I4, 4X, E10.4)           INP 9520
9390 FORMAT (1X, A8, 4X, I4, 4X, E10.4, 2X, E10.4, 2X, E10.4)           INP 9530
9400 FORMAT (4X, 'NAME', 4X, 'INDEX', 5X, 'LOWKT', 7X, 'HIGHKT',        INP 9540
     .       6X, 'DHA ')                                              INP 9550
9410 FORMAT (2X, I4, 2X, E10.4)                                         INP 9560
9420 FORMAT ('  MINERAL TO BE DISSOLVED/PRECIPITATED TO SATURATION:',  INP 9570
     .       ' ', A8, 5X, ' Index number: ',I3)                       INP 9580
9430 FORMAT ('  MINERAL TO BE DISSOLVED/PRECIPITATED:',15X,             INP 9590
     .         A8, 5X, ' Index number: ',I3)                          INP 9600
9440 FORMAT ('  REACTION FOR SATURATION: ', 3X, 'ID#', 3X,              INP 9610
     .       'Species ', 5X, 'STOICH COEFF')                          INP 9620
9450 FORMAT ('  Step direction/scaling factor = ', E12.5)               INP 9630
9460 FORMAT (' ', 29X, I3, 3X, A8, 5X, E12.5)                           INP 9640
9470 FORMAT ('  FRACTION OF BOILING: ',F12.4)                           INP 9650
9480 FORMAT (1X,' Number of mixtures = ', I3, ' starting at',           INP 9660
     .          ' fraction of solution one = ', F12.4,                INP 9670
     .          ' using a step increment of: ', F12.4 )               INP 9680
9481 FORMAT (1X,' and reading the second water composition from',       INP 9690
     .          ' the file ',A)                                       INP 9700
9482 FORMAT (1X,' and reading the second water composition from',       INP 9710
     .        /,' the data set following this one. ')                 INP 9720
9490 FORMAT (3X, A8, 5X, E12.5)                                         INP 9730
9500 FORMAT (3X, A4, 8X, A4, 8X, A3, 8X, A6, 8X, A3)                    INP 9740
9510 FORMAT (2I2, 3E10.4, A8)                                           INP 9750
9520 FORMAT (3X, A4, 7X, A6, 5X, A3, 5X, A3, 5X, A4)                    INP 9760
9530 FORMAT (1X, A8, 5X, I2, 5X, F4.1, 5X, F8.3, 5X, 1P, E10.4)         INP 9770
9540 FORMAT (3X, A6, 7X, A3, 5X, A5, 5X, A5)                            INP 9780
9550 FORMAT (I2, 3E10.4, A8)                                            INP 9790
9560 FORMAT (1X, I2, 2X, A8, 3(5X, E10.4))                              INP 9800
9570 FORMAT (3E10.4, A8)                                                INP 9810
9580 FORMAT (1X, A8, 5X, A14, F7.2, 5X, A14, F7.2)                      INP 9820
9590 FORMAT (1X, 9(F5.2, A1, A8, A3))                                   INP 9830
9600 FORMAT (5I2, A80)                                                  INP 9840
9610 FORMAT ('  Restart information will be written to the file ',      INP 9850
     .       A)                                                       INP 9860
9710 FORMAT (' Because the Mixing option was chosen in the previous'    INP 9870
     .       ' data set,',/,                                          INP 9880
     .       ' the DISSOLUTION/PRECIPITATION option will not be',     INP 9890
     .       ' performed on this data set.')                          INP 9900
9720 FORMAT (' Because the Mixing option was chosen in the previous'    INP 9910
     .       ' data set,',/,                                          INP 9920
     .       ' the MIXING information will not be read from this'     INP 9930
     .       ' data set.')                                            INP 9940
9730 FORMAT (' Because the Mixing option was chosen in the previous'    INP 9950
     .       ' data set,',/,                                          INP 9960
     .       ' the BOILING option will not be performed on this data', INP 9970
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     .       ' set.')                                                    INP 9980
      END                                                                INP 9990



      SUBROUTINE INTIAL (OK, ALK, INFORM, RATIO, GAMMA, TEMP, HITEMP,    INT 0010
     .                   PRESS, HTOTI, OHTOTI, ICO2, IMCO3, IBMIX,      INT 0020
     .                   FCCSAT, IEXCH, ISAT, IPHNUM, JCCST)            INT 0030
C ================================================================================|INT 0040
C     This routine initializes certain values when each new data                   |INT 0050
C     set is read into solmneqf.                                                   |INT 0060
C --------------------------------------------------------------------------------|INT 0070
C     ALFA       DBL   Activity of aqueous species i                               |INT 0080
C     ALK        INT   Flag for distribution of carbonate species                  |INT 0090
C     CEC        DBL   Cation exchange capacity                                    |INT 0100
C     COEF       DBL   Stoichiometric coefficient and Id number                    |INT 0110
C     CUNITS     DBL   Analytical input concentration                              |INT 0120
C     DCH4       DBL   Concentration of CH4 lost up annulus                        |INT 0130
C     DDCH4      DBL   Concentration of CH4 lost before pH measurement             |INT 0140
C     DCO2       DBL   Concentration of CO2 lost up annulus                        |INT 0150
C     DDCO2      DBL   Concentration of CO2 lost before pH measurement             |INT 0160
C     DH2S       DBL   Concentration of H2S lost up annulus                        |INT 0170
C     DDH2S      DBL   Concentration of H2S lost before pH measurement             |INT 0180
C     DNH3       DBL   Concentration of NH3 lost up annulus                        |INT 0190
C     DDNH3      DBL   Concentration of NH3 lost before pH measurement             |INT 0200
C     DSEP       DBL   Density of oil at 15 degree C                               |INT 0210
C     FCCSAT     DBL   Tolerance factor for pH and CO2 options                     |INT 0220
C     GAMMA      DBL   Activity coefficient                                        |INT 0230
C     HITEMP     DBL   In-situ temperature                                         |INT 0240
C     HTOTI      DBL   Sum of H in system                                          |INT 0250
C     I          INT   Loop counting variable                                      |INT 0260
C     IBMIX      INT   Switch for mixing option                                    |INT 0270
C     ICO2       INT   Switch for co2 option                                       |INT 0280
C     IEXCH      INT   Switch for exchange/adsorption option                       |INT 0290
C     IMCO3      INT   Selects CO2 option                                          |INT 0300
C     INFORM     INT   Flag to print all the log K values in data base             |INT 0310
C     IOPT       INT   Switch for CO2 option                                       |INT 0320
C     IPHASE     INT   Gas/Oil/Water gas redistibution                             |INT 0330
C     IPHNUM     INT   Counter used in PHCALC                                      |INT 0340
C     IRXDP      INT   Id number of the aqueous species to be added                |INT 0350
C     ISAT       INT   Counter used in CO2OPT                                      |INT 0360
C     JCCST      INT   Switch indicating if PHOPT called 1s5 time                  |INT 0370
C     JCO3       INT   Switch to control printing of some headings                 |INT 0380
C     KT1        DBL   Equilibrium constant of the aqueous reactions               |INT 0390
C     M          DBL   Calculated molality of aqueous species                      |INT 0400
C     MBASE      DBL   Equivalence Mole Fraction (initial) on surface              |INT 0410
C     NDUM       INT   Id of mineral/aqueous complex with K(T) changed             |INT 0420
C     NMAX       INT   General array dimension to allow easy expansion             |INT 0430
C     ODUM       CHA   Switch to indicate a mineral/aqueous complex                |INT 0440
C     OHTOTI     DBL   Sum of hydroxide in system                                  |INT 0450
C     OK         INT   Error flag for Lagrange interpolation routine               |INT 0460
C     PHHIT      INT   Switch for ph iteration                                     |INT 0470
C     PPHHIT     INT   Switch for ph iterations                                    |INT 0480
C     PRESS      DBL   Total pressure                                              |INT 0490
C     RATIO      INT   Flag for printing activity ratios of elements               |INT 0500
C     RXDP       DBL   Molal amount of the aqueous species added                   |INT 0510
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C     SCO2       DBL   Sum of CO2 species                                    |INT 0520
C     TAREA      DBL   Site density per unit area                            |INT 0530
C     TCH4M      DBL   Moles CH4 distributed between oil, water, vapor       |INT 0540
C     TCO2M      DBL   Moles CO2 distributed between oil, water, vapor       |INT 0550
C     TEMP       DBL   Temperature of the solution when pH was measured      |INT 0560
C     TH2SM      DBL   Moles H2S distributed between oil, water, vapor       |INT 0570
C     XDUM       DBL   New log K(T) value                                    |INT 0580
C ---------------------------------------------------------------------------|INT 0590
                                                                             INT 0600
      INTEGER NMAX                                                           INT 0610
      PARAMETER (NMAX = 340)                                                 INT 0620
                                                                             INT 0630
      INTEGER ALK, I, IBMIX, ICO2, IDDP, IDN(10,10), IDSAT, IEXCH            INT 0640
      INTEGER IMCO3, INFORM, INSP, IPHASE, IPHNUM, IOPT, IRXDP(10)           INT 0650
      INTEGER ISAT, ISCHG(10), ISCOMP(10), JCO3, NDUM(12), OK                INT 0660
      INTEGER PHHIT, PPHHIT, RATIO                                           INT 0670
                                                                             INT 0680
      CHARACTER * 1 ODUM(12)                                                 INT 0690
                                                                             INT 0700
      DOUBLE PRECISION ALFA(NMAX), ANALM(NMAX), CEC, COEF(10,10)             INT 0710
      DOUBLE PRECISION CUNITS(NMAX), DCH4, DDCH4, DCO2, DDCO2                INT 0720
      DOUBLE PRECISION DH2S, DDH2S, DNH3, DDNH3, DP, FCCSAT, FIXIT           INT 0730
      DOUBLE PRECISION GAMMA(NMAX), HITEMP, HTOT, HTOTI, JCCST               INT 0740
      DOUBLE PRECISION KCH4OL, KCO2OL, KH2SOL, KRXN(10)                      INT 0750
      DOUBLE PRECISION KT1(NMAX), M(NMAX), MBASE(10)                         INT 0760
      DOUBLE PRECISION OHTOT, OHTOTI, PH, PRESS, DSEP, RXDP(10)              INT 0770
      DOUBLE PRECISION SAREA, SCO2, TAREA, TCH4M, TCO2M, TH2SM               INT 0780
      DOUBLE PRECISION TEMP, WROIL, XDUM(12)                                 INT 0790
                                                                             INT 0800
      COMMON /AL    / NDUM, XDUM                                             INT 0810
      COMMON /CH    / ODUM                                                   INT 0820
      COMMON /DIST  / TCO2M,  TCH4M, TH2SM, WROIL, KCH4OL, KCO2OL,           INT 0830
     .                KH2SOL, IPHASE, DSEP                                    INT 0840
      COMMON /EXCHAN/ COEF, MBASE, KRXN, CEC, TAREA, SAREA, IDN,             INT 0850
     .                ISCHG, ISCOMP, INSP                                     INT 0860
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,                 INT 0870
     .                DCH4, DDCH4, IOPT, FIXIT                                INT 0880
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                             INT 0890
      COMMON /SAT   / IDDP, IDSAT, DP, RXDP, IRXDP                           INT 0900
      COMMON /TTK   / KT1                                                    INT 0910
      COMMON /ZPH   / PHHIT, PPHHIT, JCO3, SCO2, HTOT, OHTOT                 INT 0920
                                                                             INT 0930
C ===========================================================================|INT 0940
                                                                             INT 0950
      IF (IBMIX .LE. 0) THEN                                                 INT 0960
        DO 10 I = 1, 12                                                      INT 0970
          ODUM(I) = ' '                                                      INT 0980
          NDUM(I) = 0                                                        INT 0990
          XDUM(I) = 0.0D0                                                    INT 1000
   10   CONTINUE                                                            INT 1010
                                                                             INT 1020
        DO 20 I = 1, NMAX                                                    INT 1030
          KT1(I) = 0.0D0                                                     INT 1040
   20   CONTINUE                                                            INT 1050
                                                                             INT 1060
                                                                             INT 1070
        JCCST  = 0                                                           INT 1080
        PHHIT  = 0                                                           INT 1090
```

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        INFORM = 0                                                      INT 1100
        HITEMP = 0.0D0                                                  INT 1110
        OHTOTI = 0.0D0                                                  INT 1120
        ALK    = 0                                                      INT 1130
        TEMP   = 0.0D0                                                  INT 1140
        HTOTI  = 0.0D0                                                  INT 1150
        RATIO  = 0                                                      INT 1160
        PRESS  = 0.0D0                                                  INT 1170
      END IF                                                            INT 1180
                                                                        INT 1190
      IPHNUM = 0                                                        INT 1200
      OK     = 0                                                        INT 1210
      DDCO2  = 0.0D0                                                    INT 1220
      DDH2S  = 0.0D0                                                    INT 1230
      DDNH3  = 0.0D0                                                    INT 1240
      DDCH4  = 0.0D0                                                    INT 1250
      DCO2   = 0.0D0                                                    INT 1260
      DH2S   = 0.0D0                                                    INT 1270
      DNH3   = 0.0D0                                                    INT 1280
      DCH4   = 0.0D0                                                    INT 1290
      IOPT   = 0                                                        INT 1300
      ICO2   = 0                                                        INT 1310
      IMCO3  = 0                                                        INT 1320
      FCCSAT = 0.05D0                                                   INT 1330
      TCO2M  = 0.0D0                                                    INT 1340
      TCH4M  = 0.0D0                                                    INT 1350
      TH2SM  = 0.0D0                                                    INT 1360
      IPHASE = 0                                                        INT 1370
      DSEP   = 0.0D0                                                    INT 1380
      PPHHIT = 0                                                        INT 1390
      JCO3   = 0                                                        INT 1400
      ISAT   = 0                                                        INT 1410
      IEXCH  = 0                                                        INT 1420
      CEC    = 0.0D0                                                    INT 1430
      TAREA  = 0.0D0                                                    INT 1440
                                                                        INT 1450
      DO 40 I = 1, NMAX                                                 INT 1460
        CUNITS(I) = 0.0D0                                               INT 1470
        M(I)      = 0.0D0                                               INT 1480
        ALFA(I)   = 0.0D0                                               INT 1490
        GAMMA(I)  = 1.0D0                                               INT 1500
   40 CONTINUE                                                          INT 1510
                                                                        INT 1520
      DO 50 I = 1, 10                                                   INT 1530
        RXDP(I)  = 0.0                                                  INT 1540
        IRXDP(I) = 0                                                    INT 1550
   50 CONTINUE                                                          INT 1560
                                                                        INT 1570
      RETURN                                                            INT 1580
      END                                                               INT 1590


      DOUBLE PRECISION FUNCTION KHCH4 (TK, MNACLD, P)                   KH4 0010
C ======================================================================|KH4 0020
C     Calculates the henry's law coefficient for methane                |KH4 0030
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C -----------------------------------------------------------------|KH4 0040
C     MNACLD    DBL   Sum of Molality * charge / 2                 |KH4 0050
C     P         DBL   Partial pressure of methane                  |KH4 0060
C     TK        DBL   Temperature in kelvin                        |KH4 0070
C -----------------------------------------------------------------|KH4 0080
      DOUBLE PRECISION MNACLD, TK, P                                 KH4 0090
      INTRINSIC DEXP                                                 KH4 0100
                                                                     KH4 0110
C =================================================================|KH4 0120
                                                                     KH4 0130
      KHCH4 =  26.187D0             + (0.13647D-2 * P)               KH4 0140
     .       - (26.991D-3 * TK)     + (11.69D-2         * MNACLD)   KH4 0150
     .       - (3380.7D0  / TK)     - (24.09D-2         / MNACLD)   KH4 0160
     .       - (27.79D-2  / P)      + (19.19D-5   * P   / MNACLD)   KH4 0170
     .       - (14.28D-2  * P / TK) + (27.78D-5   * TK * MNACLD)   KH4 0180
                                                                     KH4 0190
      KHCH4 = DEXP(KHCH4)                                            KH4 0200
                                                                     KH4 0210
      RETURN                                                         KH4 0220
      END                                                            KH4 0230
```

```
      DOUBLE PRECISION FUNCTION KHCO2 (T, MU)                        KHC 0010
C =================================================================|KHC 0020
C     Calculates the henry's law coefficient for CO2               |KHC 0030
C -----------------------------------------------------------------|KHC 0040
C     MU        DBL   Ionic strength of solution                   |KHC 0050
C     T         DBL   Temperature in kelvin                        |KHC 0060
C -----------------------------------------------------------------|KHC 0070
      DOUBLE PRECISION MU, T                                         KHC 0080
      INTRINSIC DEXP, DLOG                                           KHC 0090
                                                                     KHC 0100
C =================================================================|KHC 0110
                                                                     KHC 0120
      KHCO2 =  20.244D0             - (0.016323D0 * T)               KHC 0130
     .       - (1.0312D0 * MU)      - (3629.7     / T)               KHC 0140
     .       + (0.4445D0 / MU)      + (0.12806D-2 * T * MU)          KHC 0150
     .       + (255.90D0 * MU / T) - (0.16060D-2 * T / MU)           KHC 0160
                                                                     KHC 0170
      KHCO2 = DEXP(KHCO2)                                            KHC 0180
                                                                     KHC 0190
      RETURN                                                         KHC 0200
      END                                                            KHC 0210
```

```
      DOUBLE PRECISION FUNCTION KHH2S (TK, M1)                       KHH 0010
C =================================================================|KHH 0020
C     Calculates the henry's law coefficient for H2S               |KHH 0030
C -----------------------------------------------------------------|KHH 0040
C     M1        DBL   Sum of Molality * charge / 2                 |KHH 0050
C     TK        DBL   Temperature in kelvin                        |KHH 0060
C -----------------------------------------------------------------|KHH 0070
```

```
                                                                      KHH 0080
      DOUBLE PRECISION TK, M1                                         KHH 0090
      INTRINSIC DEXP                                                  KHH 0100
                                                                      KHH 0110
C ====================================================================|KHH 0120
                                                                      KHH 0130
      KHH2S =  11.416D0             - (0.007013D0 * TK)               KHH 0140
     .      + (0.2905D0 * M1)       - (2067.7D0   / TK)               KHH 0150
     .      + (.5705D0  / M1)       - (.0001574D0 * TK * M1)          KHH 0160
     .      - (46.20D0  * M1 / TK) - (.001777D0  * TK / M1)           KHH 0170
                                                                      KHH 0180
      KHH2S = DEXP(KHH2S)                                             KHH 0190
                                                                      KHH 0200
      RETURN                                                          KHH 0210
      END                                                             KHH 0220
```

```
      DOUBLE PRECISION FUNCTION KHNH3 (TK)                            KHN 0010
C ====================================================================|KHN 0020
C     Calculates the henry's law coefficient for ammonia              |KHN 0030
C --------------------------------------------------------------------|KHN 0040
C     TK        DBL   Temperature in kelvin                           |KHN 0050
C --------------------------------------------------------------------|KHN 0060
                                                                      KHN 0070
      DOUBLE PRECISION TK                                             KHN 0080
      INTRINSIC DLOG                                                  KHN 0090
                                                                      KHN 0100
C ====================================================================|KHN 0110
                                                                      KHN 0120
      KHNH3 = -1816.602D0/TK + 2.27770D0  * DLOG(TK) - 73.0179D-4 * TK KHN 0130
     .        - 6.4609                                                 KHN 0140
                                                                      KHN 0150
      KHNH3 = 10.0D0**KHNH3                                           KHN 0160
                                                                      KHN 0170
      RETURN                                                          KHN 0180
      END                                                             KHN 0190
```

```
      SUBROUTINE LAGINT (XT, YT, X, Y, MAXK, NDIM, OK)                LAG 0010
C ====================================================================|LAG 0020
C     Lagrange interpolation routine.                                 |LAG 0030
C --------------------------------------------------------------------|LAG 0040
C     Variables                                                       |LAG 0050
C -------------                                                       |LAG 0060
C     C         DBL   Calculates the interpolation constants          |LAG 0070
C     CPUMAX    DBL   Largest positive real value program uses        |LAG 0080
C     CPUMIN    DBL   Smallest positive real value program uses       |LAG 0090
C     DIF       INT   Difference between upper and lower bound        |LAG 0100
C     I         INT   Loop counting variable                          |LAG 0110
C     K         INT   Fixes the interpolation range                   |LAG 0120
C     LO        INT   Finds lower bound of interpolation range        |LAG 0130
C     MAXK      INT   Total number of values to be found              |LAG 0140
```

```
C     MID       INT   Finds midpoint of interpolation range                |LAG 0150
C     N         INT   Number of temperature points                         |LAG 0160
C     NDIM      INT   Identifies array dimension                           |LAG 0170
C     OK        INT   Error flag for Lagrange interpolation routine        |LAG 0180
C     UNO       INT   File unit assigned for output file                   |LAG 0190
C     UP        INT   Finds upper bound of interpolation range             |LAG 0200
C     W         DBL   Holds temperature values around point of interest    |LAG 0210
C     X         DBL   The temperature point of interest                    |LAG 0220
C     XT        DBL   Array of temperature values                          |LAG 0230
C     Y         DBL   Final interpolated values at given temperature       |LAG 0240
C     YT        DBL   Data array holding values for temperature point      |LAG 0250
C ---------------------------------------------------------------------    |LAG 0260
                                                                           LAG 0270
      INTEGER UNO                                                          LAG 0280
      DOUBLE PRECISION CPUMIN                                              LAG 0290
      PARAMETER (UNO = 6, CPUMIN = 1.0D-35)                                LAG 0300
                                                                           LAG 0310
      INTEGER DIF, I, K, LO, MAXK, MID, N, NDIM, OK, UP                    LAG 0320
                                                                           LAG 0330
      DOUBLE PRECISION C(4), W(10), X, XT(11), Y(NDIM), YT(NDIM,11)        LAG 0340
                                                                           LAG 0350
      INTRINSIC DABS                                                       LAG 0360
                                                                           LAG 0370
C ===================================================================    |LAG 0380
                                                                           LAG 0390
      N   = 11                                                             LAG 0400
      LO  =  1                                                             LAG 0410
      UP  =  N                                                             LAG 0420
      MID =  1                                                             LAG 0430
                                                                           LAG 0440
      DO 10 I = 1, MAXK                                                    LAG 0450
        Y(I) = 0.0                                                         LAG 0460
   10 CONTINUE                                                             LAG 0470
                                                                           LAG 0480
      IF (X.GT.XT(N) .OR. X.LT.XT(1)) GO TO 90                             LAG 0490
      OK = 1                                                               LAG 0500
                                                                           LAG 0510
   20 CONTINUE                                                             LAG 0520
      DIF = UP - LO                                                        LAG 0530
      IF (DIF .LE .2) GO TO 30                                             LAG 0540
      MID = (UP + LO + 1) / 2                                              LAG 0550
      GO TO 40                                                             LAG 0560
                                                                           LAG 0570
   30 CONTINUE                                                             LAG 0580
      IF (DIF .EQ. 0) GO TO 70                                             LAG 0590
      MID = LO + 1                                                         LAG 0600
                                                                           LAG 0610
   40 CONTINUE                                                             LAG 0620
      IF ((DABS(X-XT(MID))) .LT. CPUMIN) GO TO 70                          LAG 0630
      IF ((X-XT(MID)) .LT. 0.0D0) GO TO 50                                 LAG 0640
                                                                           LAG 0650
C ---------------------------------------------------------------------    |LAG 0660
C     X > XT(MID)                                                          |LAG 0670
C ---------------                                                          |LAG 0680
                                                                           LAG 0690
      LO = MID                                                             LAG 0700
      GO TO 20                                                             LAG 0710
                                                                           LAG 0720
```

```
   50 CONTINUE                                                          LAG 0730
      IF ((DABS(X-XT(MID-1))) .GT. CPUMIN) GO TO 60                     LAG 0740
                                                                        LAG 0750
C -----------------------------------------------------------------------|LAG 0760
C     X = XT(MID-1)                                                     |LAG 0770
C -----------------                                                     |LAG 0780
                                                                        LAG 0790
      MID = MID - 1                                                     LAG 0800
      GO TO 70                                                          LAG 0810
                                                                        LAG 0820
   60 CONTINUE                                                          LAG 0830
      IF ((XT(MID-1)-X) .LT. CPUMIN) GO TO 70                           LAG 0840
                                                                        LAG 0850
C -----------------------------------------------------------------------|LAG 0860
C     X < XT(MID-1)                                                     |LAG 0870
C -----------------                                                     |LAG 0880
                                                                        LAG 0890
      UP = MID                                                          LAG 0900
      GO TO 20                                                          LAG 0910
                                                                        LAG 0920
   70 CONTINUE                                                          LAG 0930
      K = MID - 2                                                       LAG 0940
      IF (K .LT. 1) K = 1                                               LAG 0950
      IF ((K+3) .GT. N) K = N - 3                                       LAG 0960
                                                                        LAG 0970
      W(1)  = X       - XT(K)                                           LAG 0980
      W(2)  = X       - XT(K+1)                                         LAG 0990
      W(3)  = X       - XT(K+2)                                         LAG 1000
      W(4)  = X       - XT(K+3)                                         LAG 1010
      W(5)  = XT(K)   - XT(K+1)                                         LAG 1020
      W(6)  = XT(K)   - XT(K+2)                                         LAG 1030
      W(7)  = XT(K)   - XT(K+3)                                         LAG 1040
      W(8)  = XT(K+1) - XT(K+2)                                         LAG 1050
      W(9)  = XT(K+1) - XT(K+3)                                         LAG 1060
      W(10) = XT(K+2) - XT(K+3)                                         LAG 1070
                                                                        LAG 1080
      DO 80 I = 1, MAXK                                                 LAG 1090
        C(1) =  YT(I,K)   / (W(5) * W(6) * W(7))                        LAG 1100
        C(2) = -YT(I,K+1) / (W(5) * W(8) * W(9))                        LAG 1110
        C(3) =  YT(I,K+2) / (W(6) * W(8) * W(10))                       LAG 1120
        C(4) = -YT(I,K+3) / (W(7) * W(9) * W(10))                       LAG 1130
                                                                        LAG 1140
        Y(I) = C(1) * W(2) * W(3) * W(4) + C(2) * W(1) * W(3) * W(4) +  LAG 1150
     .         C(3) * W(1) * W(2) * W(4) + C(4) * W(1) * W(2) * W(3)    LAG 1160
   80 CONTINUE                                                          LAG 1170
                                                                        LAG 1180
      RETURN                                                            LAG 1190
                                                                        LAG 1200
C -----------------------------------------------------------------------|LAG 1210
C     Error messages                                                    |LAG 1220
C -----------------                                                     |LAG 1230
   90 CONTINUE                                                          LAG 1240
      OK = 0                                                            LAG 1250
                                                                        LAG 1260
      IF (X .GT. XT(N)) WRITE (UNO, 100) X, XT(N)                       LAG 1270
                                                                        LAG 1280
  100 FORMAT (//, ' ', 'X-OUT IN LAGINT X=', E13.6, 2X, 'XT(N)=', E13.6)LAG 1290
                                                                        LAG 1300
```

```
      IF (X .LT. XT(1)) WRITE (UNO, 110) X, XT(1)                        LAG 1310
  110 FORMAT (//, ' ', 'X-OUT IN LAGINT X=', E13.6, 2X, 'XT(1)=', E13.6)LAG 1320
                                                                         LAG 1330
      RETURN                                                             LAG 1340
      END                                                                LAG 1350




      INTEGER FUNCTION LENGTH (STRING)                                   LEN 0010
C ===================================================================|LEN 0020
C     Returns the length of the non-blank portion of a character     |LEN 0030
C       variable                                                     |LEN 0040
C -------------------------------------------------------------------|LEN 0050
C     L          INT   Length pointer                                |LEN 0060
C     STRING     CHA   Variable for which the length is to be determined|LEN 0070
C -------------------------------------------------------------------|LEN 0080
      INTEGER L                                                          LEN 0090
      CHARACTER * 80  STRING                                             LEN 0100
                                                                         LEN 0110
C ===================================================================|LEN 0120
                                                                         LEN 0130
      L = 80                                                             LEN 0140
                                                                         LEN 0150
   10 CONTINUE                                                           LEN 0160
      IF (L .GT. 1  .AND.  STRING(L:L) .EQ. ' ') THEN                    LEN 0170
        L = L - 1                                                        LEN 0180
        GO TO 10                                                         LEN 0190
      END IF                                                             LEN 0200
                                                                         LEN 0210
      IF (STRING(L:L) .NE. ' ') THEN                                     LEN 0220
        LENGTH = L                                                       LEN 0230
      ELSE                                                               LEN 0240
        LENGTH = 1                                                       LEN 0250
      END IF                                                             LEN 0260
                                                                         LEN 0270
      RETURN                                                             LEN 0280
                                                                         LEN 0290
      END                                                                LEN 0300




      SUBROUTINE MIXER (TEMP, M1, PRESS, DENS, ICALL, ISALT, IRUN,       MIX 0010
     .                  MXSP, FCCSAT, PH2O, IPRIN2, MXMNK)               MIX 0020
C ===================================================================|MIX 0030
C     Precipitation/dissolution, Mixing, and Boiling options         |MIX 0040
C -------------------------------------------------------------------|MIX 0050
C     A1MIX      DBL   HTOT, OHTOT, TIC of first solution/original water|MIX 0060
C     ADD        DBL   The amount of material being added/subtracted  |MIX 0070
C     ADDMIN     DBL   Record of the amount of mineral added          |MIX 0080
C     ADENS      DBL   Density of first water in mixing               |MIX 0090
C     ALFA       DBL   Activity of aqueous species i                  |MIX 0100
C     AMOL       DBL   Amount in moles to be added                    |MIX 0110
C     ANALM      DBL   Analyzed molality of species i                 |MIX 0120
C     ANMMIX     DBL   Stored values for first water                  |MIX 0130
```

```
C     ATEMP     DBL   Temperature of solution A                          |MIX 0140
C     B2MIX     DBL   HTOT, OHTOT, TIC of second water                   |MIX 0150
C     BDENS     DBL   Density of second water in mixing                  |MIX 0160
C     BNMMIX    DBL   Stored values for second water                     |MIX 0170
C     BTEMP     DBL   Temperature of solution B                          |MIX 0180
C     BUFFER    CHA   Buffer for Character manipulation                  |MIX 0190
C     COFFAC    DBL   Component Coef. for dissolving phase               |MIX 0200
C     CPUMIN    DBL   Smallest positive real value program uses          |MIX 0210
C     CROSS     LOG   Have we crossed the root yet?                      |MIX 0220
C     DELTA     DBL   Temperary storage to find min. component           |MIX 0230
C     DENS      DBL   Density                                           |MIX 0240
C     DFRAC1    DBL   Smallest fraction of soln 1 mixed with soln 2      |MIX 0250
C     DIF       DBL   Difference used in testing                         |MIX 0260
C     DINC      DBL   Increment of solution 1 to be added                |MIX 0270
C     DONE      LOG   Are we done?                                       |MIX 0280
C     DP        DBL   Dissolution/precipitation switch                   |MIX 0290
C     DUM2      CHA   Character array with names of gases                |MIX 0300
C     EQC       DBL   Equivalent amount of carbon in 1 mole of comp.     |MIX 0310
C     EQH       DBL   Equivalent amount of hydrogen in 1 mole of comp.   |MIX 0320
C     ERROR     LOG   Is everything ok?                                  |MIX 0330
C     EXELT     DBL   Total mass of components                           |MIX 0340
C     FBOIL     DBL   Fraction of solution boiled-off as steam           |MIX 0350
C     FCCSAT    DBL   Tolerance factor for pH and CO2 options            |MIX 0360
C     FFB       DBL   Fraction of boiling (1 / (1-fboil))                |MIX 0370
C     FMIX      DBL   Mixtures to be examined                            |MIX 0380
C     HEQ       DBL   Coef. for H containing components                  |MIX 0390
C     I         INT   Loop variable                                      |MIX 0400
C     IADD      INT   Index for positioning in adding mineral arrays     |MIX 0410
C     IBOIL     INT   Index of number of boiling points stored           |MIX 0420
C     IBTOT     INT   Count for number of boiling iterations             |MIX 0430
C     ICALL     INT   Switch for calling this routine                    |MIX 0440
C     ICD       INT   Index for mineral being dissolved                  |MIX 0450
C     ICS       INT   Index for mineral to saturate with                 |MIX 0460
C     IDDP      INT   Id number of the mineral to be dissolved/ppt       |MIX 0470
C     IDMIN     INT   Id number of the mineral to be dissolved/ppt       |MIX 0480
C     IDMIX     INT   Id number of the aqueous species to be added       |MIX 0490
C     IDSAT     INT   Id number of the mineral to be equilibrated        |MIX 0500
C     IHID      INT   Index of H containing components                   |MIX 0510
C     INDX      INT   Index used for checking components                 |MIX 0520
C     INMIX     INT   Total number of mixtures of two solution mixed     |MIX 0530
C     IPGLN     INT   Current line number of the output file             |MIX 0540
C     IPRIN2    INT   Print switch                                       |MIX 0550
C     IRUN      INT   Keeps track if this is first or second mixture     |MIX 0560
C     IRXDP     INT   Id number of the aqueous species to be added       |MIX 0570
C     ISALT     INT   Switch used in mixer to indicate option            |MIX 0580
C     ISTF      INT   Temp. storage used in reading                       MIX 0590
C     ITMIX     INT   Switch for the mineral saturation option           |MIX 0600
C     J         INT   Loop variable                                      |MIX 0610
C     JJ        INT   Loop variable and counter                          |MIX 0620
C     K         INT   Loop variable and counter                          |MIX 0630
C     KCH4      DBL   Henrys law coef for CH4                            |MIX 0640
C     KCO2      DBL   Henrys law coef for CO2                            |MIX 0650
C     KH2S      DBL   Henrys law coef for H2S                            |MIX 0660
C     KNH3      DBL   Henrys law coef for NH3                            |MIX 0670
C     LOGKT2    DBL   Log K for minerals at specified temperature        |MIX 0680
C     M         DBL   Calculated molality of aqueous species             |MIX 0690
C     M1        DBL   Sum of Molality * charge / 2                       |MIX 0700
C     MINDIM    INT   Parameter ... dimension of various arrays          |MIX 0710
```

```
C     MINDP     LOG   Switch ... dissolving a mineral?                        |MIX 0720
C     MINSAT    LOG   Switch ... saturating with a mineral?                   |MIX 0730
C     MXMNK     INT   Total number of mineral log k values                    |MIX 0740
C     MXSP      INT   Total number of aqueous species                         |MIX 0750
C     NGAST     DBL   Values guessed for root                                 |MIX 0760
C     NL        DBL   Number of moles in liquid                               |MIX 0770
C     NMAX      INT   General array dimension to allow easy expansion         |MIX 0780
C     NV        DBL   Number of moles in vapour                               |MIX 0790
C     PAGE1     CHA   Names of aqueous species                                |MIX 0800
C     PAGE3     CHA   Names of solubility constants                           |MIX 0810
C     PH2O      DBL   Pressure of water                                       |MIX 0820
C     PRESS     DBL   Total pressure                                          |MIX 0830
C     R         DBL   Gas constant                                            |MIX 0840
C     REVERS    LOG   OK to reverse direction in root finding?                |MIX 0850
C     RXDP      DBL   Molal amount of the aqueous species added               |MIX 0860
C     SIMIN     DBL   SI of mineral being saturated with.  Tested.            |MIX 0870
C     STEP      DBL   Amount of volatile to add/remove from liquid            |MIX 0880
C     STEPSZ    DBL   Scaling factor (parameter) in diss/ppt minerals         |MIX 0890
C     STF       DBL   Temp. storage used in reading                           |MIX 0900
C     STOFAC    DBL   Stoich. Coef. for material being added/removed          |MIX 0910
C     TEMP      DBL   Current temperature                                     |MIX 0920
C     TITMIX    CHA   Title for mixtures                                      |MIX 0930
C     TITR      DBL   Iteration array in DISTRB, used for guesses             |MIX 0940
C     TK        DBL   Temperature in K                                        |MIX 0950
C     TOF       CHA   Places a form feed in output file                       |MIX 0960
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                        |MIX 0970
C     TRY       DBL   Next amount of volitiles in h2o (used in boiling)       |MIX 0980
C     UNO       INT   File unit assigned for output file                      |MIX 0990
C     UNR       INT   Unit to read data file                                  |MIX 1000
C     VDEN      DBL   Vapour density                                          |MIX 1010
C     VRCH4     DBL   Volatility ratio for CH4                                |MIX 1020
C     VRCO2     DBL   Volatility ratio for CO2                                |MIX 1030
C     VRH2S     DBL   Volatility ratio for H2S                                |MIX 1040
C     VRNH3     DBL   Volatility ratio for NH3                                |MIX 1050
C     VRT       DBL   Used in calculated volatility ratio                     |MIX 1060
C     X         DBL   Temperary storage                                       |MIX 1070
C -------------------------------------------------------------------------|MIX 1080
                                                                             MIX 1090
      INTEGER MINDIM, NMAX, UNO, UNR                                         MIX 1100
      DOUBLE PRECISION CPUMIN, R, STEPSZ                                     MIX 1110
      PARAMETER (MINDIM = 20, NMAX = 340, UNO = 6, UNR = 12)                 MIX 1120
      PARAMETER (CPUMIN = 1.0D-35, R = 83.14241D-3, STEPSZ = 1.0D-02)        MIX 1130
                                                                             MIX 1140
C -------------------------------------------------------------------------|MIX 1150
C     R is 83.15 (bar cm**3 / deg mole) times divided by 1000                |MIX 1160
C     (1 kg water). The density of the gas is in cm**3/gram, hense           |MIX 1170
C     55.51 is implied.                                                      |MIX 1180
C -------------------------------------------------------------------------|MIX 1190
                                                                             MIX 1200
      INTEGER I, IADD, IBOIL, IBTOT, ICALL, ICD, ICS                         MIX 1210
      INTEGER IDDP, IDMIX(50), IDMIN(10), IDSAT, IDSP(10)                    MIX 1220
      INTEGER IHID(10), INDX, INMIX, IPAGE, IPGLN, IPRIN2                    MIX 1230
      INTEGER IRUN, IRXDP(10), ISALT, ISTF(10), ITMIX                        MIX 1240
      INTEGER J, JJ, K, MXMNK, MXSP                                          MIX 1250
                                                                             MIX 1260
      LOGICAL DONE, MINSAT, MINDP, ERROR, CROSS, REVERS                      MIX 1270
                                                                             MIX 1280
      CHARACTER *  1 TOF, CR                                                 MIX 1290
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      CHARACTER *  5 DUM2(4)                                                MIX 1300
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                  MIX 1310
      CHARACTER * 40 TITMIX, BUFFER                                         MIX 1320
                                                                            MIX 1330
      DOUBLE PRECISION ATCPRD, ADD, ADDMIN(MINDIM), ADENS, ALFA(NMAX)       MIX 1340
      DOUBLE PRECISION AMOL(50), ANALM(NMAX), ANMMIX(NMAX), ATEMP           MIX 1350
      DOUBLE PRECISION A1MIX(5), BDENS, BNMMIX(NMAX), BTEMP, B2MIX(5)       MIX 1360
      DOUBLE PRECISION COFFAC(10), CUNITS(NMAX)                             MIX 1370
      DOUBLE PRECISION DELTA, DENS, DFRAC1, DIF(4,9), DINC, DP              MIX 1380
      DOUBLE PRECISION EQC, EQH, EXELT(35)                                  MIX 1390
      DOUBLE PRECISION FBOIL, FCCSAT, FFB, FMIX(10)                         MIX 1400
      DOUBLE PRECISION HEQ(10), LOGKT1(NMAX), LOGKT2(NMAX)                  MIX 1410
      DOUBLE PRECISION KCH4, KHCH4, KCO2, KHCO2, KH2S, KHH2S                MIX 1420
      DOUBLE PRECISION KNH3, KHNH3, M(NMAX), M1, NGAST(9), NL(4), NV(4)     MIX 1430
      DOUBLE PRECISION PH, PH2O, PRESS, RXDP(10)                            MIX 1440
      DOUBLE PRECISION SIMIN(MINDIM), STEP(4), STF(10), STOFAC(10)          MIX 1450
      DOUBLE PRECISION TEMP, TITR(11), TK, TOTEL(5), TRY(4,9)               MIX 1460
      DOUBLE PRECISION VDEN, VRT, VRCH4, VRCO2, VRH2S, VRNH3, X             MIX 1470
                                                                            MIX 1480
      EXTERNAL ATCPRD, DPVT, GUESS, KHCH4, KHCO2, KHH2S, KHNH3, SORTA       MIX 1490
      EXTERNAL PAGE                                                         MIX 1500
                                                                            MIX 1510
      INTRINSIC DABS, INDEX, LEN, MIN                                       MIX 1520
                                                                            MIX 1530
      COMMON /ALOGK / LOGKT1, LOGKT2                                        MIX 1540
      COMMON /AMM   / IDMIX, AMOL, ITMIX, INMIX, DFRAC1, DINC, FBOIL        MIX 1550
      COMMON /EXTOT / EXELT, TOTEL, TITR                                    MIX 1560
      COMMON /FMFD  / TOF, CR, TITMIX                                       MIX 1570
      COMMON /FORM  / IPAGE, IPGLN                                          MIX 1580
      COMMON /MM    / ANMMIX, A1MIX, B2MIX, FMIX, BNMMIX, ADENS, BDENS,     MIX 1590
     .                ATEMP, BTEMP                                         MIX 1600
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                            MIX 1610
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                   MIX 1620
      COMMON /SAT   / IDDP, IDSAT, DP, RXDP, IRXDP                          MIX 1630
                                                                            MIX 1640
      SAVE ADDMIN, COFFAC, CROSS, DIF, DONE                                 MIX 1650
      SAVE IADD, IBOIL, IBTOT, ICS, ICD, IDMIN, IDSP                        MIX 1660
      SAVE MINDP, MINSAT, NGAST, NL, NV, REVERS, SIMIN, STEP, STOFAC        MIX 1670
      SAVE TRY, VRCH4, VRCO2, VRH2S, VRNH3                                  MIX 1680
                                                                            MIX 1690
      DATA HEQ  /1.0, 1.0, -1.0, 4.0, 2.0, -3.0, -1.0, 2.0, 1.0, 0.0/       MIX 1700
      DATA IHID /  7,   8,    9,  12,  28,   31,   32,  33,  49,   0/       MIX 1710
      DATA DUM2 /'  CO2', '  NH3', '  H2S', '  CH4'/                        MIX 1720
                                                                            MIX 1730
C ============================================================================MIX 1740
                                                                            MIX 1750
C -----------------------------------------------------------------------    MIX 1760
C     Store solution parameters if first call                                 MIX 1770
C     totel: (1) = htot;  (2) = ohtot; (3) = tic                              MIX 1780
C -----------------------------------------------------------------------    MIX 1790
                                                                            MIX 1800
      IF (ICALL .EQ. 1) THEN                                                MIX 1810
        DO 10 I = 1, 5                                                      MIX 1820
          A1MIX(I) = TOTEL(I)                                               MIX 1830
   10   CONTINUE                                                            MIX 1840
                                                                            MIX 1850
        DO 20 I = 1, MXSP + 44                                              MIX 1860
          ANMMIX(I) = ANALM(I)                                              MIX 1870
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   20   CONTINUE                                                          MIX 1880
                                                                          MIX 1890
        ADENS = DENS                                                      MIX 1900
        ATEMP = TEMP                                                      MIX 1910
      END IF                                                              MIX 1920
                                                                          MIX 1930
C -----------------------------------------------------------------------|MIX 1940
C     icall = 1; isalt = 0 -- first call for mixing two solutions       |MIX 1950
C     icall = 1; isalt = 1 -- first call for mixing species             |MIX 1960
C     icall = 1; isalt = 2 -- first call for boiling a solution         |MIX 1970
C     icall = 1; isalt = 3 -- first call for diss/precip. of a mineral  |MIX 1980
C -----------------------------------------------------------------------|MIX 1990
                                                                          MIX 2000
      IF (ICALL .EQ. 1 .AND. ISALT .EQ. 0) THEN                           MIX 2010
        IF (IPGLN .GT. 55) CALL PAGE                                      MIX 2020
        IPGLN = IPGLN + 4                                                 MIX 2030
        WRITE (UNO,1250)                                                  MIX 2040
        IRUN = 1                                                          MIX 2050
        RETURN                                                            MIX 2060
      ELSE IF (ICALL .EQ. 1 .AND. ISALT .EQ. 1 .AND. ITMIX .GT. 0) THEN   MIX 2070
        IF (IPGLN .GT. (59-8-ITMIX)) CALL PAGE                            MIX 2080
        IPGLN = IPGLN + 5                                                 MIX 2090
        WRITE (UNO, 1070)                                                 MIX 2100
        DO 40 I = 1, ITMIX                                                MIX 2110
          INDX = IDMIX(I)                                                 MIX 2120
          IF (INDX .EQ. 11) INDX = 12                                     MIX 2130
          EQH = 0.0D00                                                    MIX 2140
          DO 30 J = 1,9                                                   MIX 2150
            IF (INDX .EQ. IHID(J)) EQH = HEQ(J)                           MIX 2160
   30     CONTINUE                                                        MIX 2170
          IF (DABS(EQH) .GT. CPUMIN) TOTEL(1) = TOTEL(1) +                MIX 2180
     .                                          (EQH * AMOL(I))          MIX 2190
                                                                          MIX 2200
          EQC = 0.0                                                       MIX 2210
          IF (INDX .EQ.   7) EQC = 1.0                                    MIX 2220
          IF (INDX .EQ.  98) EQC = 1.0                                    MIX 2230
          IF (INDX .EQ. 207) EQC = 1.0                                    MIX 2240
          IF (INDX .EQ. 208) EQC = 2.0                                    MIX 2250
          IF (INDX .EQ. 209) EQC = 3.0                                    MIX 2260
          IF (DABS(EQC) .GT. CPUMIN) TOTEL(3) = TOTEL(3) +                MIX 2270
     .                                          (EQC * AMOL(I))          MIX 2280
                                                                          MIX 2290
          ANALM(INDX) = ANALM(INDX) + AMOL(I)                             MIX 2300
          IPGLN = IPGLN + 1                                               MIX 2310
          WRITE (UNO,1080) INDX, PAGE1(INDX), AMOL(I), EQH, EQC           MIX 2320
                                                                          MIX 2330
          IF (ANALM(INDX) .LT. 0.0 .AND. ANMMIX(INDX) .GT. 0.0) THEN      MIX 2340
            WRITE (UNO, 1100) PAGE1(INDX), AMOL(I), ANMMIX(INDX)          MIX 2350
            STOP                                                          MIX 2360
          END IF                                                          MIX 2370
                                                                          MIX 2380
   40     CONTINUE                                                        MIX 2390
          IPGLN = IPGLN + 3                                               MIX 2400
          WRITE (UNO,1090)                                                MIX 2410
          ICALL = 3                                                       MIX 2420
          J = 0                                                           MIX 2430
                                                                          MIX 2440
          DO 50 I = 1, 28                                                 MIX 2450
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          J = J + 1                                                      MIX 2460
          IF (J .EQ.   8) J = 12                                         MIX 2470
          IF (J .EQ.  17) J = 18                                         MIX 2480
          IF (J .EQ.  19) J = 21                                         MIX 2490
          IF (J .EQ.  24) J = 25                                         MIX 2500
          IF (J .EQ.  34) J = 48                                         MIX 2510
          IF (J .EQ.  49) J = 169                                        MIX 2520
          IF (J .EQ. 170) J = 210                                        MIX 2530
          EXELT(I)  = ANALM(J)                                           MIX 2540
   50   CONTINUE                                                        MIX 2550
                                                                        MIX 2560
        EXELT(29)  = ANALM(7)                                           MIX 2570
        EXELT(30)  = ANALM(246)                                         MIX 2580
        EXELT(31)  = ANALM(265)                                         MIX 2590
        EXELT(32)  = ANALM(136)                                         MIX 2600
        EXELT(33)  = ANALM(MXSP+1)                                      MIX 2610
        EXELT(34)  = ANALM(MXSP+16)                                     MIX 2620
        EXELT(35)  = ANALM(MXSP+31)                                     MIX 2630
                                                                        MIX 2640
        TITR( 1) = EXELT(29)                                            MIX 2650
        TITR( 2) = EXELT( 6)                                            MIX 2660
        TITR( 3) = EXELT(22)                                            MIX 2670
        TITR( 4) = EXELT(21)                                            MIX 2680
        TITR( 5) = EXELT( 5)                                            MIX 2690
        TITR( 6) = EXELT(26)                                            MIX 2700
        TITR( 7) = EXELT(25)                                            MIX 2710
        TITR( 8) = EXELT(30)                                            MIX 2720
        TITR( 9) = EXELT(31)                                            MIX 2730
        TITR(10) = EXELT(33)                                            MIX 2740
        TITR(11) = EXELT(34)                                            MIX 2750
                                                                        MIX 2760
        RETURN                                                          MIX 2770
      END IF                                                            MIX 2780
                                                                        MIX 2790
C ------------------------------------------------------------------------|MIX 2800
C     Precipitation / dissolution of a mineral                          |MIX 2810
C ------------------------------------------------------------------------|MIX 2820
                                                                        MIX 2830
C ------------------------------------------------------------------------|MIX 2840
C     On first call, read the dissolution reactions of the minerals,    |MIX 2850
C     one at a time, and store the one required. If we are dissolving   |MIX 2860
C     /ppt a fixed amount of mineral, this will be the only call.       |MIX 2870
C ------------------------------------------------------------------------|MIX 2880
                                                                        MIX 2890
C ------------------------------------------------------------------------|MIX 2900
C     The following open statement have been changed out by             |MIX 2910
C     Ernie Perkins (ORSD, ARC) in order to allow an command            |MIX 2920
C     proceedure under VMS 4.5 on DEC VAX's to assign the files         |MIX 2930
C     external to the program.                                          |MIX 2940
C ------------------------------------------------------------------------|MIX 2950
                                                                        MIX 2960
      IF ((ISALT .EQ. 3 .OR. (ISALT .EQ. 1 .AND. ITMIX .LT. 0)) .AND.   MIX 2970
     .     ICALL .EQ. 1) THEN                                           MIX 2980
          ANMMIX(7) = TOTEL(3)                                          MIX 2990
        OPEN (UNR, FILE = 'RXN.TBL', STATUS = 'OLD', IOSTAT = K)        MIX 3000
C        OPEN (UNR, STATUS = 'OLD', shared, readonly, IOSTAT = K)       MIX 3010
        IF (K .NE. 0) THEN                                              MIX 3020
          IF (IPGLN .GE. 55) CALL PAGE                                  MIX 3030
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            IPGLN = IPGLN + 4                                                   MIX 3040
            WRITE (UNO, 1030)                                                   MIX 3050
            STOP                                                                MIX 3060
          END IF                                                                MIX 3070
                                                                                MIX 3080
          MINSAT = .FALSE.                                                      MIX 3090
          MINDP  = .FALSE.                                                      MIX 3100
          IF (IDDP  .EQ. 0) MINDP  = .TRUE.                                     MIX 3110
          IF (IDSAT .EQ. 0) MINSAT = .TRUE.                                     MIX 3120
                                                                                MIX 3130
          ERROR = .FALSE.                                                       MIX 3140
          DO 80 J = 1, MXMNK                                                    MIX 3150
            READ (UNR, 1000, IOSTAT=K) I, (STF(JJ), ISTF(JJ), JJ=1,10)          MIX 3160
            IF (K .NE. 0) THEN                                                  MIX 3170
              IF (IPGLN .GT. 55) CALL PAGE                                      MIX 3180
              IPGLN = IPGLN + 5                                                 MIX 3190
              WRITE (UNO, 1040) J                                               MIX 3200
              STOP                                                              MIX 3210
            END IF                                                              MIX 3220
            IF (.NOT. MINSAT) THEN                                              MIX 3230
              IF (IDSAT .EQ. I) THEN                                            MIX 3240
                MINSAT = .TRUE.                                                 MIX 3250
                ICS = 0                                                         MIX 3260
                DO 60 K = 1, 10                                                 MIX 3270
                  IDSP(K)   = ISTF(K)                                           MIX 3280
                  COFFAC(K) = STF(K)                                            MIX 3290
                  IF (DABS(COFFAC(K)) .GT. CPUMIN) ICS = K                      MIX 3300
   60             CONTINUE                                                      MIX 3310
                IF (STF(1) .GT. 900.) THEN                                      MIX 3320
                  ERROR = .TRUE.                                                MIX 3330
                  IF (IPGLN .GT. 56) CALL PAGE                                  MIX 3340
                  IPGLN = IPGLN + 3                                             MIX 3350
                  WRITE (UNO, 1050) PAGE3(I)                                    MIX 3360
                END IF                                                          MIX 3370
              END IF                                                            MIX 3380
            END IF                                                              MIX 3390
            IF (.NOT. MINDP) THEN                                               MIX 3400
              IF (IDDP .EQ. I) THEN                                             MIX 3410
                MINDP = .TRUE.                                                  MIX 3420
                ICD = 0                                                         MIX 3430
                DO 70 K = 1, 10                                                 MIX 3440
                  IDMIN(K)  = ISTF(K)                                           MIX 3450
                  STOFAC(K) = STF(K)                                            MIX 3460
                  IF (DABS(STOFAC(K)) .GT. CPUMIN) ICD=K                        MIX 3470
   70             CONTINUE                                                      MIX 3480
                IF (STF(1) .GT. 900.) THEN                                      MIX 3490
                  ERROR = .TRUE.                                                MIX 3500
                  IF (IPGLN .GT. 56) CALL PAGE                                  MIX 3510
                  IPGLN = IPGLN + 3                                             MIX 3520
                  WRITE (UNO, 1050) PAGE3(I)                                    MIX 3530
                END IF                                                          MIX 3540
              END IF                                                            MIX 3550
            END IF                                                              MIX 3560
                                                                                MIX 3570
C ---------------------------------------------------------------------------|MIX 3580
C     In the absence of an ANSI standard WHILE statement                     |MIX 3590
C ---------------------------------------------------------------------------|MIX 3600
                                                                                MIX 3610
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          IF (MINSAT .AND. MINDP) GO TO 90                                MIX 3620
   80     CONTINUE                                                        MIX 3630
                                                                          MIX 3640
          IF (.NOT. MINSAT) THEN                                          MIX 3650
            IF (IPGLN .GT. 54) CALL PAGE                                  MIX 3660
            IPGLN = IPGLN + 5                                             MIX 3670
            WRITE (UNO, 1010) IDSAT                                       MIX 3680
          END IF                                                          MIX 3690
                                                                          MIX 3700
          IF (.NOT. MINDP) THEN                                           MIX 3710
            IF (IPGLN .GT. 54) CALL PAGE                                  MIX 3720
            IPGLN = IPGLN + 5                                             MIX 3730
            WRITE (UNO, 1020) IDDP                                        MIX 3740
          END IF                                                          MIX 3750
                                                                          MIX 3760
          IF ((.NOT. MINDP .OR. .NOT. MINSAT) .OR. ERROR) STOP            MIX 3770
                                                                          MIX 3780
   90     CONTINUE                                                        MIX 3790
          IF (IDSAT .EQ. 0) MINSAT = .FALSE.                              MIX 3800
          IF (IDDP  .EQ. 0) MINDP  = .FALSE.                              MIX 3810
                                                                          MIX 3820
          CLOSE (UNR)                                                     MIX 3830
                                                                          MIX 3840
        END IF                                                            MIX 3850
                                                                          MIX 3860
C ---------------------------------------------------------------------|MIX 3870
C     The appropriate reactions have been found.  Make titles.          |MIX 3880
C     Prepare the first step/take the first step                        |MIX 3890
C                                                                       |MIX 3900
C     IDDP > 0  IDSAT > 0 ITMIX = 0 Dissolve/ppt IDDP til saturation    |MIX 3910
C                                   with IDSAT                          |MIX 3920
C     IDDP = 0  IDSAT > 0 ITMIX = 0 dissolve/remove aqueous components  |MIX 3930
C                                   til saturation with IDSAT           |MIX 3940
C     IDDP > 0  IDSAT = 0 ITMIX < 0 dissolve a specified amount of      |MIX 3950
C                                   IDSAT (note that this is specified  |MIX 3960
C                                   by ICALL=1, ISALT=1, and ITMIX<0)   |MIX 3970
C ---------------------------------------------------------------------|MIX 3980
                                                                        MIX 3990
        IF (ISALT .EQ. 3 .AND. ITMIX .EQ. 0 .AND. MINSAT                MIX 4000
       .                 .AND. ICALL .EQ. 1 .AND. MINDP ) THEN          MIX 4010
          IF (DP .LT. (CPUMIN * (-1.0))) THEN                           MIX 4020
            TITMIX = PAGE3(IDDP)//' PRECIPITATED         '              MIX 4030
          ELSE IF (DP .GT. CPUMIN) THEN                                 MIX 4040
            TITMIX = PAGE3(IDDP)//' DISSOLVED            '              MIX 4050
          ELSE                                                          MIX 4060
            TITMIX = PAGE3(IDDP)//' PPT/DISS             '              MIX 4070
          END IF                                                        MIX 4080
        ELSE IF (ISALT .EQ. 3 .AND. ITMIX .EQ. 0 .AND. MINSAT           MIX 4090
       .                    .AND. ICALL .EQ. 1 .AND. .NOT. MINDP) THEN  MIX 4100
                                                                        MIX 4110
C ---------------------------------------------------------------------|MIX 4120
C     If we are adding components, make up name, use * for              |MIX 4130
C     non-trivial blanks, remove all other blanks, then                 |MIX 4140
C     change * to blank                                                 |MIX 4150
C ---------------------------------------------------------------------|MIX 4160
                                                                        MIX 4170
          K   = 1                                                       MIX 4180
          ICD = 0                                                       MIX 4190
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      DO 130 I = 1, 10                                                  MIX 4200
        IF (IRXDP(I) .NE. 0) THEN                                       MIX 4210
          IDMIN(I) = IRXDP(I)                                           MIX 4220
          ICD = ICD + 1                                                 MIX 4230
          STOFAC(I) = RXDP(I)                                           MIX 4240
        END IF                                                          MIX 4250
        IF (IRXDP(I) .NE. 0 .AND. K .LE. LEN(TITMIX)) THEN              MIX 4260
          IF (K .NE. 1) THEN                                            MIX 4270
            BUFFER(1:1)   = '*'                                         MIX 4280
          ELSE                                                          MIX 4290
            BUFFER(1:1)   = ' '                                         MIX 4300
          END IF                                                        MIX 4310
          WRITE (BUFFER(2:11),'(F10.3)') RXDP(I)                        MIX 4320
          BUFFER(12:22) = ' (' // PAGE1(IRXDP(I)) // ')'                MIX 4330
                                                                        MIX 4340
100       CONTINUE                                                      MIX 4350
          JJ = INDEX(BUFFER,'0 ')                                       MIX 4360
          IF (JJ .NE. 0) THEN                                           MIX 4370
            BUFFER(JJ:JJ) = ' '                                         MIX 4380
            GO TO 100                                                   MIX 4390
          END IF                                                        MIX 4400
110       CONTINUE                                                      MIX 4410
          JJ = INDEX(BUFFER,'. ')                                       MIX 4420
          IF (JJ .NE. 0) THEN                                           MIX 4430
            BUFFER(JJ:JJ) = ' '                                         MIX 4440
            GO TO 110                                                   MIX 4450
          END IF                                                        MIX 4460
          DO 120 JJ = 1, 22                                             MIX 4470
            IF (BUFFER(JJ:JJ) .NE. ' ' .AND.                            MIX 4480
     .                        K .LE. LEN(TITMIX)) THEN                  MIX 4490
              TITMIX(K:K) = BUFFER(JJ:JJ)                               MIX 4500
              K = K + 1                                                 MIX 4510
            ELSE IF (K .GT. LEN(TITMIX)) THEN                           MIX 4520
              K = LEN(TITMIX)                                           MIX 4530
              TITMIX(K-2:K) = '...'                                     MIX 4540
              K = K + 10                                                MIX 4550
              GO TO 110                                                 MIX 4560
            END IF                                                      MIX 4570
120       CONTINUE                                                      MIX 4580
        END IF                                                          MIX 4590
130   CONTINUE                                                          MIX 4600
                                                                        MIX 4610
      DO 140 I = 1, K                                                   MIX 4620
        IF (TITMIX(I:I) .EQ. '*') TITMIX(I:I) = ' '                     MIX 4630
140   CONTINUE                                                          MIX 4640
                                                                        MIX 4650
    ELSE IF (ITMIX .LT. 0 .AND. ICALL .EQ. 1 .AND. ISALT .EQ. 1 ) THENMIX 4660
        IF (IPGLN .GT. (59-8-ITMIX)) CALL PAGE                          MIX 4670
        IPGLN = IPGLN + 5                                               MIX 4680
        WRITE (UNO,1110) PAGE3(IDDP)                                    MIX 4690
        DO 160 I = 1, 10                                                MIX 4700
          INDX = IDMIN(I)                                               MIX 4710
          IF (INDX .LE. 0) GO TO 160                                    MIX 4720
          IF (INDX .EQ. 11) INDX = 12                                   MIX 4730
                                                                        MIX 4740
          EQH = 0.0D00                                                  MIX 4750
          DO 150 J = 1, 9                                               MIX 4760
            IF (INDX .EQ. IHID(J)) EQH = HEQ(J)                         MIX 4770
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150     CONTINUE                                                        MIX 4780
        IF (DABS(EQH) .GT. CPUMIN) TOTEL(1) = TOTEL(1) + (AMOL(1) *     MIX 4790
     .                                        STOFAC(I) *EQC)           MIX 4800
                                                                        MIX 4810
        EQC = 0.0                                                       MIX 4820
        IF (INDX .EQ.   7) EQC = 1.0                                    MIX 4830
        IF (INDX .EQ.  98) EQC = 1.0                                    MIX 4840
        IF (INDX .EQ. 207) EQC = 1.0                                    MIX 4850
        IF (INDX .EQ. 208) EQC = 2.0                                    MIX 4860
        IF (INDX .EQ. 209) EQC = 3.0                                    MIX 4870
        IF (DABS(EQC) .GT. CPUMIN) TOTEL(3) = TOTEL(3) + (AMOL(1) *     MIX 4880
     .                                        STOFAC(I) * EQC)          MIX 4890
                                                                        MIX 4900
        ANALM(INDX) = ANALM(INDX) + (AMOL(1) * STOFAC(I))               MIX 4910
        IPGLN = IPGLN + 1                                               MIX 4920
        WRITE (UNO,1080) INDX, PAGE1(INDX), (AMOL(1)*STOFAC(I)),        MIX 4930
     .                   EQH, EQC                                       MIX 4940
                                                                        MIX 4950
        IF (ANALM(INDX) .LT. 0.0 .AND. ANMMIX(INDX) .GT. 0.0) THEN      MIX 4960
          WRITE (UNO, 1100) PAGE1(INDX), (AMOL(I) * STOFAC(I)),         MIX 4970
     .                      ANMMIX(INDX)                              MIX 4980
          STOP                                                          MIX 4990
        END IF                                                          MIX 5000
                                                                        MIX 5010
160     CONTINUE                                                        MIX 5020
        IPGLN = IPGLN + 3                                               MIX 5030
        WRITE (UNO,1090)                                                MIX 5040
        ICALL = 3                                                       MIX 5050
                                                                        MIX 5060
        J = 0                                                           MIX 5070
        DO 170 I = 1, 28                                                MIX 5080
          J = J + 1                                                     MIX 5090
          IF (J .EQ.   8) J = 12                                        MIX 5100
          IF (J .EQ.  17) J = 18                                        MIX 5110
          IF (J .EQ.  19) J = 21                                        MIX 5120
          IF (J .EQ.  24) J = 25                                        MIX 5130
          IF (J .EQ.  34) J = 48                                        MIX 5140
          IF (J .EQ.  49) J = 169                                       MIX 5150
          IF (J .EQ. 170) J = 210                                       MIX 5160
          EXELT(I)  = ANALM(J)                                          MIX 5170
170     CONTINUE                                                        MIX 5180
                                                                        MIX 5190
        EXELT(29)  = ANALM(7)                                           MIX 5200
        EXELT(30)  = ANALM(246)                                         MIX 5210
        EXELT(31)  = ANALM(265)                                         MIX 5220
        EXELT(32)  = ANALM(136)                                         MIX 5230
        EXELT(33)  = ANALM(MXSP+1)                                      MIX 5240
        EXELT(34)  = ANALM(MXSP+16)                                     MIX 5250
        EXELT(35)  = ANALM(MXSP+31)                                     MIX 5260
                                                                        MIX 5270
        TITR( 1) = EXELT(29)                                            MIX 5280
        TITR( 2) = EXELT( 6)                                            MIX 5290
        TITR( 3) = EXELT(22)                                            MIX 5300
        TITR( 4) = EXELT(21)                                            MIX 5310
        TITR( 5) = EXELT( 5)                                            MIX 5320
        TITR( 6) = EXELT(26)                                            MIX 5330
        TITR( 7) = EXELT(25)                                            MIX 5340
        TITR( 8) = EXELT(30)                                            MIX 5350
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        TITR( 9) = EXELT(31)                                                MIX 5360
        TITR(10) = EXELT(33)                                                MIX 5370
        TITR(11) = EXELT(34)                                                MIX 5380
        RETURN                                                              MIX 5390
      ELSE IF (ICALL .EQ. 1 .AND. ISALT .EQ. 3) THEN                        MIX 5400
        IF (IPGLN .GT. 55) CALL PAGE                                        MIX 5410
          IPGLN = IPGLN + 4                                                 MIX 5420
          WRITE (UNO, 1060) ITMIX, IDSAT, IDDP                              MIX 5430
          STOP                                                              MIX 5440
      END IF                                                                MIX 5450
                                                                            MIX 5460
      IF (IDDP .NE. 0 .AND. IPRIN2 .NE. 0) THEN                             MIX 5470
        IF (IPGLN .GT. 56) CALL PAGE                                        MIX 5480
        IPGLN = IPGLN + 2                                                   MIX 5490
        WRITE (UNO,1120) PAGE3(IDDP), TITMIX(9:25)                          MIX 5500
      END IF                                                                MIX 5510
                                                                            MIX 5520
C -----------------------------------------------------------------------|MIX 5530
C     Prepare first steps ....                                            |MIX 5540
C -----------------------------------------------------------------------|MIX 5550
                                                                            MIX 5560
      IF (ISALT .EQ. 3 .AND. ITMIX .EQ. 0 .AND. ICALL .EQ. 1) THEN          MIX 5570
        IADD = 1                                                            MIX 5580
        JJ   = 1                                                            MIX 5590
        SIMIN(IADD)  = ATCPRD (ICS, IDSP, COFFAC, ALFA)                     MIX 5600
        SIMIN(IADD)  = SIMIN(IADD)  - LOGKT2(IDSAT)                         MIX 5610
        ADDMIN(IADD) = 0.0                                                  MIX 5620
        IF (DABS(SIMIN(IADD)) .LT. FCCSAT) THEN                             MIX 5630
          ICALL = 1                                                         MIX 5640
          IF (IPGLN .GT. 55) CALL PAGE                                      MIX 5650
          IPGLN = IPGLN + 3                                                 MIX 5660
          WRITE (UNO,1150) TITMIX, ADDMIN(IADD)                             MIX 5670
          RETURN                                                            MIX 5680
        END IF                                                              MIX 5690
        J = 0                                                               MIX 5700
        DELTA = 1000.0                                                      MIX 5710
        DO 190 I = 1, 10                                                    MIX 5720
          IF (IDSP(I) .NE. 0) THEN                                          MIX 5730
            IF (M(IDSP(I)) .LT. DELTA .AND.                                 MIX 5740
     .          M(IDSP(I)) .GT. CPUMIN) THEN                                MIX 5750
              DO 180 K = 1, 10                                              MIX 5760
                IF (IDMIN(K) .EQ. IDSP(I)) THEN                             MIX 5770
                  IF (STOFAC(K) .GT. 0) THEN                                MIX 5780
                    J = 1                                                   MIX 5790
                  ELSE                                                      MIX 5800
                    J = -1                                                  MIX 5810
                  END IF                                                    MIX 5820
                  DELTA = M(IDSP(I))                                        MIX 5830
                END IF                                                      MIX 5840
  180         CONTINUE                                                      MIX 5850
            END IF                                                          MIX 5860
          END IF                                                            MIX 5870
  190   CONTINUE                                                            MIX 5880
                                                                            MIX 5890
        IF (DABS(DP) .GT. CPUMIN) THEN                                      MIX 5900
          ADD    = STEPSZ * DP                                              MIX 5910
          REVERS = .FALSE.                                                  MIX 5920
        ELSE IF ((SIMIN(IADD) .LT. 0.0 .AND. J .GE. 0) .OR.                 MIX 5930
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     .           (SIMIN(IADD) .GT. 0.0 .AND. J .LT. 0)) THEN          MIX 5940
            ADD    = STEPSZ                                          MIX 5950
            REVERS = .TRUE.                                          MIX 5960
          ELSE                                                       MIX 5970
            ADD    = STEPSZ * (-1.0)                                 MIX 5980
            REVERS = .TRUE.                                          MIX 5990
          END IF                                                     MIX 6000
          IF (DABS(DP) .LT. CPUMIN) DP = 1.0D00                      MIX 6010
          ADDMIN(IADD+1) = ADD                                       MIX 6020
          CROSS = .FALSE.                                            MIX 6030
                                                                     MIX 6040
        ELSE IF (ISALT .EQ. 3 .AND. ICALL .GT. 1) THEN               MIX 6050
          IADD = IADD + 1                                            MIX 6060
          SIMIN(IADD)  = ATCPRD (ICS, IDSP, COFFAC, ALFA)            MIX 6070
          SIMIN(IADD)  = SIMIN(IADD)  - LOGKT2(IDSAT)                MIX 6080
          IF (DABS(SIMIN(IADD)) .LT. FCCSAT) THEN                    MIX 6090
            ICALL = 1                                                MIX 6100
            IF (IPGLN .GT. 55) CALL PAGE                             MIX 6110
            IPGLN = IPGLN + 3                                        MIX 6120
            WRITE (UNO,1150) TITMIX, ADDMIN(IADD)                    MIX 6130
            RETURN                                                   MIX 6140
          END IF                                                     MIX 6150
                                                                     MIX 6160
          IF (.NOT. CROSS) THEN                                      MIX 6170
            IF ((SIMIN(IADD) * SIMIN(IADD-1)) .LT. 0.0) THEN         MIX 6180
              CROSS = .TRUE.                                         MIX 6190
            ELSE IF (DABS(SIMIN(IADD)) .LT. DABS(SIMIN(IADD-1))) THEN MIX 6200
              ADD    = ADDMIN(IADD) * 10.0                           MIX 6210
              REVERS = .FALSE.                                       MIX 6220
            ELSE IF (REVERS) THEN                                    MIX 6230
              ADD    = ADD * (-0.5)                                  MIX 6240
              IF ((DABS(ADD - ADDMIN(IADD))) .LT. 1.0E-12) THEN      MIX 6250
                WRITE (UNO, 1140) PAGE3(IDSAT), SIMIN(IADD), ADDMIN(IADD) MIX 6260
                STOP                                                 MIX 6270
              END IF                                                 MIX 6280
            ELSE                                                     MIX 6290
              ADD = (ADDMIN(IADD) - ADDMIN(IADD-1)) / 2.0            MIX 6300
              IF ((DABS(ADD) - DABS(ADDMIN(IADD))).LT.1.0E-12) THEN  MIX 6310
                WRITE (UNO, 1140) PAGE3(IDSAT), SIMIN(IADD), ADDMIN(IADD) MIX 6320
                STOP                                                 MIX 6330
              END IF                                                 MIX 6340
            END IF                                                   MIX 6350
          END IF                                                     MIX 6360
          JJ = IADD                                                  MIX 6370
          IF (CROSS) THEN                                            MIX 6380
            CALL SORTA(ADDMIN, SIMIN, IADD, JJ)                      MIX 6390
                                                                     MIX 6400
            DO 200 I = 2, IADD                                       MIX 6410
              J = I - 1                                              MIX 6420
              IF ((SIMIN(I) * SIMIN(J)) .LT. 0.0) GO TO 210          MIX 6430
200         CONTINUE                                                 MIX 6440
                                                                     MIX 6450
          ELSE                                                       MIX 6460
            J = 6                                                    MIX 6470
          END IF                                                     MIX 6480
210       IF (IADD .GT. 6) THEN                                      MIX 6490
            IF (J .GT. 3) THEN                                       MIX 6500
              DO 220 I = 1, IADD-1                                   MIX 6510
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              SIMIN(I)  = SIMIN(I+1)                                    MIX 6520
              ADDMIN(I) = ADDMIN(I+1)                                   MIX 6530
  220       CONTINUE                                                    MIX 6540
            JJ = JJ - 1                                                 MIX 6550
            J  = J  - 1                                                 MIX 6560
          END IF                                                        MIX 6570
          IADD = IADD - 1                                               MIX 6580
        END IF                                                          MIX 6590
        IF (CROSS) THEN                                                 MIX 6600
          CALL GUESS(ADDMIN, SIMIN, ADD, IADD)                          MIX 6610
          X = DABS(ADDMIN(J) - ADDMIN(J+1)) / 10000.0D00                MIX 6620
          IF (DABS (ADDMIN(J)   - ADD) .LT. X    .OR.                   MIX 6630
     .        DABS (ADDMIN(J+1) - ADD) .LT. X )  THEN                   MIX 6640
              ADD = (ADDMIN(J) + ADDMIN(J+1)) / 2.0                     MIX 6650
          END IF                                                        MIX 6660
        END IF                                                          MIX 6670
        ADDMIN(IADD+1) = ADD                                            MIX 6680
      END IF                                                            MIX 6690
                                                                        MIX 6700
C -------------------------------------------------------------------|MIX 6710
C     Change the original solution parameters for the new step and    |MIX 6720
C     go back to calculate species distribution                       |MIX 6730
C -------------------------------------------------------------------|MIX 6740
                                                                        MIX 6750
      IF (ISALT .EQ. 3) THEN                                            MIX 6760
  230   CONTINUE                                                        MIX 6770
        EQC = 0.0                                                       MIX 6780
        EQH = 0.0                                                       MIX 6790
        ANALM(7)  = TOTEL(3)                                            MIX 6800
        ANALM(98) = 0.0                                                 MIX 6810
        IF (DABS(DP) .LT. CPUMIN) DP = 1.0D00                           MIX 6820
        DO 240 I = 1, ICD                                               MIX 6830
          J = IDMIN(I)                                                  MIX 6840
          IF (J .EQ. 0) GO TO 240                                       MIX 6850
          IF (J .EQ. 11) J = 12                                         MIX 6860
          IF (     J .EQ.  7 .OR. J .EQ.  8 .OR. J .EQ. 49) THEN        MIX 6870
              EQH = EQH + (STOFAC(I) * ADD)                             MIX 6880
          ELSE IF (J .EQ. 28 .OR. J .EQ. 33 .OR. J .EQ. 97) THEN        MIX 6890
              EQH = EQH + (STOFAC(I) * ADD * 2.0D00)                    MIX 6900
          ELSE IF (J .EQ. 12) THEN                                      MIX 6910
              EQH = EQH + (STOFAC(I) * ADD * 4.0D00)                    MIX 6920
          ELSE IF (J .EQ. 32 .OR. J .EQ. 9) THEN                        MIX 6930
              EQH = EQH - (STOFAC(I) * ADD)                             MIX 6940
          ELSE IF (J .EQ. 31) THEN                                      MIX 6950
              EQH = EQH - (STOFAC(I) * ADD * 3.0D00)                    MIX 6960
          END IF                                                        MIX 6970
                                                                        MIX 6980
          IF (J .EQ.   7) EQC = (ADD * STOFAC(I)      ) + EQC           MIX 6990
          IF (J .EQ.  97) EQC = (ADD * STOFAC(I)      ) + EQC           MIX 7000
          IF (J .EQ.  98) EQC = (ADD * STOFAC(I)      ) + EQC           MIX 7010
          IF (J .EQ. 207) EQC = (ADD * STOFAC(I)      ) + EQC           MIX 7020
          IF (J .EQ. 208) EQC = (ADD * STOFAC(I) * 2.0) + EQC           MIX 7030
          IF (J .EQ. 209) EQC = (ADD * STOFAC(I) * 3.0) + EQC           MIX 7040
          IF (J .EQ.  97 .OR. J .EQ.  98 .OR. J .EQ. 207 .OR.           MIX 7050
     .        J .EQ. 208 .OR. J .EQ. 209) J = 7                         MIX 7060
                                                                        MIX 7070
          ANALM(J) = ANMMIX(J) + (ADD * STOFAC(I))                      MIX 7080
                                                                        MIX 7090
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      IF (J .NE. 8 .AND. J .NE. 9    .AND. J .NE. 10 .AND.          MIX 7100
     .    (ADD * STOFAC(I)) .LT. 0.0 .AND.                          MIX 7110
     .           ANMMIX(J) .LE. CPUMIN) THEN                        MIX 7120
        WRITE (UNO, 1160)                                          MIX 7130
        STOP                                                       MIX 7140
      END IF                                                       MIX 7150
      IF (J .NE. 8 .AND. J .NE. 9 .AND. J .NE. 10                  MIX 7160
     .           .AND. ANALM(J) .LE. 0.0) THEN                     MIX 7170
        ADD = (ANMMIX(J) / STOFAC(I)) * (-1.0)                     MIX 7180
        ADD = ADD - (ADD / (DABS(DP) * 10.0**(IADD+3)))            MIX 7190
        ADDMIN(IADD+1) = ADD                                       MIX 7200
        GO TO 230                                                  MIX 7210
      END IF                                                       MIX 7220
                                                                   MIX 7230
240   CONTINUE                                                     MIX 7240
      TOTEL(1) = A1MIX(1) + EQH                                    MIX 7250
      TOTEL(3) = A1MIX(3) + EQC                                    MIX 7260
      IF (TOTEL(3) .GT. CPUMIN) THEN                               MIX 7270
        ANALM(7)  = TOTEL(3)                                       MIX 7280
        ANALM(98) = 0.0                                            MIX 7290
      ELSE IF (A1MIX(3) .GT. CPUMIN) THEN                          MIX 7300
        ADD = ADD / 0.9                                            MIX 7310
        ADDMIN(IADD+1) = ADD                                       MIX 7320
        GO TO 230                                                  MIX 7330
      END IF                                                       MIX 7340
      ICALL = 3                                                    MIX 7350
                                                                   MIX 7360
      IF (IPRIN2 .NE. 0) THEN                                      MIX 7370
        IF (IPGLN .GT. 55) CALL PAGE                               MIX 7380
        IPGLN = IPGLN + 3                                          MIX 7390
        IF (IDDP .NE. 0) THEN                                      MIX 7400
          WRITE (UNO,1130) PAGE3(IDSAT), SIMIN(JJ), TITMIX(1:40), ADD MIX 7410
        ELSE                                                       MIX 7420
          WRITE (UNO,1130) PAGE3(IDSAT), SIMIN(JJ), TITMIX(1:40), ADD MIX 7430
        END IF                                                     MIX 7440
      END IF                                                       MIX 7450
                                                                   MIX 7460
      J = 0                                                        MIX 7470
      DO 250 I = 1, 28                                             MIX 7480
        J = J + 1                                                  MIX 7490
        IF (J .EQ.   8) J = 12                                     MIX 7500
        IF (J .EQ.  17) J = 18                                     MIX 7510
        IF (J .EQ.  19) J = 21                                     MIX 7520
        IF (J .EQ.  24) J = 25                                     MIX 7530
        IF (J .EQ.  34) J = 48                                     MIX 7540
        IF (J .EQ.  49) J = 169                                    MIX 7550
        IF (J .EQ. 170) J = 210                                    MIX 7560
        EXELT(I)  = ANALM(J)                                       MIX 7570
250   CONTINUE                                                     MIX 7580
                                                                   MIX 7590
      EXELT(29)  = ANALM(7)                                        MIX 7600
      EXELT(30)  = ANALM(246)                                      MIX 7610
      EXELT(31)  = ANALM(265)                                      MIX 7620
      EXELT(32)  = ANALM(136)                                      MIX 7630
      EXELT(33)  = ANALM(MXSP+1)                                   MIX 7640
      EXELT(34)  = ANALM(MXSP+16)                                  MIX 7650
      EXELT(35)  = ANALM(MXSP+31)                                  MIX 7660
                                                                   MIX 7670
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        TITR( 1) = EXELT(29)                                                MIX 7680
        TITR( 2) = EXELT( 6)                                                MIX 7690
        TITR( 3) = EXELT(22)                                                MIX 7700
        TITR( 4) = EXELT(21)                                                MIX 7710
        TITR( 5) = EXELT( 5)                                                MIX 7720
        TITR( 6) = EXELT(26)                                                MIX 7730
        TITR( 7) = EXELT(25)                                                MIX 7740
        TITR( 8) = EXELT(30)                                                MIX 7750
        TITR( 9) = EXELT(31)                                                MIX 7760
        TITR(10) = EXELT(33)                                                MIX 7770
        TITR(11) = EXELT(34)                                                MIX 7780
        RETURN                                                              MIX 7790
      END IF                                                                MIX 7800
                                                                            MIX 7810
C -------------------------------------------------------------------------|MIX 7820
C     Boiling routine  -- Icall = 1 on the first call only                  |MIX 7830
C -------------------------------------------------------------------------|MIX 7840
                                                                            MIX 7850
      IF (ISALT .EQ. 2) THEN                                                MIX 7860
        FFB = 1.0 - FBOIL                                                   MIX 7870
        IF (ICALL .EQ. 1) THEN                                              MIX 7880
          WRITE (BUFFER, 1230) FBOIL                                        MIX 7890
          READ (BUFFER, '(A)') TITMIX                                       MIX 7900
          IF (IPGLN .GT. 53) CALL PAGE                                      MIX 7910
          IPGLN = IPGLN + 4                                                 MIX 7920
          WRITE (UNO,1170) FBOIL                                            MIX 7930
                                                                            MIX 7940
C -------------------------------------------------------------------------|MIX 7950
C    Calculate the concentration of non-volatile species after boiling     |MIX 7960
C -------------------------------------------------------------------------|MIX 7970
                                                                            MIX 7980
          DO 260 I = 1, MXSP+30                                             MIX 7990
            ANALM(I) = ANMMIX(I) / FFB                                      MIX 8000
  260     CONTINUE                                                          MIX 8010
                                                                            MIX 8020
          J = 0                                                             MIX 8030
          DO 270 I = 1, 28                                                  MIX 8040
            J = J + 1                                                       MIX 8050
            IF (J .EQ.   8) J = 12                                          MIX 8060
            IF (J .EQ.  17) J = 18                                          MIX 8070
            IF (J .EQ.  19) J = 21                                          MIX 8080
            IF (J .EQ.  24) J = 25                                          MIX 8090
            IF (J .EQ.  34) J = 48                                          MIX 8100
            IF (J .EQ.  49) J = 169                                         MIX 8110
            IF (J .EQ. 170) J = 210                                         MIX 8120
            EXELT(I)  = ANALM(J)                                            MIX 8130
  270     CONTINUE                                                          MIX 8140
                                                                            MIX 8150
          EXELT(29)  = ANALM(7)                                             MIX 8160
          EXELT(30)  = ANALM(246)                                           MIX 8170
          EXELT(31)  = ANALM(265)                                           MIX 8180
          EXELT(32)  = ANALM(136)                                           MIX 8190
          EXELT(33)  = ANALM(MXSP+1)                                        MIX 8200
          EXELT(34)  = ANALM(MXSP+16)                                       MIX 8210
          EXELT(35)  = ANALM(MXSP+31)                                       MIX 8220
                                                                            MIX 8230
          TITR( 1) = EXELT(29)                                              MIX 8240
          TITR( 2) = EXELT( 6)                                              MIX 8250
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          TITR( 3) = EXELT(22)                                                  MIX 8260
          TITR( 4) = EXELT(21)                                                  MIX 8270
          TITR( 5) = EXELT( 5)                                                  MIX 8280
          TITR( 6) = EXELT(26)                                                  MIX 8290
          TITR( 7) = EXELT(25)                                                  MIX 8300
          TITR( 8) = EXELT(30)                                                  MIX 8310
          TITR( 9) = EXELT(31)                                                  MIX 8320
          TITR(10) = EXELT(33)                                                  MIX 8330
          TITR(11) = EXELT(34)                                                  MIX 8340
                                                                                MIX 8350
C ------------------------------------------------------------------------|MIX 8360
C     If steam is being added, change appropriate parameters. quit        |MIX 8370
C ------------------------------------------------------------------------|MIX 8380
                                                                                MIX 8390
          IF (FBOIL .LT. 0.D0) THEN                                             MIX 8400
            TOTEL(1)  = TOTEL(1) / FFB                                          MIX 8410
            TOTEL(2)  = TOTEL(2) / FFB                                          MIX 8420
            TOTEL(3)  = TOTEL(3) / FFB                                          MIX 8430
            ANALM(7)  = TOTEL(3)                                                MIX 8440
            ANALM(98) = 0.0                                                     MIX 8450
            EXELT(29) = ANALM(7)                                                MIX 8460
            TITR( 1)  = EXELT(29)                                               MIX 8470
            ICALL = 3                                                           MIX 8480
            RETURN                                                              MIX 8490
          END IF                                                                MIX 8500
                                                                                MIX 8510
C ------------------------------------------------------------------------|MIX 8520
C     Calculate the partitioning of volatile species (co2,nh3,h2s,ch4)     |MIX 8530
C ------------------------------------------------------------------------|MIX 8540
                                                                                MIX 8550
          TK   = TEMP + 273.15                                                  MIX 8560
          KH2S = KHH2S(TK, M1)                                                  MIX 8570
          KNH3 = KHNH3(TK)                                                      MIX 8580
          KCO2 = KHCO2(TK, M1)                                                  MIX 8590
          IF (PRESS .LT. PH2O) PRESS = PH2O                                     MIX 8600
                                                                                MIX 8610
          X = 1.0D00                                                            MIX 8620
          KCH4 = KHCH4(TK, M1, X)                                               MIX 8630
                                                                                MIX 8640
C ------------------------------------------------------------------------|MIX 8650
C     Calculate vapor density (routine taken from drummond's program)      |MIX 8660
C     Calculate volatility ratios                                          |MIX 8670
C ------------------------------------------------------------------------|MIX 8680
                                                                                MIX 8690
          M1 = M1 - 1.0D00                                                      MIX 8700
          CALL DPVT (TEMP, M1, PRESS, VDEN)                                     MIX 8710
          M1 = M1 + 1.0D00                                                      MIX 8720
                                                                                MIX 8730
          VRT   = VDEN * R * (TEMP + 273.15)                                    MIX 8740
          VRCO2 = KCO2 / VRT                                                    MIX 8750
          VRNH3 = KNH3 / VRT                                                    MIX 8760
          VRH2S = KH2S / VRT                                                    MIX 8770
          VRCH4 = KCH4 / VRT                                                    MIX 8780
          IF (IPGLN .GT. 51) CALL PAGE                                          MIX 8790
          IPGLN = IPGLN + 6                                                     MIX 8800
          WRITE (UNO,1190) '  KH2S = ', KH2S,   '  KNH3 = ', KNH3,            MIX 8810
     .                     '  KCO2 = ', KCO2,   '  KCH4 = ', KCH4,            MIX 8820
     .                     ' VRCO2 = ', VRCO2, ' VRNH3 = ', VRNH3,            MIX 8830
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     .                    ' VRH2S = ', VRH2S, ' VRCH4 = ', VRCH4,      MIX 8840
     .                    '   VRT = ', VRT,    '  VDEN = ', VDEN       MIX 8850
                                                                         MIX 8860
          IBTOT = 1                                                      MIX 8870
          IBOIL = 1                                                      MIX 8880
                                                                         MIX 8890
          DO 280 I = 1, 4                                                MIX 8900
            NV(I)   = 0.0                                                MIX 8910
            NL(I)   = 0.0                                                MIX 8920
            STEP(I) = 0.0                                                MIX 8930
280       CONTINUE                                                       MIX 8940
                                                                         MIX 8950
          IF (A1MIX(3) .GT. CPUMIN) THEN                                 MIX 8960
            TRY(1,IBOIL) = TOTEL(3)                                      MIX 8970
            NL(1)        = TOTEL(3)                                      MIX 8980
            NV(1)        = VRCO2 * (M(97) / FFB) * FBOIL                 MIX 8990
            DIF(1,IBOIL) = A1MIX(3) - (TOTEL(3) * FFB + NV(1))           MIX 9000
            STEP(1)      = A1MIX(3) / ((TOTEL(3) * FFB) + NV(1))         MIX 9010
            NL(1)        = (STEP(1) - 1.0D00) * NL(1)                    MIX 9020
                                                                         MIX 9030
            IF (NL(1) .LT. CPUMIN) THEN                                  MIX 9040
              NL(1)   = 0.1   * TRY(1,IBOIL)                             MIX 9050
              STEP(1) = NL(1) - TRY(1,IBOIL)                             MIX 9060
            END IF                                                       MIX 9070
                                                                         MIX 9080
            IF (NL(1) .GT. A1MIX(3) * FFB) THEN                          MIX 9090
              NL(1)   = 0.9   * A1MIX(3) * FFB                           MIX 9100
              STEP(1) = NL(1) - TRY(1,IBOIL)                             MIX 9110
            END IF                                                       MIX 9120
          END IF                                                         MIX 9130
                                                                         MIX 9140
          IF (ANMMIX(32)  .GT. CPUMIN) THEN                              MIX 9150
            TRY(2,IBOIL) = ANALM(32)                                     MIX 9160
            NL(2)        = ANALM(32)                                     MIX 9170
            NV(2)        = VRNH3 * (M(147) / FFB) * FBOIL                MIX 9180
            DIF(2,IBOIL) = ANMMIX(32) - (ANALM(32) * FFB + NV(2))        MIX 9190
            STEP(2)      = ANMMIX(32) / ((ANALM(32) * FFB) + NV(2))      MIX 9200
            NL(2)        = (STEP(2) - 1.0D00) * NL(2)                    MIX 9210
                                                                         MIX 9220
            IF (NL(2) .LT. CPUMIN) THEN                                  MIX 9230
              NL(2)   = 0.1   * TRY(2,IBOIL)                             MIX 9240
              STEP(2) = NL(2) - TRY(2,IBOIL)                             MIX 9250
            END IF                                                       MIX 9260
                                                                         MIX 9270
            IF (NL(2) .GT. (ANMMIX(32) * FFB)) THEN                      MIX 9280
              NL(2)   = 0.9   * ANMMIX(32) * FFB                         MIX 9290
              STEP(2) = NL(2) - TRY(2,IBOIL)                             MIX 9300
            END IF                                                       MIX 9310
          END IF                                                         MIX 9320
                                                                         MIX 9330
          IF (ANMMIX(33)  .GT. CPUMIN) THEN                              MIX 9340
            TRY(3,IBOIL) = ANALM(33)                                     MIX 9350
            NL(3)        = ANALM(33)                                     MIX 9360
            NV(3)        = VRH2S * (M(33) / FFB) * FBOIL                 MIX 9370
            DIF(3,IBOIL) = ANMMIX(33) - (ANALM(33) * FFB + NV(3))        MIX 9380
            STEP(3)      = ANMMIX(33) / ((ANALM(33) * FFB) + NV(3))      MIX 9390
            NL(3)        = (STEP(3) - 1.0D00) * NL(3)                    MIX 9400
                                                                         MIX 9410
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          IF (NL(3) .LT. CPUMIN) THEN                                    MIX 9420
            NL(3)   = 0.1   * TRY(3,IBOIL)                               MIX 9430
            STEP(3) = NL(3) - TRY(3,IBOIL)                               MIX 9440
          END IF                                                         MIX 9450
                                                                         MIX 9460
          IF (NL(2) .GT. (ANMMIX(33) * FFB)) THEN                        MIX 9470
            NL(3)   = 0.9   * ANMMIX(33) * FFB                           MIX 9480
            STEP(3) = NL(3) - TRY(3,IBOIL)                               MIX 9490
          END IF                                                         MIX 9500
        END IF                                                           MIX 9510
                                                                         MIX 9520
        IF (ANMMIX(285)  .GT. CPUMIN) THEN                               MIX 9530
          TRY(4,IBOIL) = ANALM(285)                                      MIX 9540
          NL(4)        = ANALM(285)                                      MIX 9550
          NV(4)        = VRCH4 * (M(285) / FFB) * FBOIL                  MIX 9560
          DIF(4,IBOIL) = ANMMIX(285) - (ANALM(285)*FFB + NV(4))          MIX 9570
          STEP(4)      = ANALM(285) / ((ANMMIX(285) * FFB) + NV(4))      MIX 9580
          NL(4)        = (STEP(4) - 1.0D00) * NL(4)                      MIX 9590
                                                                         MIX 9600
          IF (NL(4) .LT. CPUMIN) THEN                                    MIX 9610
            NL(4)   = 0.1   * TRY(4,IBOIL)                               MIX 9620
            STEP(4) = NL(4) - TRY(4,IBOIL)                               MIX 9630
          END IF                                                         MIX 9640
                                                                         MIX 9650
          IF (NL(4) .GT. (ANMMIX(285) * FFB)) THEN                       MIX 9660
            NL(4)   = 0.9   * ANMMIX(285) * FFB                          MIX 9670
            STEP(4) = NL(4) - TRY(4,IBOIL)                               MIX 9680
          END IF                                                         MIX 9690
        END IF                                                           MIX 9700
      END IF                                                             MIX 9710
                                                                         MIX 9720
      IF (ICALL .EQ. 3) THEN                                             MIX 9730
        IBOIL = IBOIL + 1                                                MIX 9740
        IBTOT = IBTOT + 1                                                MIX 9750
        IF (IBTOT .GT. 3) THEN                                           MIX 9760
          IBOIL = 3                                                      MIX 9770
          DO 300 J = 1, 4                                                MIX 9780
            DO 290 I = 2, IBOIL                                          MIX 9790
              TRY(J,I-1) = TRY(J,I)                                      MIX 9800
              DIF(J,I-1) = DIF(J,I)                                      MIX 9810
290         CONTINUE                                                     MIX 9820
300       CONTINUE                                                       MIX 9830
        END IF                                                           MIX 9840
                                                                         MIX 9850
        TRY(1,IBOIL) = TOTEL(3)                                          MIX 9860
        NV(1)        = VRCO2 * M(97) * FBOIL                             MIX 9870
        DIF(1,IBOIL) = A1MIX(3) - ((TOTEL(3) * FFB) + NV(1))             MIX 9880
                                                                         MIX 9890
        TRY(2,IBOIL) = ANALM(32)                                         MIX 9900
        NV(2)        = VRNH3 * M(147) * FBOIL                            MIX 9910
        DIF(2,IBOIL) = ANMMIX(32) - ((ANALM(32) * FFB) + NV(2))          MIX 9920
                                                                         MIX 9930
        TRY(3,IBOIL) = ANALM(33)                                         MIX 9940
        NV(3)        = VRH2S * M(33) * FBOIL                             MIX 9950
        DIF(3,IBOIL) = ANMMIX(33) - ((ANALM(33) * FFB) + NV(3))          MIX 9960
                                                                         MIX 9970
        TRY(4,IBOIL) = ANALM(285)                                        MIX 9980
        NV(4)        = VRCH4 * M(285) * FBOIL                            MIX 9990
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      DIF(4,IBOIL) = ANMMIX(285) - ((ANALM(285) * FFB) + NV(4))      MIX10000
                                                                     MIX10010
      DONE = .TRUE.                                                  MIX10020
                                                                     MIX10030
      DO 310 I = 1,  4                                               MIX10040
        IF (I .EQ. 1) THEN                                           MIX10050
          X = AlMIX(3)                                               MIX10060
        ELSE IF (I .EQ. 2) THEN                                      MIX10070
          X = ANMMIX(32)                                             MIX10080
        ELSE IF (I .EQ. 3) THEN                                      MIX10090
          X = ANMMIX(33)                                             MIX10100
        ELSE IF (I .EQ. 4) THEN                                      MIX10110
          X = ANMMIX(285)                                            MIX10120
        END IF                                                       MIX10130
                                                                     MIX10140
        IF (X .GT. CPUMIN) THEN                                      MIX10150
          IF (DABS(DIF(I,IBOIL) / X ) .GT. 0.01 .AND.                MIX10160
     .        DABS(STEP(I)) .GT. (X * 0.01) .AND. IBTOT .LT. 20)     MIX10170
     .      DONE = .FALSE.                                           MIX10180
                                                                     MIX10190
          IF ((DIF(I,IBOIL) * DIF(I,(IBOIL-1))) .LT. 0.0) THEN       MIX10200
            STEP(I) = STEP(I) * (-0.5)                               MIX10210
          ELSE IF (DABS(DIF(I,IBOIL)) .GT. DABS(DIF(I,(IBOIL-1))))   MIX10220
     .      THEN                                                     MIX10230
            STEP(I) = STEP(I) * (-0.8)                               MIX10240
          END IF                                                     MIX10250
                                                                     MIX10260
          IF ((NL(I) + STEP(I)) .LE. 0.0) THEN                       MIX10270
            STEP(I) = NL(I) * (-0.90)                                MIX10280
          ELSE IF ((NL(I) + STEP(I)) .GE. (X/FFB)) THEN              MIX10290
            STEP(I) = ((X/FFB) - NL(I)) * 0.90                       MIX10300
          END IF                                                     MIX10310
                                                                     MIX10320
          NL(I) = NL(I) + STEP(I)                                    MIX10330
          NV(I) = X - (NL(I) * FFB)                                  MIX10340
        END IF                                                       MIX10350
  310 CONTINUE                                                       MIX10360
                                                                     MIX10370
      IF (DONE) THEN                                                 MIX10380
        NGAST(1) = AlMIX(3)                                          MIX10390
        NGAST(2) = ANMMIX(32)                                        MIX10400
        NGAST(3) = ANMMIX(33)                                        MIX10410
        NGAST(4) = ANMMIX(285)                                       MIX10420
                                                                     MIX10430
        NL(1) = ANALM(7)                                             MIX10440
        NL(2) = ANALM(32)                                            MIX10450
        NL(3) = ANALM(33)                                            MIX10460
        NL(4) = ANALM(285)                                           MIX10470
                                                                     MIX10480
        IF (IPGLN .GT. 48) CALL PAGE                                 MIX10490
        IPGLN = IPGLN + 10                                           MIX10500
        WRITE (UNO,1180) FBOIL                                       MIX10510
        WRITE (UNO,1210)                                             MIX10520
                                                                     MIX10530
        DO 320 I = 1, 4                                              MIX10540
          IF (NGAST(I) .GT. CPUMIN) THEN                             MIX10550
            NV(I) = NGAST(I) - (NL(I) * FFB)                         MIX10560
            X     = NV(I) * 100.00 / NGAST(I)                        MIX10570
```

```
            ELSE                                                        MIX10580
              X = 0.0                                                   MIX10590
              NL(I) = 0.0                                               MIX10600
              NV(I) = 0.0                                               MIX10610
            END IF                                                      MIX10620
            WRITE (UNO,1220) DUM2(I), NGAST(I), (NL(I) * FFB),          MIX10630
     .                       NL(I), NV(I), X                            MIX10640
320       CONTINUE                                                      MIX10650
          ICALL = 1                                                     MIX10660
          RETURN                                                        MIX10670
        END IF                                                          MIX10680
      END IF                                                            MIX10690
                                                                        MIX10700
      IF (IPRIN2 .NE. 0) THEN                                           MIX10710
        IF (IPGLN .GT. 50) CALL PAGE                                    MIX10720
        IPGLN = IPGLN + 10                                              MIX10730
        WRITE (UNO, 1200)                                               MIX10740
     .       NV(1), (NL(1)*FFB), NL(1), PAGE1(97),  M(97),              MIX10750
     .       NV(2), (NL(2)*FFB), NL(2), PAGE1(147), M(147),             MIX10760
     .       NV(3), (NL(3)*FFB), NL(3), PAGE1(33),  M(33),              MIX10770
     .       NV(4), (NL(4)*FFB), NL(4), PAGE1(285), M(285)              MIX10780
      END IF                                                            MIX10790
                                                                        MIX10800
      TOTEL(1)   = (A1MIX(1)    - (NV(1) * 2.0)                         MIX10810
     .                          - (NV(3) * 2.0))          / FFB         MIX10820
      TOTEL(2)   = (A1MIX(2)    - NV(2))                  / FFB         MIX10830
      TOTEL(3)   = NL(1)                                                MIX10840
      ANALM(32)  = NL(2)                                                MIX10850
      ANALM(33)  = NL(3)                                                MIX10860
      ANALM(285) = NL(4)                                                MIX10870
      ANALM(7)   = TOTEL(3)                                             MIX10880
      ANALM(98)  = 0.0                                                  MIX10890
                                                                        MIX10900
      EXELT(24) = ANALM(32)                                             MIX10910
      EXELT(25) = ANALM(33)                                             MIX10920
      EXELT(29) = ANALM(7)                                              MIX10930
                                                                        MIX10940
      TITR( 1) = EXELT(29)                                              MIX10950
      TITR( 7) = EXELT(25)                                              MIX10960
                                                                        MIX10970
      ICALL = 3                                                         MIX10980
      RETURN                                                            MIX10990
    END IF                                                              MIX11000
                                                                        MIX11010
C ---------------------------------------------------------------------|MIX11020
C     The following routine is for mixing two solutions                |MIX11030
C     Store the parameters of the second solution                      |MIX11040
C ---------------------------------------------------------------------|MIX11050
                                                                        MIX11060
    IF (ICALL .EQ. 2) THEN                                              MIX11070
      DO 330 I = 1, 10                                                  MIX11080
        FMIX(I) = 0.0D0                                                 MIX11090
        IF (I .LE. 5) B2MIX(I) = TOTEL(I)                               MIX11100
330   CONTINUE                                                          MIX11110
                                                                        MIX11120
      DO 340 I = 1, MXSP+30                                             MIX11130
        BNMMIX(I) = ANALM(I)                                            MIX11140
340   CONTINUE                                                          MIX11150
```

```
                                                                      MIX11160
        BDENS = DENS                                                  MIX11170
        BTEMP = TEMP                                                  MIX11180
                                                                      MIX11190
C -------------------------------------------------------------------|MIX11200
C     Calculate the no. of mixtures to be processed and the           |MIX11210
C     proportions of the two solutions in each of the mixtures        |MIX11220
C -------------------------------------------------------------------|MIX11230
                                                                      MIX11240
        IF (INMIX .LE. 0) INMIX = 1                                   MIX11250
        IF (DABS(DINC) .LT. CPUMIN) DINC = DFRAC1                     MIX11260
                                                                      MIX11270
        INMIX = MIN(INMIX, 10)                                        MIX11280
        DO 350 I = 1, INMIX                                           MIX11290
          IF (I .EQ. 1) THEN                                          MIX11300
            FMIX(I) = DFRAC1                                          MIX11310
          ELSE                                                        MIX11320
            FMIX(I) = FMIX(I-1) + DINC                                MIX11330
          END IF                                                      MIX11340
          IF (FMIX(I) .LT. 0.0 .OR. FMIX(I) .GT. 1.00D00) THEN        MIX11350
            INMIX = I - 1                                             MIX11360
            GO TO 360                                                 MIX11370
          END IF                                                      MIX11380
  350   CONTINUE                                                      MIX11390
                                                                      MIX11400
  360   CONTINUE                                                      MIX11410
        IRUN = 0                                                      MIX11420
        CALL PAGE                                                     MIX11430
        IPGLN = IPGLN + 7                                             MIX11440
        WRITE (UNO,1240) DFRAC1, INMIX, DINC                          MIX11450
      END IF                                                          MIX11460
                                                                      MIX11470
      ICALL = 3                                                       MIX11480
                                                                      MIX11490
      RETURN                                                          MIX11500
                                                                      MIX11510
 1000 FORMAT(I3,/,10(F10.4,I4))                                       MIX11520
 1010 FORMAT(//,' ***** Mineral with i.d. number = ',I4,/,            MIX11530
     .          '       which will be dissolved/precipitated,',/,    MIX11540
     .          '       could not be found in the reaction file.')   MIX11550
 1020 FORMAT(//,' ***** Mineral with i.d. number = ',I4,/,            MIX11560
     .          '       which the solution will be brought to',      MIX11570
     .                 ' equilibrium with',/,                       MIX11580
     .          '       could not be found in the reaction file.')   MIX11590
 1030 FORMAT(//,' ***** OPEN failed for phase reactions file',        MIX11600
     .             ' (often called RXN.TBL or something similar)',   MIX11610
     .        /,'       in routine MIXER.  Check that the file ',    MIX11620
     .             ' exists ... ')                                  MIX11630
 1040 FORMAT(//,' ***** ERROR reading the reaction data file in ',    MIX11640
     .          'routine MIXER.  The error occurred while',         MIX11650
     .        /,' trying to read the ',I5,'th line.  Either the file',MIX11660
     .          ' is corrupted or the end of file was reached',     MIX11670
     .        /,' without having found the minerals to dissolve'    MIX11680
     .         ,' or precipitate.')                                 MIX11690
 1050 FORMAT(//,' ***** No reaction data for ',A8, '******',         MIX11700
     .          ' Correct and rerun')                               MIX11710
 1060  FORMAT(//,' ***** Illegal values of ITMIX, IDSAT, IDDP passed',MIX11720
     .         /,'       to MIXER when IBMIX = 0. Values are ',     MIX11730
```

```
     .           3(I2,1X), 'respectively.')                                  MIX11740
1070 FORMAT(//, '*** Net amount of salt/(aqueous component) to be',         MIX11750
     .           '  added the solution *****', //,                          MIX11760
     .           ' SP #                MOLALITY       EQH    EQC')          MIX11770
1080 FORMAT(I4,2X,A,2X,D16.8,2X,F5.2,2X,F5.2)                               MIX11780
1090 FORMAT('  ****************************************',//)                 MIX11790
1100 FORMAT(//,' *********ERROR*********ERROR**********',                   MIX11800
     .        /,4X, A, ' was removed from the solution (',E12.5,            MIX11810
     .         ') but this drove the moles negative.',                     MIX11820
     .        /,' In this solution, no more than ', E12.5,                 MIX11830
     .         ' moles can be removed. ')                                  MIX11840
1110 FORMAT(//, '*** Net amount of mineral ',A,' to be',                    MIX11850
     .           '  added the solution ... modeled using *****', //,       MIX11860
     .           ' SP #                MOLALITY       EQH    EQC')          MIX11870
1120 FORMAT(/,2X,A8,' will be ',A13,' to saturation ')                      MIX11880
1130 FORMAT(/,' Saturation Index (SI) = (',A,') = ',E10.4,                  MIX11890
     .       /,' Reaction Step (moles of ',A,') = ',E10.4)                 MIX11900
1140 FORMAT(//,'  ***  Saturation with ',A,' not possible. ',               MIX11910
     .        /,'       SI minimum found at SI = ',E12.5,                  MIX11920
     .        /,'       At last try, there was ',E12.5,                    MIX11930
     .         ' moles of material added.',                               MIX11940
     .        /,'       This may also be caused by specifying DP',         MIX11950
     .        /,'       to be negative when only a positive value',       MIX11960
     .        /,'       works (or vice versa) or DP was too small of',    MIX11970
     .        /,'       a value.')                                         MIX11980
1150 FORMAT(/,' Total moles of ',A25,' to achieve saturation: ',E10.4,      MIX11990
     .       /)                                                            MIX12000
1160 FORMAT(/,' Attempt to have a negative amount of a component',          MIX12010
     .       /,' Check what is being added/removed from the water .')      MIX12020
1170 FORMAT(//,'  **** This solution is to be boiled off ****',             MIX12030
     .       /,'       Fraction of boiling = ',F7.2)                       MIX12040
1180 FORMAT(  '  *******  BOILING CALCULATIONS  ******* ',//,              MIX12050
     .         5X, 'Fraction of solution lost by boiling: ',F5.2)          MIX12060
1190 FORMAT(//,'  Parameters used in Boiling ..... ',                       MIX12070
     .       /,4(5X,A,E12.5), /,4(5X,A,E12.5), /,2(5X,A,E12.5))           MIX12080
1200 FORMAT(/,' For the next step, projected amount in the',                MIX12090
     .         17X,'using the current values in the',                      MIX12100
     .       /,10X,'vapour',11X,'liquid',11X,'liquid',                     MIX12110
     .         10X,'aqueous solution of the species'                       MIX12120
     .       /,10X,'(moles)',10X,'(moles)',9X,'(molality)',                MIX12130
     .         23X,'(molality)',                                           MIX12140
     .       /,' CO2 = ',3(E12.5,5X),2X,A8,7X,E12.5,                       MIX12150
     .       /,' NH3 = ',3(E12.5,5X),2X,A8,7X,E12.5,                       MIX12160
     .       /,' H2S = ',3(E12.5,5X),2X,A8,7X,E12.5,                       MIX12170
     .       /,' CH4 = ',3(E12.5,5X),2X,A8,7X,E12.5,                       MIX12180
     .       /)                                                            MIX12190
1210 FORMAT(/, 14X,' Gas species', 5X,'Total Moles   ',                     MIX12200
     .          5X,'Moles in Liquid', 3X,'Molality in Liquid',             MIX12210
     .          4X,'Moles in Vapour',                                      MIX12220
     .          4X,'% Lost in Vapour', /)                                  MIX12230
1220 FORMAT(20X, A5, 5(5X,E12.5,3X),5X,F12.5)                               MIX12240
1230 FORMAT( '(fraction of boiling :- ',2X,F4.2,')')                        MIX12250
1240 FORMAT(//, ' **** Mixing of the two previous solutions in',            MIX12260
     .          ' the following proportions: ', /,                         MIX12270
     .       5X,' Initial fraction of solution 1 = ',F7.4,/,               MIX12280
     .      17X,' Number of mixtures = ',I3,/,                             MIX12290
     .          ' and the increment between solutions = ',F7.4,/)          MIX12300
1250 FORMAT(//, ' *****This solution is to be mixed with the',              MIX12310
```

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            ' next solution.....', /)                                    MIX12320
                                                                         MIX12330
      END                                                                MIX12340



      SUBROUTINE NACALC (TC, CM, PE, RLG, P, GL0)                        NAC 0010
C ==========================================================================|NAC 0020
C     Program chaos2.f4-a routine for calculating thermo. properties       |NAC 0030
C     of nacl(aq) using pitzer's new model.  0.0=osmotic;                  |NAC 0040
C --------------------------------------------------------------------------|NAC 0050
C     AC        DBL   Charge of the anions                                 |NAC 0060
C     ALPHA     DBL   Coefficient of thermal expansion                     |NAC 0070
C     AN        DBL   Number of anions                                     |NAC 0080
C     AP        DBL   Debye-huckel osmotic parameter                       |NAC 0090
C     AVN       DBL   Avogadro's number                                    |NAC 0100
C     B0        DBL   Beta zero parameter                                  |NAC 0110
C     B1        DBL   Beta one parameter                                   |NAC 0120
C     BETAL     DBL   Coefficient of compressibility                       |NAC 0130
C     BK        DBL   Boltzmann's constant in erg/deg                      |NAC 0140
C     C         DBL   C sub fee parameter                                  |NAC 0150
C     CC        DBL   Charge of the cations                                |NAC 0160
C     CI        DBL   Ionic Strength                                       |NAC 0170
C     CM        DBL   Sum of Molality * charge / 2                         |NAC 0180
C     CN        DBL   Number of cations                                    |NAC 0190
C     DC        DBL   Dielectric constant of water                         |NAC 0200
C     DCDT      DBL   Derivative of dielectic constant water T             |NAC 0210
C     DW        DBL   Density of water                                     |NAC 0220
C     E         DBL   Electron charge in esu                               |NAC 0230
C     F1I       DBL   Intermediate storage variable                        |NAC 0240
C     F2I       DBL   Intermediate storage variable                        |NAC 0250
C     F3I       DBL   Intermediate storage variable                        |NAC 0260
C     F4I       DBL   Intermediate storage variable                        |NAC 0270
C     GL0       DBL   Gibbs free energy per mole                           |NAC 0280
C     I         INT   Loop variable                                        |NAC 0290
C     P         DBL   Fit constants                                        |NAC 0300
C     P0        DBL   Vapor pressure                                       |NAC 0310
C     PE        DBL   Pressure in bars                                     |NAC 0320
C     PHI       DBL   Osmotic coefficient                                  |NAC 0330
C     PI        DBL   The constant Pi                                      |NAC 0340
C     PX        DBL   Calculated pressure of water                         |NAC 0350
C     RLG       DBL   Natural log of the activity coefficient              |NAC 0360
C     SCI       DBL   Square root of the ionic strength                    |NAC 0370
C     T         DBL   Temperature in kelvin                                |NAC 0380
C     TC        DBL   Temperature in celcius                               |NAC 0390
C     VF1       DBL   Intermediate storage variable                        |NAC 0400
C     VF2       DBL   Intermediate storage variable                        |NAC 0410
C     VF3       DBL   Intermediate storage variable                        |NAC 0420
C     XP0       DBL   Intermediate storage variable                        |NAC 0430
C     XP1       DBL   Intermediate storage variable                        |NAC 0440
C     XP2       DBL   Intermediate storage variable                        |NAC 0450
C     XP3       DBL   Intermediate storage variable                        |NAC 0460
C     XP4       DBL   Intermediate storage variable                        |NAC 0470
C     XP5       DBL   Intermediate storage variable                        |NAC 0480
C     XP6       DBL   Intermediate storage variable                        |NAC 0490
C     XP7       DBL   Intermediate storage variable                        |NAC 0500
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C     XP8       DBL   Intermediate storage variable                    |NAC 0510
C     XP9       DBL   Intermediate storage variable                    |NAC 0520
C     XS        DBL   Intermediate storage variable                    |NAC 0530
C ---------------------------------------------------------------------|NAC 0540
                                                                       NAC 0550
      INTEGER I                                                        NAC 0560
                                                                       NAC 0570
      DOUBLE PRECISION AC, ALPHA, AN, AP, AVN                          NAC 0580
      DOUBLE PRECISION B0, B1, BETAL, BK                               NAC 0590
      DOUBLE PRECISION C, CC, CI, CM, CN                               NAC 0600
      DOUBLE PRECISION DC, DCDT, DW, E                                 NAC 0610
      DOUBLE PRECISION F1I, F2I, F3I, F4I, GL0                         NAC 0620
      DOUBLE PRECISION P(60), P0, PE, PI, PHI, PX                      NAC 0630
      DOUBLE PRECISION RLG, SCI, T, TC                                 NAC 0640
      DOUBLE PRECISION VF1, VF2, VF3, XS                               NAC 0650
      DOUBLE PRECISION XP0, XP1, XP2, XP3, XP4, XP5, XP6, XP7, XP8, XP9 NAC 0660
                                                                       NAC 0670
      EXTERNAL PSAT, WAPVT, WDBP                                       NAC 0680
                                                                       NAC 0690
      INTRINSIC DABS, DEXP, DLOG, DSQRT                                NAC 0700
                                                                       NAC 0710
      DATA AVN, BK, E, PI /6.02251D+23, 1.38054D-16,                   NAC 0720
     .                     4.80298D-10, 3.1415926D+0/                  NAC 0730
                                                                       NAC 0740
C =====================================================================|NAC 0750
                                                                       NAC 0760
C ---------------------------------------------------------------------|NAC 0770
C     CC & AC = Cation and anion charge                                |NAC 0780
C ---------------------------------------------------------------------|NAC 0790
                                                                       NAC 0800
      CC = P(54)                                                       NAC 0810
      AC = P(55)                                                       NAC 0820
                                                                       NAC 0830
C ---------------------------------------------------------------------|NAC 0840
C     CN & AN = Number of cations and anions                           |NAC 0850
C ---------------------------------------------------------------------|NAC 0860
                                                                       NAC 0870
      CN = P(56)                                                       NAC 0880
      AN = P(57)                                                       NAC 0890
                                                                       NAC 0900
C ---------------------------------------------------------------------|NAC 0910
C     TC = Temp(C); CM = Molality; CI = Ionic Strength                 |NAC 0920
C ---------------------------------------------------------------------|NAC 0930
                                                                       NAC 0940
      T  = TC + 273.15D+0                                              NAC 0950
      CI = (CC**2 * CN + AC**2 * AN) * CM / 2.0                        NAC 0960
                                                                       NAC 0970
C ---------------------------------------------------------------------|NAC 0980
C     Calculate saturation vapor pressure, P0                          |NAC 0990
C ---------------------------------------------------------------------|NAC 1000
                                                                       NAC 1010
      CALL PSAT (TC, P0)                                               NAC 1020
                                                                       NAC 1030
C ---------------------------------------------------------------------|NAC 1040
C     If desired, set PE = P0                                          |NAC 1050
C ---------------------------------------------------------------------|NAC 1060
                                                                       NAC 1070
      IF (PE .LT. 1.0) PE = P0                                         NAC 1080
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                                                                      NAC 1090
C ---------------------------------------------------------------------|NAC 1100
C     Set PE = One bar. if temp. less than 100C                        |NAC 1110
C ---------------------------------------------------------------------|NAC 1120
                                                                      NAC 1130
      IF (TC .LT. 100.1) PE = 1.0                                     NAC 1140
                                                                      NAC 1150
      XP0 = P(18) + (P(19) * PE) + (P(20) * PE**2) + (P(21) * PE**3)  NAC 1160
      XP1 = P(23) + (P(24) * PE) + (P(25) * PE**2) + (P(26) * PE**3)  NAC 1170
      XP2 = P(27) + (P(28) * PE) + (P(29) * PE**2)                    NAC 1180
      XP3 = P(30) + (P(31) * PE) + (P(32) * PE**2) + (P(33) * PE**3)  NAC 1190
      XP4 = P(34) + (P(35) * PE) + (P(36) * PE**2) + (P(37) * PE**3)  NAC 1200
      XP5 = P(43) + (P(44) * PE)                                      NAC 1210
      XP6 = P(46) + (P(47) * PE)                                      NAC 1220
      XP7 = P(48) + (P(49) * PE)                                      NAC 1230
      XP8 = P(50) + (P(51) * PE)                                      NAC 1240
      XP9 = P(52) + (P(53) * PE)                                      NAC 1250
                                                                      NAC 1260
C ---------------------------------------------------------------------|NAC 1270
C     Initialize loop to calculate density, DW                         |NAC 1280
C ---------------------------------------------------------------------|NAC 1290
                                                                      NAC 1300
      DW = 1.0                                                        NAC 1310
      PX = 1.0                                                        NAC 1320
      DO 10 I = 1, 100                                                NAC 1330
        CALL WAPVT (TC, DW, PX, BETAL, GL0, ALPHA)                    NAC 1340
        XS = DW                                                       NAC 1350
        DW = DW / DEXP(BETAL * (PX - PE))                             NAC 1360
        IF (DABS((DW-XS)/XS) .LT. 1.0D-10) GO TO 20                   NAC 1370
   10 CONTINUE                                                        NAC 1380
                                                                      NAC 1390
C ---------------------------------------------------------------------|NAC 1400
C     Calculate dielectric properties of water                         |NAC 1410
C ---------------------------------------------------------------------|NAC 1420
                                                                      NAC 1430
   20 CONTINUE                                                        NAC 1440
      CALL WDBP (TC, PE, DC, DCDT)                                    NAC 1450
                                                                      NAC 1460
C ---------------------------------------------------------------------|NAC 1470
C     AP = Debye-huckel osmotic parameter                              |NAC 1480
C ---------------------------------------------------------------------|NAC 1490
                                                                      NAC 1500
      AP = (1.0 / 3.0) * DSQRT(2.0 * PI * AVN * DW / 1000.0) *        NAC 1510
           (E**2 / (DC * BK * T))**1.5                                NAC 1520
                                                                      NAC 1530
C ---------------------------------------------------------------------|NAC 1540
C     Calculate functions of ionic strength                            |NAC 1550
C ---------------------------------------------------------------------|NAC 1560
                                                                      NAC 1570
      SCI = DSQRT(CI)                                                 NAC 1580
      F1I = DEXP(-2.0 * SCI)                                          NAC 1590
                                                                      NAC 1600
C ---------------------------------------------------------------------|NAC 1610
C     Is RLG a heat quantity ?                                         |NAC 1620
C ---------------------------------------------------------------------|NAC 1630
                                                                      NAC 1640
      F2I = SCI / (1.0 + 1.2 * SCI)                                   NAC 1650
      F3I = (2.0 / 1.2) * DLOG(1.0 + 1.2 * SCI)                       NAC 1660
```

```
      F4I = (1.0 - (1.0 + 2.0 * SCI - 4.0 * CI / 2.0) * F1I) /          NAC 1670
     .      (4.0 * CI)                                                  NAC 1680
                                                                        NAC 1690
C -------------------------------------------------------------------|NAC 1700
C     Calculate valence factors                                       |NAC 1710
C -------------------------------------------------------------------|NAC 1720
                                                                        NAC 1730
      VF1 = CC * AC                                                     NAC 1740
      VF2 = 2.0 * CN * AN / (CN + AN)                                   NAC 1750
      VF3 = 2.0 * (CN * AN)**1.5 / (CN + AN)                            NAC 1760
                                                                        NAC 1770
C -------------------------------------------------------------------|NAC 1780
C     B0, B1, & C are parameters BETA0, BETA1, & C(superscript phi) in |NAC 1790
C     pitzer's equations. B0, B1, & C are calculated as functions of  |NAC 1800
C     temp. In terms of the adjustable parameters, P(I)               |NAC 1810
C -------------------------------------------------------------------|NAC 1820
                                                                        NAC 1830
      B0 = P(17) / T + XP0 + P(22) * DLOG(T) + XP1 * T + XP2 * T**2 +   NAC 1840
     .     XP3 / (T - 227.0) + XP4 / (680.0 - T)                        NAC 1850
      B1 = P(38) / T + P(39) + P(40) * T + P(41) / (T - 227.0)          NAC 1860
      C = P(42) / T + XP5 + P(45) * DLOG(T) + XP6 * T + XP7 * T**2 +    NAC 1870
     .    XP8 / (T - 227.0) + XP9 / (680.0 - T)                         NAC 1880
                                                                        NAC 1890
C -------------------------------------------------------------------|NAC 1900
C     PHI = Osmotic Coefficient                                       |NAC 1910
C -------------------------------------------------------------------|NAC 1920
                                                                        NAC 1930
      PHI = 1.0 - VF1 * AP * F2I + CM * VF2 * (B0 + B1 * F1I) +         NAC 1940
     .      CM**2 * VF3 * C                                           NAC 1950
                                                                        NAC 1960
C -------------------------------------------------------------------|NAC 1970
C     RLG = Ln Gamma                                                  |NAC 1980
C -------------------------------------------------------------------|NAC 1990
                                                                        NAC 2000
      RLG = -VF1 * AP * (F2I + F3I) + CM * 2.0 * VF2 *                  NAC 2010
     .      (B0 + B1 * F4I) + 1.5 * CM**2 * VF3 * C                   NAC 2020
                                                                        NAC 2030
      RETURN                                                            NAC 2040
      END                                                               NAC 2050
```

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      SUBROUTINE PAGE                                                   PAG 0010
C ===================================================================|PAG 0020
C     Writes a form feed into output file, increments page number, and |PAG 0030
C       resets line count                                              |PAG 0040
C -------------------------------------------------------------------|PAG 0050
C     IPAGE     INT   Current page number of output file              |PAG 0060
C     IPGLN     INT   Current line number of the output file          |PAG 0070
C     TOF       CHA   Places a form feed in output file               |PAG 0080
C     UNO       INT   File unit assigned for output file              |PAG 0090
C -------------------------------------------------------------------|PAG 0100
                                                                        PAG 0110
      INTEGER UNO                                                       PAG 0120
      PARAMETER (UNO = 6)                                               PAG 0130
                                                                        PAG 0140
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      INTEGER IPAGE, IPGLN                                                  PAG 0150
                                                                            PAG 0160
      CHARACTER *  1 TOF, CR                                                PAG 0170
      CHARACTER * 40 TITMIX                                                 PAG 0180
                                                                            PAG 0190
      COMMON /FMFD/ TOF, CR, TITMIX                                         PAG 0200
      COMMON /FORM/ IPAGE, IPGLN                                            PAG 0210
                                                                            PAG 0220
C ==========================================================================|PAG 0230
                                                                            PAG 0240
      IPAGE = IPAGE + 1                                                     PAG 0250
      WRITE (UNO, 100) TOF, IPAGE                                           PAG 0260
      IPGLN = 4                                                             PAG 0270
                                                                            PAG 0280
      RETURN                                                                PAG 0290
                                                                            PAG 0300
  100 FORMAT (A1,60X,' PAGE - ',I4,' - ',///)                               PAG 0310
                                                                            PAG 0320
      END                                                                   PAG 0330
```

```
      SUBROUTINE PCLOGK (TCENT, PS, PRES, MXAQK, MXPC)                      PCL 0010
C ==========================================================================|PCL 0020
C     Determines the pressure correction on log K values if pressure        |PCL 0030
C       is greater than vapor pressure of water                             |PCL 0040
C ---------------------------------------------------------------------------|PCL 0050
C     A          DBL   Fit constants                                        |PCL 0060
C     AHI        DBL   Pressure correction fit parameter                    |PCL 0070
C     AL         DBL   Fit constant                                         |PCL 0080
C     ALOW       DBL   Pressure correction fit parameter                    |PCL 0090
C     B          DBL   Intermediate storage variable                        |PCL 0100
C     B0         DBL   Fit constant                                         |PCL 0110
C     B1         DBL   Fit constant                                         |PCL 0120
C     B2         DBL   Fit constant                                         |PCL 0130
C     B4         DBL   Fit constant                                         |PCL 0140
C     BB         DBL   Intermediate storage variable                        |PCL 0150
C     BB0        DBL   Fit constant                                         |PCL 0160
C     BEET0      DBL   Coefficient of isothermal compressibility of         |PCL 0170
C                        water at temperature T                             |PCL 0180
C     BET        DBL   Fit constant                                         |PCL 0190
C     BETA0      DBL   Compressibility of water at 5 degree increments      |PCL 0200
C                        starting a 5 deg. along the saturation curve       |PCL 0210
C     BHI        DBL   Pressure correction fit parameter                    |PCL 0220
C     BLOW       DBL   Pressure correction fit parameter                    |PCL 0230
C     C          DBL   Fit constant                                         |PCL 0240
C     CHI        DBL   Pressure correction fit parameter                    |PCL 0250
C     CLOW       DBL   Pressure correction fit parameter                    |PCL 0260
C     CPUMIN     DBL   Smallest positive real value program uses            |PCL 0270
C     D          DBL   Fit constant                                         |PCL 0280
C     DELK       DBL   Correction factor to log K of aqueous species        |PCL 0290
C     DELKHI     DBL   Adjusted log k at 1000 bars                          |PCL 0300
C     DELKLO     DBL   Adjusted log k at 500 bars                           |PCL 0310
C     DELVR      DBL   Change in volume at 25 degrees                       |PCL 0320
C     DELW       DBL   Log K adjustment to water reaction                   |PCL 0330
C     DLRR0      DBL   Intermediate storage variable                        |PCL 0340
```

```
C     DPR       DBL   Intermediate storage variable                          |PCL 0350
C     E         DBL   Fit constant                                           |PCL 0360
C     ER        DBL   Intermediate storage variable                          |PCL 0370
C     GAM       DBL   Fit constant                                           |PCL 0380
C     I         INT   Loop variable                                          |PCL 0390
C     ICOUNT    INT   Keeps track of number of times density is calc.        |PCL 0400
C     IDB0      INT   Temperature pointer to compressibility constant        |PCL 0410
C     J         INT   Loop variable                                          |PCL 0420
C     LOGKP     DBL   Correction factor to log K for the minerals            |PCL 0430
C     LOGKT1    DBL   Log K for aqueous species at specified temp.           |PCL 0440
C     LOGKT2    DBL   Log K for minerals at specified temperature            |PCL 0450
C     MXAQK     INT   Total number of aqueous log k values                   |PCL 0460
C     MXPC      INT   Total number of mineral pressure constants             |PCL 0470
C     N         INT   Loop variable                                          |PCL 0480
C     NH2O      DBL   Number of water ionization reactions                   |PCL 0490
C     NMAX      INT   General array dimension to allow easy expansion        |PCL 0500
C     P         DBL   Intermediate storage variable                          |PCL 0510
C     PADJ      DBL   Adjusted pressure (Total press. - Sat. press.)         |PCL 0520
C     PPP       DBL   Intermediate storage variable                          |PCL 0530
C     PR        DBL   Intermediate storage variable                          |PCL 0540
C     PRES      DBL   Total pressure                                         |PCL 0550
C     PS        DBL   Saturation pressure                                    |PCL 0560
C     R         DBL   Gas constant in cm**3 * bar / gram * deg. K            |PCL 0570
C     R0        DBL   Density of water at T along the saturation curve       |PCL 0580
C     RCAL      DBL   Gas constant in therm cal / mole * deg. K              |PCL 0590
C     RH        DBL   Intermediate storage variable                          |PCL 0600
C     RHN       DBL   Intermediate storage variable                          |PCL 0610
C     RHO       DBL   Density of water at P, T                               |PCL 0620
C     S         DBL   Intermediate storage variable                          |PCL 0630
C     T         DBL   Temperature in degrees K                               |PCL 0640
C     TAU       DBL   T / T critical                                         |PCL 0650
C     TCENT     DBL   Temperature in degrees C                               |PCL 0660
C     TEST1     DBL   Test to check for proper density                       |PCL 0670
C     TEST2     DBL   Test to check for proper pressure                      |PCL 0680
C     UNO       INT   File unit assigned for output file                     |PCL 0690
C     VH2O      DBL   Change change of water at the saturation pressure      |PCL 0700
C     VRIC      DBL   Isocoulombic volume change for the reaction            |PCL 0710
C     Y         DBL   Intermediate storage variable                          |PCL 0720
C ---------------------------------------------------------------------------|PCL 0730
                                                                             PCL 0740
      INTEGER NMAX, UNO                                                      PCL 0750
      DOUBLE PRECISION CPUMIN                                                PCL 0760
      PARAMETER (NMAX = 340, UNO = 6, CPUMIN = 1.0D-35)                      PCL 0770
                                                                             PCL 0780
      INTEGER I, ICOUNT, IDB0, J, MXAQK, MXPC, N                             PCL 0790
                                                                             PCL 0800
      DOUBLE PRECISION A(9,7), AHI(200), AL, ALOW(200)                       PCL 0810
      DOUBLE PRECISION B, B0, B1, B2, B4, BB, BB0, BEET0, BET                PCL 0820
      DOUBLE PRECISION BETA0(70), BHI(200), BLOW(200)                        PCL 0830
      DOUBLE PRECISION C, CHI(200), CLOW(200)                                PCL 0840
      DOUBLE PRECISION D, DELK, DELKHI(200), DELKLO(200), DELVR(NMAX)        PCL 0850
      DOUBLE PRECISION DELW, DLRR0, DPR, E, ER, GAM                          PCL 0860
      DOUBLE PRECISION LOGKP, LOGKT1(NMAX), LOGKT2(NMAX)                     PCL 0870
      DOUBLE PRECISION NH2O(NMAX)                                            PCL 0880
      DOUBLE PRECISION P, PADJ, PPP, PR, PRES, PS                            PCL 0890
      DOUBLE PRECISION R, R0, RCAL, RH, RHN, RHO                             PCL 0900
      DOUBLE PRECISION S, T, TAU, TCENT, TEST1, TEST2                        PCL 0910
      DOUBLE PRECISION VH2O, VRIC, Y                                         PCL 0920
```

```
                                                                      PCL 0930
      INTRINSIC DABS, DEXP, DLOG, DLOG10                              PCL 0940
                                                                      PCL 0950
      COMMON /ALOGK/ LOGKT1, LOGKT2                                   PCL 0960
      COMMON /PTK  / DELVR, NH2O, ALOW, BLOW, CLOW, AHI, BHI, CHI     PCL 0970
                                                                      PCL 0980
      DATA AL, BET, GAM /11.0, 44.3333333, 3.5/                       PCL 0990
      DATA B0, C, D /.747862916, -.354078223, .007159876/             PCL 1000
      DATA E / -.003528426/                                           PCL 1010
      DATA BB0, B1, B2 /1.127833441, -.594400123, -5.010995915/       PCL 1020
      DATA B4 / 0.636842555/                                          PCL 1030
      DATA R, RCAL, VH2O /4.61518, 1.9872, 21.1/                      PCL 1040
                                                                      PCL 1050
      DATA A /0.0, 0.0,  68833.257944332, 0.0, 0.0, 0.0, 0.0,         PCL 1060
     .        0.0, 0.0, -5306.2968529023, 178638.32875422,             PCL 1070
     .       -2563743.6613260,  11797433.655832, -31377774.947767,    PCL 1080
     .        46561826.115608, -31555231.392127, 0.0, 6962522.0862664, PCL 1090
     .        22744.901424408, -395147.31563338,  4821257.5981415,    PCL 1100
     .       -21734810.110373,  52911910.757704, -72752773.275387,    PCL 1110
     .        47929666.384584, 0.0, -10834900.096447, -26627.944829770, PCL 1120
     .        0.0, 217572.45522644, 0.0, -707304.18082074, 0.0, 0.0,  PCL 1130
     .        0.0, 0.0, 7877.9333020687, 338038.84280753,             PCL 1140
     .       -3418301.6969660,  10829952.168620, -13802577.177877,    PCL 1150
     .        4177424.6148294,  4091266.4781209, 0.0, -2272282.7401688, PCL 1160
     .        0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,           PCL 1170
     .       -698.30527374994, -138550.50202703,  1222315.6417448,    PCL 1180
     .       -2544199.8064049, -2510991.4369001,  14016358.244614,    PCL 1190
     .       -13626369.388386,  0.0,              3836548.6000660/    PCL 1200
                                                                      PCL 1210
      DATA BETA0 /49.48,  48.26,  47.19,  46.33,  45.60,  45.06,  44.69,PCL 1220
     .            44.46,  44.35,  44.36,  44.48,  44.69,  45.01,  45.41,PCL 1230
     .            45.89,  46.46,  47.10,  47.82,  48.62,  49.50,  50.46,PCL 1240
     .            51.50,  52.62,  53.83,  55.12,  56.51,  57.99,  59.58,PCL 1250
     .            61.28,  63.09,  65.03,  67.10,  69.32,  71.69,  74.24,PCL 1260
     .            76.96,  79.89,  83.04,  86.43,  90.09,  94.77,  99.45,PCL 1270
     .           104.12, 108.80, 113.48, 120.78, 128.07, 135.37, 142.46,PCL 1280
     .           149.96, 162.28, 174.59, 186.91, 199.22, 211.54, 235.04,PCL 1290
     .           258.55, 282.05, 305.55, 329.06, 384.78, 440.50, 496.21,PCL 1300
     .           551.93, 607.65, 825.89,1044.13,1262.37,1480.61,1698.85/PCL 1310
                                                                      PCL 1320
C =====================================================================|PCL 1330
                                                                      PCL 1340
      IDB0   = TCENT / 5                                              PCL 1350
      BEET0  = BETA0(IDB0) / 10.0**6.0                                PCL 1360
      T      = TCENT + 273.15                                         PCL 1370
      TAU    = T / 647.073                                            PCL 1380
      ICOUNT = 1                                                      PCL 1390
      P      = PS                                                     PCL 1400
                                                                      PCL 1410
   10 CONTINUE                                                        PCL 1420
      B  = B0  + C * DLOG(TAU) + D / TAU**3 + E / TAU**5              PCL 1430
      BB = BB0 + B1 / TAU + B2 / TAU**2 + B4 / TAU**4                 PCL 1440
      RH = 1.0                                                        PCL 1450
      IF (P .LT. PS) RH = 0.001                                       PCL 1460
      PPP = P - 1.0D0                                                 PCL 1470
      IF(DABS(PPP) .LT. 1.0D-10 .AND. T .GT. 647.25) RH = 0.001       PCL 1480
                                                                      PCL 1490
      DO 40 I = 1, 100                                                PCL 1500
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      Y   = RH * B / 4.0                                                  PCL 1510
      ER  = DEXP(-RH)                                                     PCL 1520
      PR  = 0.0                                                           PCL 1530
      DPR = 0.0                                                           PCL 1540
      DO 30 N = 1, 9                                                      PCL 1550
        S = A(N,1)                                                        PCL 1560
        DO 20 J = 2, 7                                                    PCL 1570
          S = S + A(N,J) / TAU**(J-1)                                     PCL 1580
   20   CONTINUE                                                          PCL 1590
        PR  = PR  + S * (1 - ER)**(N-1)                                   PCL 1600
        DPR = DPR + S * (1 - ER)**(N-1) * (2 + RH * (N * ER - 1) /        PCL 1610
              (1 - ER))                                                   PCL 1620
   30   CONTINUE                                                          PCL 1630
      PR  = RH**2 * ER * PR  + RH * R * T * ((1 +     AL * Y +           PCL 1640
                BET * Y**2) / (1-Y)**3 + 4 * Y * (BB / B - GAM))        PCL 1650
      DPR = RH    * ER * DPR +      R * T * ((1 + 2 * AL * Y +           PCL 1660
            3 * BET * Y**2) / (1-Y)**3 + 3 * Y * (1 + AL * Y +          PCL 1670
                BET * Y**2) / (1-Y)**4 + 8 * Y * (BB / B - GAM))        PCL 1680
      RHN = RH + (P - PR) / DPR                                           PCL 1690
      TEST1 = DABS((RHN - RH) / RHN)                                      PCL 1700
      TEST2 = DABS((P - PR) / P)                                          PCL 1710
      IF (TEST1 .LT. 1.0D-6 .AND. TEST2 .LT. 1.0D-5) GO TO 50             PCL 1720
      RH = RHN                                                            PCL 1730
   40 CONTINUE                                                            PCL 1740
                                                                          PCL 1750
      WRITE (UNO, 100) T, P, RHN                                          PCL 1760
      RETURN                                                              PCL 1770
                                                                          PCL 1780
   50 CONTINUE                                                            PCL 1790
      IF (ICOUNT .EQ. 1) THEN                                             PCL 1800
        R0 = RHN                                                          PCL 1810
        P  = PRES                                                         PCL 1820
        ICOUNT = ICOUNT + 1                                               PCL 1830
        GO TO 10                                                          PCL 1840
      END IF                                                              PCL 1850
                                                                          PCL 1860
      RHO = RHN                                                           PCL 1870
                                                                          PCL 1880
C -----------------------------------------------------------------------|PCL 1890
C     Calculate the effect of pressure on logk of water                   |PCL 1900
C -----------------------------------------------------------------------|PCL 1910
                                                                          PCL 1920
      DLRR0 = DLOG10(RHO / R0)                                            PCL 1930
      DELW = -19.0D0 * DLRR0                                              PCL 1940
      LOGKT1(2) = LOGKT1(2) - DELW                                        PCL 1950
                                                                          PCL 1960
C -----------------------------------------------------------------------|PCL 1970
C     Adjust the logk of other species for the effect of pressure         |PCL 1980
C -----------------------------------------------------------------------|PCL 1990
                                                                          PCL 2000
      DLRR0 = DLRR0 / (RCAL * T * BEET0)                                  PCL 2010
                                                                          PCL 2020
      DO 60 I = 1, MXAQK                                                  PCL 2030
        IF (DABS(DELVR(I) - 0.D0) .LT. 1.0D-10) GO TO 60                  PCL 2040
        VRIC = DELVR(I) + NH2O(I) * VH2O                                  PCL 2050
        DELK = (VRIC /(-41.84D0) * DLRR0) - NH2O(I) * DELW                PCL 2060
        LOGKT1(I) = LOGKT1(I) + DELK                                      PCL 2070
   60 CONTINUE                                                            PCL 2080
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                                                                      PCL 2090
C -----------------------------------------------------------------|PCL 2100
C     Adjust the logk of minerals using helgeson's data            |PCL 2110
C -----------------------------------------------------------------|PCL 2120
                                                                      PCL 2130
      PADJ = PRES - PS                                                PCL 2140
      DO 90 I = 1, MXPC                                               PCL 2150
        DELKLO(I) = ALOW(I) + BLOW(I) * TCENT + CLOW(I) * TCENT**6    PCL 2160
        DELKHI(I) = AHI(I)  + BHI(I)  * TCENT + CHI(I)  * TCENT**6    PCL 2170
                                                                      PCL 2180
        IF ((500.0D0-PADJ) .LT. CPUMIN) THEN                          PCL 2190
          LOGKP = DELKLO(I) + ((DELKHI(I) - DELKLO(I)) *              PCL 2200
     .            (PADJ - 500.0D0)) / 500.0D0                         PCL 2210
        ELSE                                                          PCL 2220
          LOGKP = DELKLO(I) * PADJ / 500.0D0                          PCL 2230
        END IF                                                        PCL 2240
                                                                      PCL 2250
        LOGKT2(I) = LOGKT2(I) + LOGKP                                 PCL 2260
   90 CONTINUE                                                        PCL 2270
                                                                      PCL 2280
      RETURN                                                          PCL 2290
                                                                      PCL 2300
  100 FORMAT (/, ' ** CONVERGENCE ON DENSITY NOT ACHIEVED ***', /,    PCL 2310
     .           '   PRESSURE CORRECTION FOR AQUEOUS AND SOLID',      PCL 2320
     .           ' EQUILIBRIA WILL NOT BE IMPLEMENTED ')              PCL 2330
                                                                      PCL 2340
      END                                                             PCL 2350
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      SUBROUTINE PHCALC (TEMP, HITEMP, CONV2, ITIC, ITWR, ISALT,      PHC 0010
     .                   IPHNUM, IPRIN2, *, *, *, *)                  PHC 0020
C ================================================================|PHC 0030
C     Calculates pH when ever conditions change                    |PHC 0040
C -----------------------------------------------------------------|PHC 0050
C     ALFA      DBL   Activity of aqueous species i                 |PHC 0060
C     CO2F      DBL   Sum of CO2 plus CO2 lost from solution        |PHC 0070
C     CONV2     DBL   Convergence test                              |PHC 0080
C     CROSS     LOG   Have we crossed root yet?                     |PHC 0090
C     CUNITS    DBL   Analytical input concentration                |PHC 0100
C     DCO2      DBL   Concentration of CO2 lost before pH measurement |PHC 0110
C     DH2S      DBL   Concentration of H2S lost before pH measurement |PHC 0120
C     DIFTRY    DBL   Difference from root                          |PHC 0130
C     DNH3      DBL   Concentration of NH3 lost before pH measurement |PHC 0140
C     DONE      LOG   Are we done yet?                              |PHC 0150
C     HITEMP    DBL   In-situ temperature                           |PHC 0160
C     HTOT      DBL   Total hydronium                               |PHC 0170
C     HTOTI     DBL   Initial total hydronium                       |PHC 0180
C     I         INT   Loop counter                                  |PHC 0190
C     II        INT   Counter and pointer                           |PHC 0200
C     IOPT      INT   Switch for CO2 option                         |PHC 0210
C     IPGLN     INT   Current line number of the output file        |PHC 0220
C     IPHNUM    INT   Counter used in PHCALC                        |PHC 0230
C     IPRIN2    INT   Flag for printing hydronium balance           |PHC 0240
C     ISALT     INT   Switch for what option                        |PHC 0250
C     ITIC      INT   Hitemp distribution of carbonate species      |PHC 0260
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C     ITWR      INT   Switch to control printing of some headings       |PHC 0270
C     JCO3      INT   Switch to control printing of some headings       |PHC 0280
C     JJ        INT   Pointer to last point(s) calculated               |PHC 0290
C     M         DBL   Calculated molality of aqueous species            |PHC 0300
C     NDIM      INT   Identifies array dimension                        |PHC 0310
C     NMAX      INT   General array dimension to allow easy expansion   |PHC 0320
C     OHTOT     DBL   Current sum of all OH- in solution                |PHC 0330
C     OHTOTI    DBL   Target sum of all OH- in solution                 |PHC 0340
C     PH        DBL   Measured pH of the solution                       |PHC 0350
C     PHHIT     INT   HITEMP switch, used to control PHCALC             |PHC 0360
C     PHINC     DBL   Parameter.  Used to scale size of step            |PHC 0370
C     PHTRY     DBL   Values of pH tried                                |PHC 0380
C     PPHHIT    INT   Switch to control calling PHCALC                  |PHC 0390
C     SCO2      DBL   Sum of CO2 species                                |PHC 0400
C     TEMP      DBL   Temperature of the solution when pH was measured  |PHC 0410
C     TEST1     DBL   Current Hydronium-hydroxide balance               |PHC 0420
C     TEST2     DBL   H - OH balance to shoot for                       |PHC 0430
C     TEST3     DBL   Test of how far are we from root                  |PHC 0440
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                  |PHC 0450
C     UNO       INT   File unit assigned for output file                |PHC 0460
C ---------------------------------------------------------------------|PHC 0470
                                                                        PHC 0480
      INTEGER NDIM, NMAX, UNO                                           PHC 0490
      DOUBLE PRECISION PHINC                                            PHC 0500
      PARAMETER (NDIM = 5, NMAX = 340, UNO = 6, PHINC = 1.0)            PHC 0510
                                                                        PHC 0520
      INTEGER I, II, IOPT, IPAGE, IPGLN, IPHNUM, IPRIN2, ISALT          PHC 0530
      INTEGER ITIC, ITWR, JCO3, JJ, PHHIT, PPHHIT                       PHC 0540
                                                                        PHC 0550
      LOGICAL CROSS, DONE                                               PHC 0560
                                                                        PHC 0570
      CHARACTER *  1 TOF, CR                                            PHC 0580
      CHARACTER * 40 TITMIX                                             PHC 0590
                                                                        PHC 0600
      DOUBLE PRECISION ALFA(NMAX), ANALM(NMAX), CO2F, CONV2             PHC 0610
      DOUBLE PRECISION CUNITS(NMAX), DCH4, DDCH4, DCO2, DDCO2           PHC 0620
      DOUBLE PRECISION DH2S, DDH2S, DNH3, DDNH3, DIFTRY(NDIM)           PHC 0630
      DOUBLE PRECISION EXELT(35), FIXIT, HITEMP, HTOT, HTOTI            PHC 0640
      DOUBLE PRECISION M(NMAX), OHTOT, OHTOTI, PH, PHTRY(NDIM)          PHC 0650
      DOUBLE PRECISION SCO2, TEMP, TEST1, TEST2, TEST3                  PHC 0660
      DOUBLE PRECISION TITR(11), TOTEL(5)                               PHC 0670
                                                                        PHC 0680
      EXTERNAL GUESS, PAGE, SORTA                                       PHC 0690
                                                                        PHC 0700
      INTRINSIC DABS, DLOG10, DSIGN                                     PHC 0710
                                                                        PHC 0720
      COMMON /EXTOT / EXELT, TOTEL, TITR                                PHC 0730
      COMMON /FMFD  / TOF, CR, TITMIX                                   PHC 0740
      COMMON /FORM  / IPAGE, IPGLN                                      PHC 0750
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,            PHC 0760
                      DCH4, DDCH4, IOPT, FIXIT                          PHC 0770
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                        PHC 0780
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                               PHC 0790
      COMMON /ZPH   / PHHIT, PPHHIT, JCO3, SCO2, HTOT, OHTOT            PHC 0800
                                                                        PHC 0810
      SAVE CROSS, DIFTRY, JJ, PHTRY                                     PHC 0820
                                                                        PHC 0830
C =====================================================================|PHC 0840
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                                                                      PHC 0850
      DONE = .FALSE.                                                  PHC 0860
      IF (PPHHIT .NE. 1 .AND. PHHIT .EQ. 1) THEN                      PHC 0870
        IF (IPHNUM .LE. 0) THEN                                       PHC 0880
          CROSS = .FALSE.                                             PHC 0890
        END IF                                                        PHC 0900
                                                                      PHC 0910
C -----------------------------------------------------------------|PHC 0920
C     If this is the first round of Hi-T, initialize, and exit to  |PHC 0930
C     re-calculate the log K values and to setup the mass-balance  |PHC 0940
C     criteria.                                                    |PHC 0950
C -----------------------------------------------------------------|PHC 0960
                                                                      PHC 0970
        IF (DABS(TEMP - HITEMP) .GT. 1.0D-10) THEN                    PHC 0980
          TEMP     = HITEMP                                         PHC 0990
          HTOTI    = HTOT                                           PHC 1000
          OHTOTI   = OHTOT                                          PHC 1010
          TOTEL(1) = HTOTI                                          PHC 1020
          TOTEL(2) = OHTOTI                                         PHC 1030
          TOTEL(3) = CO2F                                           PHC 1040
          IF (ITIC .EQ. 1) ITIC = 2                                 PHC 1050
          RETURN 1                                                  PHC 1060
        END IF                                                      PHC 1070
                                                                    PHC 1080
        ITWR  = 1                                                   PHC 1090
                                                                    PHC 1100
C -----------------------------------------------------------------|PHC 1110
C     Get and test for convergence.                                |PHC 1120
C     Use a difference if solution is neutral to avoid             |PHC 1130
C     a divide by zero.                                            |PHC 1140
C -----------------------------------------------------------------|PHC 1150
                                                                    PHC 1160
        TEST1 = HTOT  - OHTOT                                       PHC 1170
        TEST2 = HTOTI - OHTOTI + (2.D0 * DCO2) + (2.0D0 * DH2S) - DNH3  PHC 1180
        TEST3 = TEST1 - TEST2                                       PHC 1190
        IF (DABS(TEST2) .GT. 1.0D-10 .AND. DABS(TEST1) .GT. 1.0D-10)  PHC 1200
          THEN                                                      PHC 1210
          TEST3 = TEST3 / TEST2                                     PHC 1220
        ELSE                                                        PHC 1230
          IF      (DABS(TEST1) .GT. 1.0D-10) THEN                   PHC 1240
              TEST3 = TEST3 / TEST1                                 PHC 1250
          ELSE IF (DABS(TEST2) .GT. 1.0D-35) THEN                   PHC 1260
              TEST3 = TEST3 / DSIGN(1.0D-10, TEST2)                 PHC 1270
          ELSE                                                      PHC 1280
              TEST3 = TEST3 / 1.0D-10                               PHC 1290
          END IF                                                    PHC 1300
        END IF                                                      PHC 1310
                                                                    PHC 1320
        IPHNUM  = IPHNUM  + 1                                       PHC 1330
        JJ      = IPHNUM                                            PHC 1340
        IF (IPHNUM .EQ. 0) THEN                                     PHC 1350
          ALFA(8)  = 10.0D00**(-PH)                                 PHC 1360
          RETURN 2                                                  PHC 1370
        END IF                                                      PHC 1380
                                                                    PHC 1390
C -----------------------------------------------------------------|PHC 1400
C     Store Values and Check if root has been found or crossed.    |PHC 1410
C -----------------------------------------------------------------|PHC 1420
```

```
                                                                      PHC 1430
        PHTRY(IPHNUM)  = - DLOG10(ALFA(8))                            PHC 1440
        DIFTRY(IPHNUM) = TEST3                                        PHC 1450
                                                                      PHC 1460
        IF (DABS(TEST2) .GT. 1.0D-08 .AND. DABS(TEST1) .GT. 1.0D-08)  PHC 1470
     .    THEN                                                       PHC 1480
          IF (DABS(DIFTRY(IPHNUM)) .LT. CONV2) DONE = .TRUE.          PHC 1490
        ELSE                                                          PHC 1500
          IF ((DABS(DIFTRY(IPHNUM))*1.0D-08) .LT. 1.0D-09) DONE = .TRUE.PHC 1510
        END IF                                                        PHC 1520
                                                                      PHC 1530
        IF (IPHNUM .GT. 1 .AND. .NOT. CROSS) THEN                     PHC 1540
          IF ((DIFTRY(IPHNUM) * DIFTRY(IPHNUM-1)) .LT. 0.0)           PHC 1550
     .      CROSS = .TRUE.                                           PHC 1560
        END IF                                                        PHC 1570
                                                                      PHC 1580
C -------------------------------------------------------------------|PHC 1590
C     If root has been found, sort into order                        |PHC 1600
C -------------------------------------------------------------------|PHC 1610
                                                                      PHC 1620
        IF (CROSS) THEN                                               PHC 1630
          CALL SORTA (PHTRY, DIFTRY, IPHNUM, JJ)                      PHC 1640
          IF (.NOT. DONE .AND. JJ .GT. 1) THEN                        PHC 1650
            IF ((DIFTRY(JJ) * DIFTRY(JJ-1)) .LT. 0.0) THEN            PHC 1660
              IF (DABS(PHTRY(JJ) - PHTRY(JJ-1)) .LT. 5.0E-4)          PHC 1670
     .          DONE = .TRUE.                                        PHC 1680
            END IF                                                    PHC 1690
          END IF                                                      PHC 1700
                                                                      PHC 1710
          IF (.NOT. DONE .AND. JJ .LT. IPHNUM) THEN                   PHC 1720
            IF ((DIFTRY(JJ) * DIFTRY(JJ+1)) .LT. 0.0) THEN            PHC 1730
              IF (DABS(PHTRY(JJ) - PHTRY(JJ+1)) .LT. 5.0E-4)          PHC 1740
     .          DONE = .TRUE.                                        PHC 1750
            END IF                                                    PHC 1760
          END IF                                                      PHC 1770
        END IF                                                        PHC 1780
                                                                      PHC 1790
C -------------------------------------------------------------------|PHC 1800
C     Due to small size only keep last NDIM-1 points                 |PHC 1810
C -------------------------------------------------------------------|PHC 1820
                                                                      PHC 1830
        IF (IPHNUM .EQ. NDIM .AND. .NOT. DONE) THEN                   PHC 1840
          IF (.NOT. CROSS) THEN                                       PHC 1850
            IPHNUM = (NDIM-1)                                         PHC 1860
            DO 100 I = 1, (NDIM-1)                                    PHC 1870
              PHTRY(I)  = PHTRY(I+1)                                  PHC 1880
              DIFTRY(I) = DIFTRY(I+1)                                 PHC 1890
  100       CONTINUE                                                  PHC 1900
            JJ = JJ - 1                                               PHC 1910
          END IF                                                      PHC 1920
                                                                      PHC 1930
          IF (CROSS) THEN                                             PHC 1940
            DO 110 I = 1, (IPHNUM - 1)                                PHC 1950
              IF ((DIFTRY(I) * DIFTRY(I+1)) .LT. 0.0) II = I          PHC 1960
  110       CONTINUE                                                  PHC 1970
                                                                      PHC 1980
            IF (II .GT. (IPHNUM / 2) .AND.  JJ .NE. 1) THEN           PHC 1990
              DO 120 I = 1, (NDIM-1)                                  PHC 2000
```

```
                PHTRY(I)  = PHTRY(I+1)                                    PHC 2010
                DIFTRY(I) = DIFTRY(I+1)                                   PHC 2020
  120         CONTINUE                                                    PHC 2030
              JJ = JJ - 1                                                 PHC 2040
              IPHNUM = NDIM - 1                                           PHC 2050
            ELSE                                                          PHC 2060
              IPHNUM = NDIM - 1                                           PHC 2070
            END IF                                                        PHC 2080
          END IF                                                          PHC 2090
        END IF                                                            PHC 2100
                                                                          PHC 2110
C -------------------------------------------------------------------|PHC 2120
C     If root not yet crossed, keep trucking                        |PHC 2130
C -------------------------------------------------------------------|PHC 2140
                                                                          PHC 2150
        IF ( .NOT. DONE .AND. .NOT. CROSS) THEN                           PHC 2160
          PH  = PHTRY(IPHNUM)                                             PHC 2170
          IF (IPHNUM .EQ. 1) THEN                                         PHC 2180
            PH = PH - (DSIGN(1.0D00, (TEST2 - TEST1)) * PHINC)            PHC 2190
          ELSE                                                            PHC 2200
            IF (DABS(DIFTRY(IPHNUM)) .GT. DABS(DIFTRY(IPHNUM-1))) THEN    PHC 2210
              PH = DIFTRY(IPHNUM)                                         PHC 2220
              DIFTRY(IPHNUM) = DIFTRY(IPHNUM-1)                           PHC 2230
              DIFTRY(IPHNUM-1) = PH                                       PHC 2240
              PH = PHTRY(IPHNUM)                                          PHC 2250
              PHTRY(IPHNUM) = PHTRY(IPHNUM-1)                             PHC 2260
              PHTRY(IPHNUM-1) = PH                                        PHC 2270
              PH = (2.0 * PHTRY(IPHNUM)) - PHTRY(IPHNUM-1)                PHC 2280
              JJ = IPHNUM -1                                              PHC 2290
            ELSE                                                          PHC 2300
              PH = (2.0 * PHTRY(IPHNUM)) - PHTRY(IPHNUM-1)                PHC 2310
            END IF                                                        PHC 2320
          END IF                                                          PHC 2330
          ALFA(8)  = 10.0D00**(-PH)                                       PHC 2340
        END IF                                                            PHC 2350
                                                                          PHC 2360
C -------------------------------------------------------------------|PHC 2370
C     If root has been crossed, get new value of pH                 |PHC 2380
C -------------------------------------------------------------------|PHC 2390
                                                                          PHC 2400
        IF ( .NOT. DONE .AND. CROSS) THEN                                 PHC 2410
          CALL GUESS (PHTRY, DIFTRY, PH, IPHNUM)                          PHC 2420
          ALFA(8) = 10.0D00**(-PH)                                        PHC 2430
        END IF                                                            PHC 2440
                                                                          PHC 2450
C -------------------------------------------------------------------|PHC 2460
C     Go and try again.  Print if necessary                         |PHC 2470
C -------------------------------------------------------------------|PHC 2480
                                                                          PHC 2490
        IF ( .NOT. DONE) THEN                                             PHC 2500
          IF (IPRIN2 .NE. 0) THEN                                         PHC 2510
            IF (IPGLN .GT. 56) CALL PAGE                                  PHC 2520
            WRITE (UNO,1000) TEST2, TEST1, (TEST1 - TEST2), DIFTRY(JJ),   PHC 2530
                             PHTRY(JJ), PH, (PH - PHTRY(JJ))              PHC 2540
            IPGLN = IPGLN + 3                                             PHC 2550
          END IF                                                          PHC 2560
          RETURN 2                                                        PHC 2570
        END IF                                                            PHC 2580
```

```
                                                                      PHC 2590
C -----------------------------------------------------------------|PHC 2600
C     Root has been found.  Update appropriate variables and exit  |PHC 2610
C -----------------------------------------------------------------|PHC 2620
                                                                      PHC 2630
        PH     = PHTRY(JJ)                                            PHC 2640
        IPHNUM = 0                                                    PHC 2650
        IF (JCO3  .EQ. 1 .AND. IOPT .NE. 0) RETURN                    PHC 2660
        IF (ISALT .GE. 2) RETURN 4                                    PHC 2670
        PPHHIT = 1                                                    PHC 2680
      END IF                                                          PHC 2690
                                                                      PHC 2700
      IF (PPHHIT .EQ. 1) THEN                                         PHC 2710
        IF (IOPT .EQ. 1) RETURN                                       PHC 2720
        TEST1 = HTOT  - OHTOT                                         PHC 2730
        TEST2 = HTOTI - OHTOTI + (2.D0 * DCO2) + (2.0D0 * DH2S) - DNH3  PHC 2740
        IF (IPRIN2 .NE. 0) THEN                                       PHC 2750
            IF (IPGLN .GT. 53) CALL PAGE                              PHC 2760
            WRITE (UNO,1010) PH, TEST2, TEST1, (TEST2 - TEST1)        PHC 2770
            IPGLN = IPGLN + 5                                         PHC 2780
        END IF                                                        PHC 2790
        IF (JCO3 .EQ. 1) THEN                                         PHC 2800
          TOTEL(1) = TOTEL(1) + 2.0*DCO2                              PHC 2810
          TOTEL(3) = TOTEL(3) +     DCO2                              PHC 2820
        END IF                                                        PHC 2830
        RETURN 3                                                      PHC 2840
      END IF                                                          PHC 2850
                                                                      PHC 2860
C -----------------------------------------------------------------|PHC 2870
C     Store some parameters for use in mixing / printing            |PHC 2880
C -----------------------------------------------------------------|PHC 2890
                                                                      PHC 2900
      IF (HTOTI .LT. 1.D-35) THEN                                     PHC 2910
        TOTEL(1) = HTOT                                               PHC 2920
        TOTEL(2) = OHTOT                                              PHC 2930
      ELSE                                                            PHC 2940
        TOTEL(1) = HTOTI                                              PHC 2950
        TOTEL(2) = OHTOTI                                             PHC 2960
      END IF                                                          PHC 2970
                                                                      PHC 2980
      TOTEL(3) = SCO2                                                 PHC 2990
      TOTEL(4) = PH                                                   PHC 3000
                                                                      PHC 3010
      IF (JCO3 .EQ. 1) THEN                                           PHC 3020
        TOTEL(1) = TOTEL(1) + 2.0*DCO2                                PHC 3030
        TOTEL(3) = TOTEL(3) +     DCO2                                PHC 3040
        RETURN 2                                                      PHC 3050
      END IF                                                          PHC 3060
                                                                      PHC 3070
      RETURN                                                          PHC 3080
                                                                      PHC 3090
 1000 FORMAT (/, '  (HTOTI-OHTOTI) =',D16.8,' (HTOT-OHTOT) =',D16.8,  PHC 3100
     .           '   Difference = ',D16.8,'  Test = ',D16.8,          PHC 3110
     .         /, '   pH was: ', F8.4, '   New pH is: ', F8.4,        PHC 3120
     .           '   Change = ', E12.5)                               PHC 3130
 1010 FORMAT (//,'  **** Convergence Achieved at pH=', F8.4,          PHC 3140
     .          /,' (HTOTI-OHTOTI) = ',D16.8,                        PHC 3150
     .            '  (HTOT-OHTOT) = ', D16.8,                        PHC 3160
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                  Difference = ', D16.8, //)                                PHC 3170
                                                                            PHC 3180
      END                                                                   PHC 3190



      SUBROUTINE PHOPT (ICCSAT, FCCSAT, ITWR, JCCST, *)                     PHO 0010
C ==========================================================================|PHO 0020
C     The following routine achieves CALCITE, DOLOMITE or SIDERITE          |PHO 0030
C     saturation by adjusting pH. "ICCSAT" is equivalent to "IPHSAT"        |PHO 0040
C     in the manual.                                                        |PHO 0050
C --------------------------------------------------------------------------|PHO 0060
C     ALFA       DBL   Activity of aqueous species i                        |PHO 0070
C     CROSS      LOG   Have we crossed root yet?                            |PHO 0080
C     FCCSAT     DBL   Zero test                                            |PHO 0090
C     HFAC       DBL   Number of hydrogen ions in reaction from mineral     |PHO 0100
C                        to dominate species                                |PHO 0110
C     I          INT   Loop Variable and pointer                            |PHO 0120
C     ICCSAT     INT   Switch for pH option                                 |PHO 0130
C     IDK        INT   Index for log K of mineral (Cal, Dol, Sid)           |PHO 0140
C     IID        INT   Index of dominate carbonate species                  |PHO 0150
C     IPGLN      INT   Current line number of the output file               |PHO 0160
C     ITWR       INT   Switch to control printing of some headings          |PHO 0170
C     JCCST      INT   Switch indicating if PHOPT called lst time           |PHO 0180
C     JJ         INT   Pointer to last value calculated                     |PHO 0190
C     KTF        DBL   Number of Carbonate groups in reaction               |PHO 0200
C     LOGKT1     DBL   Log K for aqueous species at specified temp.         |PHO 0210
C     LOGKT2     DBL   Log K for minerals at specified temperature          |PHO 0220
C     LTTIAP     DBL   Log of activity product                              |PHO 0230
C     M          DBL   Calculated molality of aqueous species               |PHO 0240
C     MAXCO2     DBL   Temp storage to determinate domin. Carb. species     |PHO 0250
C     NMAX       INT   General array dimension to allow easy expansion      |PHO 0260
C     NUM        INT   Number of SI/ pH points in arrays                    |PHO 0270
C     PH         DBL   Measured pH of the solution                          |PHO 0280
C     PHTRY      DBL   Values of pH tried                                   |PHO 0290
C     REVERS     LOG   Do we need to reverse to find root?                  |PHO 0300
C     SATNAM     CHA   Name of mineral to be saturated with                 |PHO 0310
C     SI         DBL   Current SI value                                     |PHO 0320
C     SITRY      DBL   Values of SIs obtained                               |PHO 0330
C     STEP       DBL   Value used to change pH by                           |PHO 0340
C     TOFAR      LOG   Have we gone too far?                                |PHO 0350
C     TTIAP      DBL   Activity product                                     |PHO 0360
C     TTKT       DBL   Log K for reaction                                   |PHO 0370
C     UNO        INT   File unit assigned for output file                   |PHO 0380
C --------------------------------------------------------------------------|PHO 0390
                                                                            PHO 0400
      INTEGER NMAX, UNO                                                     PHO 0410
      PARAMETER (NMAX = 340, UNO = 6)                                       PHO 0420
                                                                            PHO 0430
      INTEGER I, IAQ, ICCSAT, IDK, IID, IPAGE, IPGLN, ITWR                  PHO 0440
      INTEGER JJ, JCCST, NUM                                                PHO 0450
                                                                            PHO 0460
      LOGICAL CROSS, TOFAR, REVERS                                          PHO 0470
                                                                            PHO 0480
      CHARACTER * 8 SATNAM(3)                                               PHO 0490
                                                                            PHO 0500
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```
      DOUBLE PRECISION ALFA(NMAX), ANALM(NMAX), CUNITS(NMAX), FCCSAT    PHO 0510
      DOUBLE PRECISION HFAC, KTF, LOGKT1(NMAX), LOGKT2(NMAX), LTTIAP    PHO 0520
      DOUBLE PRECISION M(NMAX), MAXCO2, PH, PHTRY(5), SI, SITRY(5)      PHO 0530
      DOUBLE PRECISION STEP, TTIAP, TTKT                                PHO 0540
                                                                        PHO 0550
      EXTERNAL GUESS, PAGE, SORTA                                       PHO 0560
                                                                        PHO 0570
      INTRINSIC DABS, DLOG10, DSIGN                                     PHO 0580
                                                                        PHO 0590
      COMMON /ALOGK/ LOGKT1, LOGKT2                                     PHO 0600
      COMMON /FORM / IPAGE, IPGLN                                       PHO 0610
      COMMON /MOLS / PH, ANALM, M, ALFA, CUNITS                         PHO 0620
                                                                        PHO 0630
      SAVE CROSS, NUM, PHTRY, REVERS, SITRY, STEP, TOFAR                PHO 0640
                                                                        PHO 0650
      DATA SATNAM / 'CALCITE ', 'DOLOMITE', 'SIDERITE'/                 PHO 0660
                                                                        PHO 0670
C ======================================================================|PHO 0680
                                                                        PHO 0690
C ----------------------------------------------------------------------|PHO 0700
C     Scan for the most abundant CO2 species                            |PHO 0710
C ----------------------------------------------------------------------|PHO 0720
                                                                        PHO 0730
      MAXCO2 = M(7)                                                     PHO 0740
      HFAC   = ALFA(8)                                                  PHO 0750
      IID    = 7                                                        PHO 0760
                                                                        PHO 0770
      DO 10 IAQ = 97, 98                                                PHO 0780
        IF (M(IAQ) .GT. MAXCO2) THEN                                    PHO 0790
          IF (IAQ .EQ. 97) HFAC = ALFA(8) ** 2.0                        PHO 0800
          IF (IAQ .EQ. 98) HFAC = 1.0                                   PHO 0810
          MAXCO2 = M(IAQ)                                               PHO 0820
          IID    = IAQ                                                  PHO 0830
        END IF                                                          PHO 0840
   10 CONTINUE                                                          PHO 0850
                                                                        PHO 0860
C ----------------------------------------------------------------------|PHO 0870
C     ICCSAT = 1 for Calcite; = 2 for Dolomite; = 3 for Siderite        |PHO 0880
C                                                                       |PHO 0890
C     Assign the appropriate SI based on ICCSAT AND the most abundant   |PHO 0900
C     CO2 species                                                       |PHO 0910
C ----------------------------------------------------------------------|PHO 0920
                                                                        PHO 0930
      IF (ICCSAT .EQ. 1) THEN                                           PHO 0940
        TTIAP  = ALFA(1) * ALFA(IID) / HFAC                             PHO 0950
        LTTIAP = DLOG10(TTIAP)                                          PHO 0960
        IDK    = 24                                                     PHO 0970
        KTF    = 1.0                                                    PHO 0980
      ELSE IF (ICCSAT .EQ. 2) THEN                                      PHO 0990
        TTIAP  = ALFA(1) * ALFA(2) * ALFA(IID)**2 / HFAC**2             PHO 1000
        LTTIAP = DLOG10(TTIAP)                                          PHO 1010
        IDK    = 41                                                     PHO 1020
        KTF    = 2.0                                                    PHO 1030
      ELSE                                                              PHO 1040
        TTIAP  = ALFA(18) * ALFA(IID) / HFAC                            PHO 1050
        LTTIAP = DLOG10(TTIAP)                                          PHO 1060
        IDK    = 146                                                    PHO 1070
        KTF    = 1.0                                                    PHO 1080
```

```
      END IF                                                              PHO 1090
                                                                          PHO 1100
      IF (IID .EQ. 98) TTKT = LOGKT2(IDK)                                 PHO 1110
      IF (IID .EQ. 7)  TTKT = LOGKT2(IDK) - KTF * LOGKT1(1)               PHO 1120
      IF (IID .EQ. 97) TTKT = LOGKT2(IDK) - KTF * LOGKT1(1)               PHO 1130
     .                                     - KTF * LOGKT1(72)             PHO 1140
                                                                          PHO 1150
C -------------------------------------------------------------------    |PHO 1160
C     First time here, initialize various switches, and get first       |PHO 1170
C     step.                                                             |PHO 1180
C -------------------------------------------------------------------    |PHO 1190
                                                                          PHO 1200
      IF (JCCST .LT. 1) THEN                                              PHO 1210
        WRITE (UNO,1001) SATNAM(ICCSAT)                                   PHO 1220
        IPGLN  = IPGLN + 3                                                PHO 1230
        IF (IPGLN .GT. 57) CALL PAGE                                      PHO 1240
        NUM    = 0                                                        PHO 1250
        STEP   = -0.5                                                     PHO 1260
        CROSS  = .FALSE.                                                  PHO 1270
        TOFAR  = .FALSE.                                                  PHO 1280
        REVERS = .FALSE.                                                  PHO 1290
        JCCST  = 1                                                        PHO 1300
        IF (IID .EQ. 98) THEN                                             PHO 1310
          STEP = 0.5                                                      PHO 1320
          IF ((LTTIAP - TTKT) .GE. 0.0) STEP = -1.0                       PHO 1330
        ELSE                                                              PHO 1340
          KTF = 1.0                                                       PHO 1350
          IF (IID .EQ. 97) KTF = 2.0                                      PHO 1360
                                                                          PHO 1370
          IF      (IDK .EQ. 24) THEN                                      PHO 1380
            STEP = TTKT - DLOG10(ALFA(1)) - DLOG10(ALFA(IID))             PHO 1390
            STEP = STEP - (KTF * PH)                                      PHO 1400
            STEP = STEP * 1.01 / KTF                                      PHO 1410
          ELSE IF (IDK .EQ. 41) THEN                                      PHO 1420
            STEP = TTKT - DLOG10(ALFA(1)) - DLOG10(ALFA(2))               PHO 1430
     .                 - (2.0 * DLOG10(ALFA(IID)))                       PHO 1440
            STEP = STEP - (2.0 * KTF * PH)                                PHO 1450
            STEP = STEP * 1.01 / (KTF * 2.0)                              PHO 1460
          ELSE IF (IDK .EQ. 146) THEN                                     PHO 1470
            STEP = TTKT - DLOG10(ALFA(18)) - DLOG10(ALFA(IID))            PHO 1480
            STEP = STEP - (KTF * PH)                                      PHO 1490
            STEP = STEP * 1.01 / KTF                                      PHO 1500
          END IF                                                          PHO 1510
        END IF                                                            PHO 1520
      END IF                                                              PHO 1530
                                                                          PHO 1540
C -------------------------------------------------------------------    |PHO 1550
C     Check for saturation using the SI                                 |PHO 1560
C     If saturation not achieved, adjust pH                             |PHO 1570
C -------------------------------------------------------------------    |PHO 1580
                                                                          PHO 1590
      SI = LTTIAP - TTKT                                                  PHO 1600
      IF (DABS(SI) .GT. FCCSAT) THEN                                      PHO 1610
        NUM = NUM + 1                                                     PHO 1620
        PHTRY(NUM) = PH                                                   PHO 1630
        SITRY(NUM) = SI                                                   PHO 1640
        JJ = NUM                                                          PHO 1650
                                                                          PHO 1660
```

```
IF (NUM .GT. 1 .AND. .NOT. CROSS) THEN                          PHO 1670
  IF ((SI * SITRY(NUM-1)) .LT. 0.0) CROSS = .TRUE.              PHO 1680
END IF                                                          PHO 1690
                                                                PHO 1700
IF ( .NOT. CROSS) THEN                                          PHO 1710
  IF (NUM .GT. 1) THEN                                          PHO 1720
    IF (DABS(SI) - DABS(SITRY(NUM-1)) .LE. 0.0) THEN            PHO 1730
      STEP = STEP * 1.5                                         PHO 1740
      REVERS = .FALSE.                                          PHO 1750
    ELSE                                                        PHO 1760
      PH = PHTRY(NUM-1)                                         PHO 1770
      SI = SITRY(NUM-1)                                         PHO 1780
      PHTRY(NUM-1) = PHTRY(NUM)                                 PHO 1790
      SITRY(NUM-1) = SITRY(NUM)                                 PHO 1800
      PHTRY(NUM) = PH                                           PHO 1810
      SITRY(NUM) = SI                                           PHO 1820
      JJ = NUM - 1                                              PHO 1830
                                                                PHO 1840
      IF ( REVERS ) THEN                                        PHO 1850
        STEP = STEP * (-0.3)                                    PHO 1860
      ELSE                                                      PHO 1870
        IF (NUM .EQ. 2) THEN                                    PHO 1880
          STEP = STEP * (-1.0)                                  PHO 1890
        ELSE                                                    PHO 1900
          STEP = STEP * (0.5)                                   PHO 1910
        END IF                                                  PHO 1920
      END IF                                                    PHO 1930
                                                                PHO 1940
      REVERS = .TRUE.                                           PHO 1950
    END IF                                                      PHO 1960
  END IF                                                        PHO 1970
                                                                PHO 1980
  IF (DABS(STEP) .GT. 1.5) STEP = DSIGN(1.5D00, STEP)           PHO 1990
  PH = PHTRY(NUM) + STEP                                        PHO 2000
                                                                PHO 2010
  IF (TOFAR) THEN                                               PHO 2020
    WRITE (UNO,1002) SATNAM(ICCSAT), PH                         PHO 2030
    IPGLN = IPGLN + 3                                           PHO 2040
    IF (IPGLN .GT. 57) CALL PAGE                                PHO 2050
    RETURN                                                      PHO 2060
  END IF                                                        PHO 2070
                                                                PHO 2080
  IF (DABS(STEP) .LT. 0.01) THEN                                PHO 2090
    WRITE (UNO,1003) SATNAM(ICCSAT), PH                         PHO 2100
    IPGLN = IPGLN + 3                                           PHO 2110
    IF (IPGLN .GT. 57) CALL PAGE                                PHO 2120
    RETURN                                                      PHO 2130
  END IF                                                        PHO 2140
                                                                PHO 2150
  IF (PH .LT.  0.1) THEN                                        PHO 2160
    PH = 0.1                                                    PHO 2170
    TOFAR = .TRUE.                                              PHO 2180
  END IF                                                        PHO 2190
                                                                PHO 2200
  IF (PH .GT. 13.9) THEN                                        PHO 2210
    PH = 13.9                                                   PHO 2220
    TOFAR = .TRUE.                                              PHO 2230
  END IF                                                        PHO 2240
```

```
                                                                      PHO 2250
        IF (NUM .EQ. 4) THEN                                          PHO 2260
          DO 20 I = 2, 5                                              PHO 2270
            PHTRY(I-1) = PHTRY(I)                                     PHO 2280
            SITRY(I-1) = SITRY(I)                                     PHO 2290
 20       CONTINUE                                                    PHO 2300
          NUM = NUM - 1                                               PHO 2310
          JJ  = JJ  - 1                                               PHO 2320
        END IF                                                        PHO 2330
      END IF                                                          PHO 2340
                                                                      PHO 2350
      IF ( CROSS ) THEN                                               PHO 2360
        CALL SORTA (PHTRY, SITRY, NUM, JJ)                            PHO 2370
        IF (NUM .GT. 3) THEN                                          PHO 2380
          IF ((SITRY(3) * SITRY(4)) .LT. 0.0) THEN                    PHO 2390
            DO 30 I = 2, 4                                            PHO 2400
              SITRY(I-1) = SITRY(I)                                   PHO 2410
              PHTRY(I-1) = PHTRY(I)                                   PHO 2420
 30         CONTINUE                                                  PHO 2430
            NUM = NUM - 1                                             PHO 2440
            JJ  = JJ - 1                                              PHO 2450
          ELSE IF ((SITRY(1) * SITRY(2)) .LT. 0.0) THEN               PHO 2460
            NUM = NUM -1                                              PHO 2470
          ELSE IF (DABS(SITRY(1)) .GT. DABS(SITRY(4))) THEN           PHO 2480
            DO 40 I = 2, 4                                            PHO 2490
              SITRY(I-1) = SITRY(I)                                   PHO 2500
              PHTRY(I-1) = PHTRY(I)                                   PHO 2510
 40         CONTINUE                                                  PHO 2520
            NUM = NUM - 1                                             PHO 2530
            JJ  = JJ - 1                                              PHO 2540
          ELSE                                                        PHO 2550
            NUM = NUM - 1                                             PHO 2560
          END IF                                                      PHO 2570
        END IF                                                        PHO 2580
                                                                      PHO 2590
        CALL GUESS (PHTRY, SITRY, PH, NUM)                            PHO 2600
                                                                      PHO 2610
      END IF                                                          PHO 2620
                                                                      PHO 2630
      ALFA(8) = 10.0**(-PH)                                           PHO 2640
      WRITE (UNO,1004) SATNAM(ICCSAT), SITRY(JJ), PHTRY(JJ), PH       PHO 2650
      IPGLN = IPGLN + 3                                               PHO 2660
      IF (IPGLN .GT. 57) CALL PAGE                                    PHO 2670
      ITWR  = 1                                                       PHO 2680
      RETURN 1                                                        PHO 2690
    END IF                                                            PHO 2700
                                                                      PHO 2710
    RETURN                                                            PHO 2720
                                                                      PHO 2730
1001 FORMAT (/ ,' Begining ',A8,' saturation by adjusting pH ',/)     PHO 2740
1002 FORMAT (//,' ***** ',A8,' saturation NOT POSSIBLE for PH',       PHO 2750
   .           ' between 0.1 and 13.9;  Last pH tried = ',F6.3)      PHO 2760
1003 FORMAT (//,' ***** ',A8,' saturation NOT POSSIBLE for pH',       PHO 2770
   .           ' of ',F6.3,' as a staddle point seems to have',      PHO 2780
   .           ' been reached here.')                                PHO 2790
1004 FORMAT (/ ,' Log SI (',A8,') = ',E13.4,' at a pH of ',F6.3,      PHO 2800
   .           ' Trying a new pH of ',F6.3,/)                        PHO 2810
    END                                                               PHO 2820
```

```
      SUBROUTINE PITZER (A, MU, MXSP, TEMP1, PGDCA, PGDNA, PG, TEMP,     PIT 0010
                         PALFA, CO2TIT, Z, FLAG1)                        PIT 0020
C ==========================================================================|PIT 0030
C     This routine calculates the pitzer activity coefficients.           |PIT 0040
C --------------------------------------------------------------------------|PIT 0050
C     Local constants                                                      |PIT 0060
C -------------------                                                     |PIT 0070
C     CPUMIN            DBL    Smallest value machine can represent      |PIT 0080
C     NANI              INT    Number of Anions                          |PIT 0090
C     NCAT              INT    Number of Cations                         |PIT 0100
C     NMAX              INT    Number of aqueous species declariton      |PIT 0110
C     NTEM              INT    Number of Temperatures                    |PIT 0120
C     UNP               INT    File unit of Pitzer Data                  |PIT 0130
C --------------------------------------------------------------------------|PIT 0140
C     Declare constants                                                    |PIT 0150
C ---------------------                                                    |PIT 0160
      INTEGER NANI, NCAT, NMAX, NTEM, UNP                                  PIT 0170
      DOUBLE PRECISION CPUMIN                                              PIT 0180
      PARAMETER (NCAT = 10, NANI = 5, NMAX = 340, NTEM = 11, UNP = 7)      PIT 0190
      PARAMETER (CPUMIN = 1.0D-35)                                         PIT 0200
                                                                           PIT 0210
C --------------------------------------------------------------------------|PIT 0220
C     Local variables                                                      |PIT 0230
C -------------------                                                     |PIT 0240
C     A          DBL   Molal debeye-huckel coefficient                   |PIT 0250
C     ALFA       DBL   Activity of aqueous species i                     |PIT 0260
C     ANALM      DBL   Analyzed molality of species i                    |PIT 0270
C     ANI        INT   Selects anions with pitzer data                   |PIT 0280
C     B          DBL   B coefficient                                     |PIT 0290
C     B0         DBL   Beta zero parameter for current temp              |PIT 0300
C     B00        DBL   Array of B0's for all temps                       |PIT 0310
C     B1         DBL   Beta one parameter of current temp                |PIT 0320
C     B11        DBL   Array of B1's for all temps                       |PIT 0330
C     BFEE       DBL   B sub fee coefficient                             |PIT 0340
C     BP         DBL   B prime coefficient                               |PIT 0350
C     BZ         DBL   Charge coefficient                                |PIT 0360
C     C          DBL   C coefficient                                     |PIT 0370
C     CAT        INT   Selects cations with pitzer data                  |PIT 0380
C     CO2TIT     DBL   Analyzed molality of CO3 + HCO3                   |PIT 0390
C     CP         DBL   C sub fee parameter for current temp              |PIT 0400
C     CPP        DBL   Array of CP's for all temps                       |PIT 0410
C     DIFF       DBL   Difference value for activities                   |PIT 0420
C     DONE       INT   Switch to determine when DIFF is OK               |PIT 0430
C     ETHTA      DBL   E theta function for anions                       |PIT 0440
C     ETHTAP     DBL   E theta prime function for anions                 |PIT 0450
C     ETHTC      DBL   E theta function for cations                      |PIT 0460
C     ETHTCP     DBL   E theta prime function for cations                |PIT 0470
C     F          DBL   Debye-huckel interaction term                     |PIT 0480
C     FEE        DBL   Osmotic coefficient                               |PIT 0490
C     FLAG1      INT   Water calculation flag                            |PIT 0500
C     G          DBL   Function to calculate coefficient values          |PIT 0510
C     GP         DBL   Primed function to calculate coefficient values   |PIT 0520
C     I          INT   Cation 1 loop variable                            |PIT 0530
C     II         INT   Cation loop variable                              |PIT 0540
C     ITER       INT   Iteration counter                                 |PIT 0550
C     J          INT   Cation 2 loop variable                            |PIT 0560
C     K          INT   Anion 1 loop variable                             |PIT 0570
C     KK         INT   Anion loop variable                               |PIT 0580
```

```
C     KT1       DBL   Equilibrium constants for specified temp          |PIT 0590
C     L         INT   Anion 2 loop variable                             |PIT 0600
C     LINE      CHA   Read in lines which contain no information        |PIT 0610
C     LNGA      DBL   Ln anion gamma                                    |PIT 0620
C     LNGC      DBL   Ln cation gamma                                   |PIT 0630
C     LNGDCA    DBL   Ln gamma for divalent ions with no pitzer data    |PIT 0640
C     LNGDNA    DBL   Ln gamma for monovalent ions with no pitzer data  |PIT 0650
C     LOOP      INT   Loop Variable                                     |PIT 0660
C     M         DBL   Calculated molality of aqueous species i          |PIT 0670
C     MA        DBL   Moles of Anion                                    |PIT 0680
C     MC        DBL   Moles of Cation                                   |PIT 0690
C     MU        DBL   Ionic strength of aqueous solution                |PIT 0700
C     MXSP      INT   Total number of aqueous species                   |PIT 0710
C     OHA       DBL   Hydroxide Activity                                |PIT 0720
C     PALFA     DBL   Pitzer activities                                 |PIT 0730
C     PG        DBL   Pitzer gammas                                     |PIT 0740
C     PGAMA     DBL   Pitzer Gammas for Anions                          |PIT 0750
C     PGAMC     DBL   Pitzer Gammas for Cations                         |PIT 0760
C     PGDCA     DBL   Gamma for divalent ions with no pitzer data       |PIT 0770
C     PGDNA     DBL   Gamma for monovalent ions with no pitzer data     |PIT 0780
C     PHIA      DBL   Phi anion coefficient                             |PIT 0790
C     PHIAP     DBL   Phi prime anion coefficient                       |PIT 0800
C     PHIC      DBL   Phi cation coefficient                            |PIT 0810
C     PHICP     DBL   Phi prime cation coefficient                      |PIT 0820
C     PSIA      DBL   Psi Anion-Anion-Cation parameter                  |PIT 0830
C     PSIAA     DBL   Array of PSIA for all Temps                       |PIT 0840
C     PSIC      DBL   Psi Cation-Cation-Anion parameter                 |PIT 0850
C     PSICC     DBL   Array of PSIC for all Temps                       |PIT 0860
C     SUM1      DBL   Internal sum for ln gamma calculations            |PIT 0870
C     SUM2      DBL   Internal sum for ln gamma calculations            |PIT 0880
C     SUM2A     DBL   Internal sum for ln gamma calculations            |PIT 0890
C     SUM3      DBL   Internal sum for ln gamma calculations            |PIT 0900
C     SUM4      DBL   Internal sum for ln gamma calculations            |PIT 0910
C     SUM5      DBL   Internal sum for osmotic calculations             |PIT 0920
C     SUM6      DBL   Internal sum for osmotic calculations             |PIT 0930
C     SUM6A     DBL   Internal sum for osmotic calculations             |PIT 0940
C     SUM7      DBL   Internal sum for osmotic calculations             |PIT 0950
C     SUM7A     DBL   Internal sum for osmotic calculations             |PIT 0960
C     SUM8      DBL   Internal sum for osmotic calculations             |PIT 0970
C     TEMP      DBL   Array of 11 Temperatures                          |PIT 0980
C     TEMP1     DBL   Temperature of Interest                           |PIT 0990
C     THTA      DBL   Pitzer theta anion parameter                      |PIT 1000
C     THTAA     DBL   Array of THTA for all temps                       |PIT 1010
C     THTC      DBL   Pitzer theta cation parameter                     |PIT 1020
C     THTCC     DBL   Array of THTC for all temps                       |PIT 1030
C     TP        INT   Integer equivalient to temp(i)                   |PIT 1040
C     X         DBL   Independent variable in the G functions           |PIT 1050
C     Z         INT   Charge of Aqueous Species i                       |PIT 1060
C     ZA        INT   Charge of the anions                              |PIT 1070
C     ZC        INT   Charge of the cations                             |PIT 1080
C ------------------------------------------------------------------------|PIT 1090
C     Declare variables                                                 |PIT 1100
C ---------------------                                                 |PIT 1110
      INTEGER ANI(NANI), CAT(NCAT), DONE, FLAG1                          PIT 1120
      INTEGER I, II, ITER, J, K, KK, L, LOOP                             PIT 1130
      INTEGER MXSP, TP, Z(NMAX), ZA(NANI), ZC(NCAT)                      PIT 1140
                                                                         PIT 1150
      CHARACTER * 1 LINE                                                 PIT 1160
```

```
                                                                      PIT 1170
      DOUBLE PRECISION A, ALFA(NMAX), ANALM(NMAX), B(NCAT,NANI)       PIT 1180
      DOUBLE PRECISION B0(NCAT,NANI), B00(NCAT,NANI,NTEM), B1(NCAT,NANI)PIT 1190
      DOUBLE PRECISION B11(NCAT,NANI,NTEM), BFEE(NCAT,NANI)           PIT 1200
      DOUBLE PRECISION BP(NCAT,NANI), BZ                              PIT 1210
      DOUBLE PRECISION C(NCAT,NANI), CO2TIT, CP(NCAT,NANI)            PIT 1220
      DOUBLE PRECISION CPP(NCAT,NANI,NTEM), CUNITS(NMAX), DIFF        PIT 1230
      DOUBLE PRECISION ETHTA(NANI,NANI), ETHTAP(NANI,NANI)            PIT 1240
      DOUBLE PRECISION ETHTC(NCAT,NCAT), ETHTCP(NCAT,NCAT), F, FEE    PIT 1250
      DOUBLE PRECISION G, GP, KT1(NMAX), LNGA(NANI)                   PIT 1260
      DOUBLE PRECISION LNGC(NCAT), LNGDCA, LNGDNA, M(NMAX), MA(NANI)  PIT 1270
      DOUBLE PRECISION MC(NCAT), MU, OHA, PALFA(NMAX)                 PIT 1280
      DOUBLE PRECISION PG(NMAX), PGAMA(NANI), PGAMC(NCAT), PGDCA, PGDNA PIT 1290
      DOUBLE PRECISION PH, PHIA(NANI,NANI), PHIAP(NANI,NANI)          PIT 1300
      DOUBLE PRECISION PHIC(NCAT,NCAT), PHICP(NCAT,NCAT)              PIT 1310
      DOUBLE PRECISION PSIA(NANI,NANI,NCAT), PSIAA(NANI,NANI,NCAT,NTEM) PIT 1320
      DOUBLE PRECISION PSIC(NCAT,NCAT,NANI), PSICC(NCAT,NCAT,NANI,NTEM) PIT 1330
      DOUBLE PRECISION SUM1, SUM2, SUM2A, SUM2B, SUM2C, SUM3, SUM4    PIT 1340
      DOUBLE PRECISION SUM4B, SUM4C, SUM5, SUM6, SUM6A, SUM7, SUM7A   PIT 1350
      DOUBLE PRECISION SUM8, TEMP(NTEM), TEMP1                        PIT 1360
      DOUBLE PRECISION THTA(NANI,NANI), THTAA(NANI,NANI,NTEM)         PIT 1370
      DOUBLE PRECISION THTC(NCAT,NCAT), THTCC(NCAT,NCAT,NTEM), X      PIT 1380
                                                                      PIT 1390
      EXTERNAL PTZINT                                                 PIT 1400
                                                                      PIT 1410
      INTRINSIC DABS, DEXP, DLOG, DSQRT, IABS                         PIT 1420
                                                                      PIT 1430
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                      PIT 1440
      COMMON /TTK   / KT1                                             PIT 1450
                                                                      PIT 1460
      DATA ANI /5, 6, 7, 98,  9/                                      PIT 1470
      DATA CAT /3, 4, 1,  2, 26, 15, 8, 14, 23, 27/                   PIT 1480
                                                                      PIT 1490
C ======================================================================|PIT 1500
                                                                      PIT 1510
C ----------------------------------------------------------------------|PIT 1520
C     Open data table of pitzer coefficients                           |PIT 1530
C ----------------------------------------------------------------------|PIT 1540
                                                                      PIT 1550
       OPEN (UNP, FILE = 'PIT.TBL', STATUS = 'OLD')                   PIT 1560
C       OPEN (UNP, STATUS = 'OLD', shared, readonly)                  PIT 1570
                                                                      PIT 1580
C ----------------------------------------------------------------------|PIT 1590
C     Initialize arrays of parameters and coefficients                 |PIT 1600
C ----------------------------------------------------------------------|PIT 1610
                                                                      PIT 1620
      DO 10 I = 1, NMAX                                               PIT 1630
        PG(I) = 0.0D0                                                 PIT 1640
   10 CONTINUE                                                        PIT 1650
                                                                      PIT 1660
      DO 40 I = 1, NCAT                                               PIT 1670
        DO 30 K = 1, NANI                                             PIT 1680
          B0(I,K) = 0.0D0                                             PIT 1690
          B1(I,K) = 0.0D0                                             PIT 1700
          CP(I,K) = 0.0D0                                             PIT 1710
                                                                      PIT 1720
          DO 20 TP = 1, NTEM                                          PIT 1730
            B00(I,K,TP) = 0.0D0                                       PIT 1740
```

```
          B11(I,K,TP) = 0.0D0                                          PIT 1750
          CPP(I,K,TP) = 0.0D0                                          PIT 1760
 20     CONTINUE                                                       PIT 1770
                                                                       PIT 1780
 30   CONTINUE                                                         PIT 1790
 40 CONTINUE                                                          PIT 1800
                                                                       PIT 1810
    DO 70 I = 1, NCAT                                                  PIT 1820
      DO 60 J = 1, NCAT                                                PIT 1830
        THTC(I,J) = 0.0D0                                              PIT 1840
                                                                       PIT 1850
        DO 50 TP = 1, NTEM                                             PIT 1860
          THTCC(I,J,TP) = 0.0D0                                        PIT 1870
 50     CONTINUE                                                       PIT 1880
                                                                       PIT 1890
 60   CONTINUE                                                         PIT 1900
 70 CONTINUE                                                          PIT 1910
                                                                       PIT 1920
    DO 100 K = 1, NANI                                                 PIT 1930
      DO 90 L = 1, NANI                                                PIT 1940
        THTA(K,L) = 0.0D0                                              PIT 1950
                                                                       PIT 1960
        DO 80 TP = 1, NTEM                                             PIT 1970
          THTAA(K,L,TP) = 0.0D0                                        PIT 1980
 80     CONTINUE                                                       PIT 1990
                                                                       PIT 2000
 90   CONTINUE                                                         PIT 2010
100 CONTINUE                                                          PIT 2020
                                                                       PIT 2030
    DO 140 I = 1, NCAT                                                 PIT 2040
      DO 130 J = 1, NCAT                                               PIT 2050
        DO 120 K = 1, NANI                                             PIT 2060
          PSIC(I,J,K) = 0.0D0                                          PIT 2070
                                                                       PIT 2080
          DO 110 TP = 1, NTEM                                          PIT 2090
            PSICC(I,J,K,TP) = 0.0D0                                    PIT 2100
110       CONTINUE                                                     PIT 2110
                                                                       PIT 2120
120     CONTINUE                                                       PIT 2130
130   CONTINUE                                                         PIT 2140
140 CONTINUE                                                          PIT 2150
                                                                       PIT 2160
    DO 180 K = 1, NANI                                                 PIT 2170
      DO 170 L = 1, NANI                                               PIT 2180
        DO 160 I = 1, NCAT                                             PIT 2190
          PSIA(K,L,I) = 0.0D0                                          PIT 2200
                                                                       PIT 2210
          DO 150 TP = 1, NTEM                                          PIT 2220
            PSIAA(K,L,I,TP) = 0.0D0                                    PIT 2230
150       CONTINUE                                                     PIT 2240
                                                                       PIT 2250
160     CONTINUE                                                       PIT 2260
170   CONTINUE                                                         PIT 2270
180 CONTINUE                                                          PIT 2280
                                                                       PIT 2290
    DO 190 I = 1, NCAT                                                 PIT 2300
      LNGC (I) = 0.0D0                                                 PIT 2310
      IF (I .LE. NANI) LNGA (I) = 0.0D0                                PIT 2320
```

```
  190 CONTINUE                                                          PIT 2330
                                                                        PIT 2340
C -------------------------------------------------------------------|PIT 2350
C     Read in data                                                     |PIT 2360
C -------------------------------------------------------------------|PIT 2370
                                                                        PIT 2380
      DO 195 I = 1, 3                                                   PIT 2390
        READ (UNP, '(A1)') LINE                                         PIT 2400
  195 CONTINUE                                                          PIT 2410
                                                                        PIT 2420
      DO 220 I = 1, 6                                                   PIT 2430
        DO 210 TP = 1, NTEM                                             PIT 2440
          READ (UNP, 200) (B00(I,K,TP), B11(I,K,TP), CPP(I,K,TP),       PIT 2450
                           K = 1, 4)                                    PIT 2460
  200       FORMAT (12(F10.5))                                        PIT 2470
  210     CONTINUE                                                    PIT 2480
          DO 215 J = 1, 4                                             PIT 2490
            READ (UNP, '(A1)') LINE                                   PIT 2500
  215     CONTINUE                                                    PIT 2510
  220 CONTINUE                                                        PIT 2520
                                                                      PIT 2530
      DO 240 I = 7, 10                                                PIT 2540
        DO 230 TP = 1, 2                                              PIT 2550
          READ (UNP, 200) (B00(I,K,TP), B11(I,K,TP), CPP(I,K,TP),     PIT 2560
                           K = 1, 4)                                  PIT 2570
  230     CONTINUE                                                    PIT 2580
          DO 235 J = 1, 4                                             PIT 2590
            READ (UNP, '(A1)') LINE                                   PIT 2600
  235     CONTINUE                                                    PIT 2610
  240 CONTINUE                                                        PIT 2620
                                                                      PIT 2630
      DO 260 LOOP = 1, 9                                              PIT 2640
        READ (UNP, 250) I, J, (THTCC(I,J,TP), TP = 1, 11)            PIT 2650
  250     FORMAT (2(I2), 1X, 11(F10.5))                               PIT 2660
  260 CONTINUE                                                        PIT 2670
                                                                      PIT 2680
      DO 265 I = 1, 3                                                 PIT 2690
        READ (UNP, '(A1)') LINE                                       PIT 2700
  265 CONTINUE                                                        PIT 2710
                                                                      PIT 2720
      DO 270 LOOP = 1, 9                                              PIT 2730
        READ (UNP, 250) K, L, (THTAA(K,L,TP), TP = 1, 11)            PIT 2740
  270 CONTINUE                                                        PIT 2750
                                                                      PIT 2760
      DO 275 I = 1, 3                                                 PIT 2770
        READ (UNP, '(A1)') LINE                                       PIT 2780
  275 CONTINUE                                                        PIT 2790
                                                                      PIT 2800
      DO 290 LOOP = 1, 19                                             PIT 2810
        READ (UNP, 280) I, J, K, (PSICC(I,J,K,TP), TP = 1, 11)       PIT 2820
  280     FORMAT (3(I2), 1X, 11(F10.5))                               PIT 2830
  290 CONTINUE                                                        PIT 2840
                                                                      PIT 2850
      DO 295 I = 1, 3                                                 PIT 2860
        READ (UNP, '(A1)') LINE                                       PIT 2870
  295 CONTINUE                                                        PIT 2880
                                                                      PIT 2890
      DO 300 LOOP = 1, 20                                             PIT 2900
```

```
        READ (UNP, 280) K, L, I, (PSIAA(K,L,I,TP), TP = 1, 11)          PIT 2910
  300 CONTINUE                                                          PIT 2920
                                                                        PIT 2930
      CLOSE (UNP)                                                       PIT 2940
                                                                        PIT 2950
C -----------------------------------------------------------------------|PIT 2960
C     Interpolate values from table to proper temperature               |PIT 2970
C -----------------------------------------------------------------------|PIT 2980
                                                                        PIT 2990
      CALL PTZINT (TEMP, TEMP1, B0, B00, B1, B11, CP, CPP, THTC, THTCC, PIT 3000
     .             THTA, THTAA, PSIC, PSICC, PSIA, PSIAA)               PIT 3010
                                                                        PIT 3020
C -----------------------------------------------------------------------|PIT 3030
C     Initialize E sub theta functions                                  |PIT 3040
C -----------------------------------------------------------------------|PIT 3050
                                                                        PIT 3060
      DO 320 I = 1, NCAT                                                PIT 3070
        DO 310 J = 1, NCAT                                              PIT 3080
          ETHTC(I,J)  = 0.0D0                                           PIT 3090
          ETHTCP(I,J) = 0.0D0                                           PIT 3100
  310   CONTINUE                                                        PIT 3110
  320 CONTINUE                                                          PIT 3120
                                                                        PIT 3130
      DO 340 K = 1, NANI                                                PIT 3140
        DO 330 L = 1, NANI                                              PIT 3150
          ETHTA(K,L)  = 0.0D0                                           PIT 3160
          ETHTAP(K,L) = 0.0D0                                           PIT 3170
  330   CONTINUE                                                        PIT 3180
  340 CONTINUE                                                          PIT 3190
                                                                        PIT 3200
C -----------------------------------------------------------------------|PIT 3210
C     Initialize moles and charge for anions and cations                |PIT 3220
C -----------------------------------------------------------------------|PIT 3230
                                                                        PIT 3240
      DO 350 I = 1, NCAT                                                PIT 3250
        MC(I) = 0.0D0                                                   PIT 3260
        ZC(I) = 0                                                       PIT 3270
        IF (I .LE. NANI) THEN                                           PIT 3280
          MA(I) = 0.0D0                                                 PIT 3290
          ZA(I) = 0                                                     PIT 3300
        END IF                                                          PIT 3310
  350 CONTINUE                                                          PIT 3320
                                                                        PIT 3330
C -----------------------------------------------------------------------|PIT 3340
C     To avoid zerodivide the molality of unknown components in         |PIT 3350
C     pitzer is set = 0.001 mole                                        |PIT 3360
C -----------------------------------------------------------------------|PIT 3370
                                                                        PIT 3380
      DO 360 I = 1, NCAT                                                PIT 3390
        ZC(I) = Z(CAT(I))                                               PIT 3400
        MC(I) = ANALM(CAT(I))                                           PIT 3410
        IF (FLAG1 .NE. 1 .AND. I .EQ. 7) MC(I) = ALFA(8)                PIT 3420
        IF (MC(I) .LT. CPUMIN) MC(I) = 1.0D-3                           PIT 3430
  360 CONTINUE                                                          PIT 3440
                                                                        PIT 3450
      DO 370 K = 1, NANI                                                PIT 3460
        ZA(K) = Z(ANI(K))                                               PIT 3470
        MA(K) = ANALM(ANI(K))                                           PIT 3480
```

```
        IF (FLAG1 .NE. 1 .AND. K .EQ. 5)                                PIT 3490
          MA(K) = KT1(2) * ALFA(10) / ALFA(8)                           PIT 3500
        IF (MA(K) .LT. CPUMIN) MA(K) = 1.0D-3                           PIT 3510
  370 CONTINUE                                                          PIT 3520
                                                                        PIT 3530
C -------------------------------------------------------------------|PIT 3540
C     Determine ionic strength                                        |PIT 3550
C -------------------------------------------------------------------|PIT 3560
                                                                        PIT 3570
      MU = 0.0D0                                                        PIT 3580
      BZ = 0.0D0                                                        PIT 3590
                                                                        PIT 3600
      DO 380 I = 1, MXSP + 44                                           PIT 3610
        MU = MU + ANALM(I) * Z(I)**2                                    PIT 3620
        IF (Z(I) .NE. 0) BZ = BZ + ANALM(I) * IABS(Z(I))                PIT 3630
  380 CONTINUE                                                          PIT 3640
                                                                        PIT 3650
      MU = 0.5 * MU                                                     PIT 3660
                                                                        PIT 3670
C -------------------------------------------------------------------|PIT 3680
C     Calculate g functions assuming alpha = 2.0                      |PIT 3690
C -------------------------------------------------------------------|PIT 3700
                                                                        PIT 3710
      X  = 2 * DSQRT(MU)                                                PIT 3720
      G  =  2 * (1 - (1 + X) * DEXP(-X)) / (X**2)                       PIT 3730
      GP = -2 * (1 - (1 + X + (0.5 * X**2)) * DEXP(-X)) / X**2          PIT 3740
                                                                        PIT 3750
C -------------------------------------------------------------------|PIT 3760
C     Determine B, B', and C coefficients assuming beta(2)MX = 0.0    |PIT 3770
C -------------------------------------------------------------------|PIT 3780
                                                                        PIT 3790
      DO 400 I = 1, NCAT                                                PIT 3800
        DO 390 K = 1, NANI                                              PIT 3810
          C(I,K)  = 0.0D0                                               PIT 3820
          B(I,K)  = 0.0D0                                               PIT 3830
          BP(I,K) = 0.0D0                                               PIT 3840
                                                                        PIT 3850
          IF (MC(I) .LT. CPUMIN) GO TO 400                              PIT 3860
          IF (MA(K) .LT. CPUMIN) GO TO 390                              PIT 3870
          B(I,K)  = B0(I,K) + B1(I,K) * G                               PIT 3880
          BP(I,K) = B1(I,K) * GP / MU                                   PIT 3890
                                                                        PIT 3900
          IF (ZC(I) .EQ. 0) GO TO 400                                   PIT 3910
          IF (ZA(K) .EQ. 0) GO TO 390                                   PIT 3920
          C(I,K) = CP(I,K) / (2 * ((IABS(ZC(I) * ZA(K)))**0.5))        PIT 3930
  390   CONTINUE                                                        PIT 3940
  400 CONTINUE                                                          PIT 3950
                                                                        PIT 3960
C -------------------------------------------------------------------|PIT 3970
C     Determine Phi and Phi' cation coefficients                      |PIT 3980
C -------------------------------------------------------------------|PIT 3990
                                                                        PIT 4000
      DO 420 I = 1, NCAT                                                PIT 4010
        DO 410 J = 1, NCAT                                              PIT 4020
          PHIC(I,J)  = 0.0D0                                            PIT 4030
          PHICP(I,J) = 0.0D0                                            PIT 4040
                                                                        PIT 4050
          IF (MC(I) .LT. CPUMIN) GO TO 420                              PIT 4060
```

```
          IF (MC(J) .LT. CPUMIN) GO TO 410                              PIT 4070
                                                                        PIT 4080
          PHIC(I,J)  = THTC(I,J) + ETHTC(I,J)                           PIT 4090
          PHICP(I,J) = ETHTCP(I,J)                                      PIT 4100
  410   CONTINUE                                                        PIT 4110
  420 CONTINUE                                                          PIT 4120
                                                                        PIT 4130
C -------------------------------------------------------------------|PIT 4140
C     Determine Phi and Phi' anion coefficients                       |PIT 4150
C -------------------------------------------------------------------|PIT 4160
                                                                        PIT 4170
      DO 440 K = 1, NANI                                                PIT 4180
        DO 430 L = 1, NANI                                              PIT 4190
          PHIA(K,L)  = 0.0D0                                            PIT 4200
          PHIAP(K,L) = 0.0D0                                            PIT 4210
                                                                        PIT 4220
          IF (MA(K) .LT. CPUMIN) GO TO 440                              PIT 4230
          IF (MA(L) .LT. CPUMIN) GO TO 430                              PIT 4240
                                                                        PIT 4250
          PHIA(K,L)  = THTA(K,L) + ETHTA(K,L)                           PIT 4260
          PHIAP(K,L) = ETHTAP(K,L)                                      PIT 4270
  430   CONTINUE                                                        PIT 4280
  440 CONTINUE                                                          PIT 4290
                                                                        PIT 4300
C -------------------------------------------------------------------|PIT 4310
C     Determine first summation term to solve equation for F          |PIT 4320
C -------------------------------------------------------------------|PIT 4330
                                                                        PIT 4340
      SUM1 = 0.0D0                                                      PIT 4350
                                                                        PIT 4360
      DO 460 I = 1, NCAT                                                PIT 4370
        DO 450 K = 1, NANI                                              PIT 4380
          SUM1 = SUM1 + MC(I) * MA(K) * BP(I,K)                         PIT 4390
  450   CONTINUE                                                        PIT 4400
  460 CONTINUE                                                          PIT 4410
                                                                        PIT 4420
C -------------------------------------------------------------------|PIT 4430
C     Determine second summation term to solve equation for F         |PIT 4440
C -------------------------------------------------------------------|PIT 4450
                                                                        PIT 4460
      SUM2  = 0.0D0                                                     PIT 4470
                                                                        PIT 4480
      DO 480 I = 1, (NCAT-1)                                            PIT 4490
        DO 470 J = (I+1), NCAT                                          PIT 4500
          SUM2 = SUM2 + MC(I) * MC(J) * PHICP(I,J)                      PIT 4510
  470   CONTINUE                                                        PIT 4520
  480 CONTINUE                                                          PIT 4530
                                                                        PIT 4540
C -------------------------------------------------------------------|PIT 4550
C     Determine third summation term to solve equation for F          |PIT 4560
C -------------------------------------------------------------------|PIT 4570
                                                                        PIT 4580
      SUM3 = 0.0D0                                                      PIT 4590
                                                                        PIT 4600
      DO 500 K = 1, (NANI-1)                                            PIT 4610
        DO 490 L = (K+1), NANI                                          PIT 4620
          SUM3 = SUM3 + MA(K) * MA(L) * PHIAP(K,L)                      PIT 4630
  490   CONTINUE                                                        PIT 4640
```

```
  500 CONTINUE                                                          PIT 4650
                                                                        PIT 4660
C -------------------------------------------------------------------|PIT 4670
C     Solve for F                                                      |PIT 4680
C -------------------------------------------------------------------|PIT 4690
                                                                        PIT 4700
      F = -0.768 * A * ((DSQRT(MU) / (1 + 1.2 * DSQRT(MU))) +          PIT 4710
     .    (2 / 1.2) * DLOG(1 + 1.2 * DSQRT(MU))) + SUM1 + SUM2 + SUM3  PIT 4720
                                                                        PIT 4730
C -------------------------------------------------------------------|PIT 4740
C     Start to solve for ln activity coefficient of the cations        |PIT 4750
C -------------------------------------------------------------------|PIT 4760
                                                                        PIT 4770
      ITER = 1                                                          PIT 4780
                                                                        PIT 4790
      DO 620 II = 1, NCAT                                               PIT 4800
  520   CONTINUE                                                        PIT 4810
        IF (FLAG1 .EQ. 1 .AND. II .EQ. 7 .AND. ITER .EQ. 1)             PIT 4820
     .       M(8) = ALFA(8)                                             PIT 4830
        IF (MC(II) .LT. CPUMIN) GO TO 610                               PIT 4840
                                                                        PIT 4850
C -------------------------------------------------------------------|PIT 4860
C     First summation term for cation activity coefficients            |PIT 4870
C -------------------------------------------------------------------|PIT 4880
                                                                        PIT 4890
        SUM1 = 0.0D0                                                    PIT 4900
                                                                        PIT 4910
        DO 530 K = 1, NANI                                              PIT 4920
          SUM1 = SUM1 + MA(K) * (2 * B(II,K) + BZ * C(II,K))            PIT 4930
  530   CONTINUE                                                        PIT 4940
                                                                        PIT 4950
C -------------------------------------------------------------------|PIT 4960
C     Second summantion term for cation activity coefficients          |PIT 4970
C -------------------------------------------------------------------|PIT 4980
                                                                        PIT 4990
        SUM2  = 0.0D0                                                   PIT 5000
        SUM2B = 0.0D0                                                   PIT 5010
        SUM2C = 0.0D0                                                   PIT 5020
                                                                        PIT 5030
        DO 550 J = 1, NCAT                                              PIT 5040
          IF (II .EQ. J) GO TO 550                                      PIT 5050
          SUM2A = 0.0D0                                                 PIT 5060
                                                                        PIT 5070
          DO 540 K = 1, NANI                                            PIT 5080
            IF (MC(J) .LT. CPUMIN) GO TO 540                            PIT 5090
            SUM2A = SUM2A + MA(K) * PSIC(II,J,K)                        PIT 5100
  540     CONTINUE                                                      PIT 5110
                                                                        PIT 5120
          SUM2 = SUM2 + MC(J) * (2 * PHIC(II,J) + SUM2A)                PIT 5130
                                                                        PIT 5140
          IF (J .EQ. 1 .OR. J .EQ. 3) THEN                              PIT 5150
            SUM2B = SUM2 + 1.0D-3 * (2 * PHIC(II,J) + SUM2A)            PIT 5160
            SUM2C = SUM2 + 1.0D-3 * (2 * PHIC(II,J) + SUM2A)            PIT 5170
C          ELSE                                                         PIT 5180
C            SUM2B = SUM2 + MC(J) * (2 * PHIC(II,J) + SUM2A)            PIT 5190
C            SUM2C = SUM2 + MC(J) * (2 * PHIC(II,J) + SUM2A)            PIT 5200
          END IF                                                        PIT 5210
                                                                        PIT 5220
```

```
  550   CONTINUE                                                          PIT 5230
                                                                          PIT 5240
C -------------------------------------------------------------------|PIT 5250
C     Third summantion term for cation activity coefficients          |PIT 5260
C -------------------------------------------------------------------|PIT 5270
                                                                        PIT 5280
        SUM3 = 0.0D0                                                    PIT 5290
                                                                        PIT 5300
        DO 570 K = 1, (NANI-1)
          DO 560 L = (K+1), NANI                                        PIT 5320
            SUM3 = SUM3 + MA(K) * MA(L) * PSIA(K,L,II)                  PIT 5330
  560     CONTINUE                                                      PIT 5340
  570   CONTINUE                                                        PIT 5350
                                                                        PIT 5360
C -------------------------------------------------------------------|PIT 5370
C     Fourth summantion term for cation activity coefficients         |PIT 5380
C -------------------------------------------------------------------|PIT 5390
                                                                        PIT 5400
        SUM4  = 0.0D0                                                   PIT 5410
        SUM4B = 0.0D0                                                   PIT 5420
        SUM4C = 0.0D0                                                   PIT 5430
                                                                        PIT 5440
        DO 590 I = 1, NCAT                                              PIT 5450
          DO 580 K = 1, NANI                                            PIT 5460
            SUM4 = SUM4 + MC(I) * MA(K) * C(I,K)                        PIT 5470
            IF (I .EQ. 1 .OR. I .EQ. 3) THEN                            PIT 5480
              SUM4B = SUM4 + 1.0D-3 * MA(K) * C(I,K)                    PIT 5490
              SUM4C = SUM4 + 1.0D-3 * MA(K) * C(I,K)                    PIT 5500
C            ELSE                                                       PIT 5510
C             SUM4B = SUM4 + MC(I) * MA(K) * C(I,K)                     PIT 5520
C             SUM4C = SUM4 + MC(I) * MA(K) * C(I,K)                     PIT 5530
            END IF                                                      PIT 5540
  580     CONTINUE                                                      PIT 5550
  590   CONTINUE                                                        PIT 5560
                                                                        PIT 5570
        IF      (II .EQ. 1) THEN                                        PIT 5580
          LNGDNA =     F + SUM1 + SUM2C + SUM3 +   SUM4C                PIT 5590
          PGDNA  = DEXP(LNGDNA)                                         PIT 5600
        ELSE IF (II .EQ. 3) THEN                                        PIT 5610
          LNGDCA = 4 * F + SUM1 + SUM2B + SUM3 + 2*SUM4B                PIT 5620
          PGDCA  = DEXP(LNGDCA)                                         PIT 5630
        END IF                                                          PIT 5640
                                                                        PIT 5650
C -------------------------------------------------------------------|PIT 5660
C   Add up components to solve for activity coefficient for the cation |PIT 5670
C -------------------------------------------------------------------|PIT 5680
                                                                        PIT 5690
        LNGC(II)  = ZC(II)**2 * F + SUM1 + SUM2 + SUM3 +                PIT 5700
                    IABS(ZC(II)) * SUM4                                 PIT 5710
        PGAMC(II) = DEXP(LNGC(II))                                      PIT 5720
        PALFA(CAT(II)) = MC(II) * PGAMC(II)                             PIT 5730
                                                                        PIT 5740
        IF (FLAG1 .NE. 1) GO TO 610                                     PIT 5750
                                                                        PIT 5760
        DONE = 1                                                        PIT 5770
        M(8) = ALFA(8) / PGAMC(7)                                       PIT 5780
        DIFF = PALFA(CAT(7)) - ALFA(8)                                  PIT 5790
                                                                        PIT 5800
```

```
      IF ((DABS(DIFF)-(5.0D-3*ALFA(8))) .LT. CPUMIN) GO TO 600        PIT 5810
                                                                      PIT 5820
      DONE = 0                                                        PIT 5830
      ITER = ITER + 1                                                 PIT 5840
                                                                      PIT 5850
600   CONTINUE                                                        PIT 5860
      IF (DONE .NE. 1) GO TO 520                                      PIT 5870
      OHA  = KT1(2) * ALFA(10) / ALFA(8)                              PIT 5880
      M(9) = OHA                                                      PIT 5890
                                                                      PIT 5900
610   CONTINUE                                                        PIT 5910
      PG(CAT(II)) = PGAMC(II)                                         PIT 5920
620 CONTINUE                                                          PIT 5930
                                                                      PIT 5940
C -----------------------------------------------------------------|PIT 5950
C     Start to solve for ln activity coefficient of the anions     |PIT 5960
C -----------------------------------------------------------------|PIT 5970
                                                                      PIT 5980
      KK = 1                                                          PIT 5990
630   CONTINUE                                                        PIT 6000
      IF (MA(KK) .LT. CPUMIN) GO TO 720                               PIT 6010
                                                                      PIT 6020
C -----------------------------------------------------------------|PIT 6030
C     First summation term for anion activity coefficients         |PIT 6040
C -----------------------------------------------------------------|PIT 6050
                                                                      PIT 6060
      SUM1 = 0.0D0                                                    PIT 6070
                                                                      PIT 6080
      DO 640 I = 1, NCAT                                              PIT 6090
        SUM1 = SUM1 + MC(I) * (2 * B(I,KK) + BZ * C(I,KK))            PIT 6100
640   CONTINUE                                                        PIT 6110
                                                                      PIT 6120
C -----------------------------------------------------------------|PIT 6130
C     Second summation term for anion activity coefficients        |PIT 6140
C -----------------------------------------------------------------|PIT 6150
                                                                      PIT 6160
      SUM2 = 0.0D0                                                    PIT 6170
                                                                      PIT 6180
      DO 660 L = 1, NANI                                              PIT 6190
        IF (L .EQ. KK) GO TO 660                                      PIT 6200
                                                                      PIT 6210
        SUM2A = 0.0D0                                                 PIT 6220
                                                                      PIT 6230
        DO 650 I = 1, NCAT                                            PIT 6240
          IF (MA(L) .LT. CPUMIN) GO TO 650                            PIT 6250
          SUM2A = SUM2A + MC(I) * PSIA(KK,L,I)                        PIT 6260
650     CONTINUE                                                      PIT 6270
                                                                      PIT 6280
        SUM2 = SUM2 + MA(L) * (2 * PHIA(KK,L) + SUM2A)                PIT 6290
660   CONTINUE                                                        PIT 6300
                                                                      PIT 6310
C -----------------------------------------------------------------|PIT 6320
C     Third summation term for anion activity coefficients         |PIT 6330
C -----------------------------------------------------------------|PIT 6340
                                                                      PIT 6350
      SUM3 = 0.0D0                                                    PIT 6360
                                                                      PIT 6370
      DO 680 I = 1, (NCAT-1)                                          PIT 6380
```

```
        DO 670 J = (I+1), NCAT                                          PIT 6390
          SUM3 = SUM3 + MC(I) * MC(J) * PSIC(I,J,KK)                    PIT 6400
  670     CONTINUE                                                      PIT 6410
  680   CONTINUE                                                        PIT 6420
                                                                        PIT 6430
C -------------------------------------------------------------------|PIT 6440
C     Fourth summation term for anion activity coefficients            |PIT 6450
C -------------------------------------------------------------------|PIT 6460
                                                                        PIT 6470
        SUM4 = 0.0D0                                                    PIT 6480
                                                                        PIT 6490
        DO 700 I = 1, NCAT                                              PIT 6500
          DO 690 K = 1, NANI                                            PIT 6510
            SUM4 = SUM4 + MC(I) * MA(K) * C(I,K)                        PIT 6520
  690     CONTINUE                                                      PIT 6530
  700   CONTINUE                                                        PIT 6540
                                                                        PIT 6550
C -------------------------------------------------------------------|PIT 6560
C   Add up components to solve for activity coefficient for the anion  |PIT 6570
C -------------------------------------------------------------------|PIT 6580
                                                                        PIT 6590
        LNGA(KK)  = ZA(KK)**2 * F + SUM1 + SUM2 + SUM3 +                PIT 6600
     .              IABS(ZA(KK)) * SUM4                                PIT 6610
        PGAMA(KK) = DEXP(LNGA(KK))                                      PIT 6620
        PALFA(ANI(KK)) = MA(KK) * PGAMA(KK)                             PIT 6630
                                                                        PIT 6640
        IF (FLAG1 .NE. 1) GO TO 720                                     PIT 6650
                                                                        PIT 6660
        DONE = 1                                                        PIT 6670
        M(9) = OHA / PGAMA(5)                                           PIT 6680
        DIFF = PALFA(ANI(5)) - OHA                                      PIT 6690
                                                                        PIT 6700
        IF ((DABS(DIFF)-(5.0D-3*OHA)) .LT. CPUMIN) GO TO 710            PIT 6710
                                                                        PIT 6720
        DONE = 0                                                        PIT 6730
                                                                        PIT 6740
  710   CONTINUE                                                        PIT 6750
                                                                        PIT 6760
        IF (DONE .NE. 1) GO TO 630                                      PIT 6770
                                                                        PIT 6780
  720   CONTINUE                                                        PIT 6790
                                                                        PIT 6800
        IF (KK .EQ. 4 .AND. CO2TIT .GT. CPUMIN) THEN                    PIT 6810
          MA(3) = CO2TIT / (1 + 2 * (KT1(1) * PGAMA(3)) /               PIT 6820
     .                      (PGAMA(4)*ALFA(8)))                       PIT 6830
          MA(4) = 5.0D-1 * (CO2TIT - MA(3))                             PIT 6840
                                                                        PIT 6850
          IF (DABS(PALFA(ANI(3))-MA(3)*PGAMA(3)) .GT.                   PIT 6860
     .          5.0D-3*PALFA(ANI(3))) KK = 3                            PIT 6870
          IF (KK .EQ. 3) GO TO 630                                      PIT 6880
          IF (DABS(PALFA(ANI(4))-MA(4)*PGAMA(4)) .GT.                   PIT 6890
     .          5.0D-3*PALFA(ANI(4))) GO TO 630                         PIT 6900
        END IF                                                          PIT 6910
                                                                        PIT 6920
        PG(ANI(KK)) = PGAMA(KK)                                         PIT 6930
      KK = KK + 1                                                       PIT 6940
      IF (KK .LE. 5) GO TO 630                                          PIT 6950
                                                                        PIT 6960
```

```
C -----------------------------------------------------------------|PIT 6970
C     Calculate the osmostic coefficient                           |PIT 6980
C -----------------------------------------------------------------|PIT 6990
                                                                    PIT 7000
      DO 750 I = 1, NCAT                                            PIT 7010
        DO 740 K = 1, NANI                                          PIT 7020
          BFEE(I,K) = B0(I,K) + B1(I,K) * DEXP(-2.0 * DSQRT(MU))    PIT 7030
  740   CONTINUE                                                    PIT 7040
  750 CONTINUE                                                      PIT 7050
                                                                    PIT 7060
      SUM5 = 0.0D0                                                  PIT 7070
                                                                    PIT 7080
      DO 770 I = 1, NCAT                                            PIT 7090
        DO 760 K = 1, NANI                                          PIT 7100
          SUM5 = SUM5 + (MC(I) * MA(K)) * (BFEE(I,K) + BZ * C(I,K)) PIT 7110
  760   CONTINUE                                                    PIT 7120
  770 CONTINUE                                                      PIT 7130
                                                                    PIT 7140
      SUM6 = 0.0D0                                                  PIT 7150
                                                                    PIT 7160
      DO 800 I = 1, (NCAT-1)                                        PIT 7170
        DO 790 J = (I+1), NCAT                                      PIT 7180
          SUM6A = 0.0D0                                             PIT 7190
          DO 780 K = 1, NANI                                        PIT 7200
            SUM6A = SUM6A + MA(K) * PSIC(I,J,K)                     PIT 7210
  780     CONTINUE                                                  PIT 7220
          SUM6 = SUM6 + (MC(I) * MC(J)) * (PHIC(I,J) + SUM6A)       PIT 7230
  790   CONTINUE                                                    PIT 7240
  800 CONTINUE                                                      PIT 7250
                                                                    PIT 7260
      SUM7 = 0.0D0                                                  PIT 7270
                                                                    PIT 7280
      DO 830 K = 1, (NANI-1)                                        PIT 7290
        DO 820 L = (K+1), NANI                                      PIT 7300
          SUM7A = 0.0D0                                             PIT 7310
          DO 810 I = 1, NCAT                                        PIT 7320
            SUM7A = SUM7A + MC(I) * PSIA(K,L,I)                     PIT 7330
  810     CONTINUE                                                  PIT 7340
          SUM7 = SUM7 + (MA(K) * MA(L)) * (PHIA(K,L) + SUM7A)       PIT 7350
  820   CONTINUE                                                    PIT 7360
  830 CONTINUE                                                      PIT 7370
                                                                    PIT 7380
      SUM8 = 0.0D0                                                  PIT 7390
                                                                    PIT 7400
      DO 840 I = 1, NCAT                                            PIT 7410
        SUM8 = SUM8 + MC(I)                                         PIT 7420
  840 CONTINUE                                                      PIT 7430
                                                                    PIT 7440
      DO 845 I = 1, NANI                                            PIT 7450
        SUM8 = SUM8 + MA(I)                                         PIT 7460
  845 CONTINUE                                                      PIT 7470
                                                                    PIT 7480
      FEE = (-0.768 * A * MU) / (1 + 1.2 * DSQRT(MU))               PIT 7490
      FEE = FEE + SUM5 + SUM6 + SUM7                                PIT 7500
      FEE = 1.0 + (2.0 * FEE) / SUM8                                PIT 7510
                                                                    PIT 7520
C -----------------------------------------------------------------|PIT 7530
C     Calculate the activity of water                              |PIT 7540
```

```
C -----------------------------------------------------------------|PIT 7550
                                                                   PIT 7560
      ALFA(10) = 10**(-0.007823 * SUM8 * FEE)                      PIT 7570
                                                                   PIT 7580
C -----------------------------------------------------------------|PIT 7590
C     At this time pitzer data calculated for only (na,k,ca,mg,cl,so4) |PIT 7600
C -----------------------------------------------------------------|PIT 7610
                                                                   PIT 7620
      DO 850 I = 7, NMAX                                           PIT 7630
        PALFA(I) = 0.0D0                                           PIT 7640
        PG(I)    = 0.0D0                                           PIT 7650
  850 CONTINUE                                                     PIT 7660
                                                                   PIT 7670
      RETURN                                                       PIT 7680
      END                                                          PIT 7690
```

```
      SUBROUTINE POLY (A, B, C, E, D, G, J, ROOT)                  POL 0010
C ================================================================|POL 0020
C     This routine solves the cubic equation which describes the   |POL 0030
C     partitioning between gas, oil, and water.                    |POL 0040
C     Values defined in calling routine                            |POL 0050
C  ---------------------------------------------------------------|POL 0060
                                                                   POL 0070
      INTEGER UNO                                                  POL 0080
      DOUBLE PRECISION CPUMIN                                      POL 0090
      PARAMETER (UNO = 6)                                          POL 0100
      PARAMETER (CPUMIN = 1.0D-35)                                 POL 0110
                                                                   POL 0120
      DOUBLE PRECISION A, B, C, D, E, F1, F2, F3, G, J, P          POL 0130
      DOUBLE PRECISION Q, R, S, ROOT, T, X, Z, Z1, Z2, Z3          POL 0140
                                                                   POL 0150
      INTRINSIC DABS, DACOS, DCOS, DMAX1, DSIN, DSQRT              POL 0160
                                                                   POL 0170
C ================================================================|POL 0180
                                                                   POL 0190
      X = (1.0D00 / 3.0D00)                                        POL 0200
                                                                   POL 0210
      Z1 = D + G + J - A - B - C                                   POL 0220
      Z1 = Z1 / E                                                  POL 0230
                                                                   POL 0240
      Z2 = (D * G) + (D * J) + (G * J) - (A * G) - (A * J) - (B * D)  POL 0250
     .           - (B * J) - (C * D) - (C * G)                     POL 0260
      Z2 = Z2 / (E**2)                                             POL 0270
                                                                   POL 0280
      Z3 = (D * G * J) - (A * G * J) - (B * D * J) - (C * D * G)   POL 0290
      Z3 = Z3 / (E**3)                                             POL 0300
                                                                   POL 0310
      Q = ((3.0 * Z2) - (Z1**2)) / 9.00D00                         POL 0320
                                                                   POL 0330
      R = (9.0D00 * Z1 * Z2) - (27.00D00 * Z3) - (2.0D00 * Z1**3)  POL 0340
      R = R / 54.0D00                                              POL 0350
                                                                   POL 0360
      P = Q**3 + R**2                                              POL 0370
                                                                   POL 0380
```

```
      IF (DABS(P) .LT. CPUMIN) THEN                                      POL 0390
        F1 = (2.0D00 * (R**X))                                           POL 0400
        F1 = F1 - ( X * Z1)                                              POL 0410
        F2 = (-1.0D00) * (R**X) -  (X * Z1)                              POL 0420
        F3 = F2                                                          POL 0430
      ELSE IF (P .GT. 0.0D00) THEN                                       POL 0440
        S  = (R + DSQRT(Q**3 + R**2))**X                                 POL 0450
        T  = (R - DSQRT(Q**3 + R**2))**X                                 POL 0460
        F1 = S + T - (X * Z1)                                            POL 0470
        F2 = F1                                                          POL 0480
        F3 = F1                                                          POL 0490
      ELSE IF (P .LT. 0.0D00) THEN                                       POL 0500
        Z  = DACOS(R / (DSQRT(-1.0 * Q**3)))                             POL 0510
        Z  = Z / 3.0D00                                                  POL 0520
        F1 = (2.0D00 * DSQRT(-1.0 * Q) * DCOS(Z)) - (X * Z1)             POL 0530
        F2 = ((-1.0) * DSQRT(-1.0 * Q) * DCOS(Z)) - (X * Z1)             POL 0540
     .             + (DSQRT(-3.0 * Q) * DSIN(Z))                         POL 0550
        F3 = ((-1.0) * DSQRT(-1.0 * Q) * DCOS(Z)) - (X * Z1)             POL 0560
     .           - (DSQRT(-3.0 * Q) * DSIN(Z))                           POL 0570
      END IF                                                             POL 0580
                                                                         POL 0590
      ROOT = DMAX1(F1, F2, F3)                                           POL 0600
                                                                         POL 0610
      IF (ROOT .LE. 0.0) THEN                                            POL 0620
        WRITE (UNO, 1001)                                                POL 0630
        STOP                                                             POL 0640
      END IF                                                             POL 0650
                                                                         POL 0660
      RETURN                                                             POL 0670
                                                                         POL 0680
 1001 FORMAT( //, 57('*'),/, ' *',56X,'*' ,/, ' *  ERROR .... Call ',   POL 0690
     .          'E.H. Perkins, with complete problem  *',/,             POL 0700
     .       ' *',13X,'details.  Error occurred during volatile  *',/,  POL 0710
     .       ' *',13X,'fractionation between water, oil and gas  *',/,  POL 0720
     .       ' *',13X,'phases. ',34X,'*',/, ' *',56X,'*',/, 57('*'),//) POL 0730
                                                                         POL 0740
      END                                                                POL 0750
```

```
      SUBROUTINE PRATIO (TITLE, PRESS, TEMP, DENS, UNITS, PCO2, GEOTH,  PRA 0010
                         RATIO)                                         PRA 0020
C ==========================================================================|PRA 0030
C     This routine prints mole ratios, log of active ratios, etc.         |PRA 0040
C --------------------------------------------------------------------------|PRA 0050
C     A1         DBL   Temperary storage for intermediate values         |PRA 0060
C     A2         DBL   Temperary storage for intermediate values         |PRA 0070
C     A3         DBL   Temperary storage for intermediate values         |PRA 0080
C     A4         DBL   Temperary storage for intermediate values         |PRA 0090
C     ALFA       DBL   Activity of aqueous species i                     |PRA 0100
C     ANALM      DBL   Analyzed molality of species i                    |PRA 0110
C     CO         DBL   Hold intermediate calculations                    |PRA 0120
C     CPUMIN     DBL   Smallest positive real value program uses         |PRA 0130
C     CR         CHA   Inserts carriage returns in output                |PRA 0140
C     CUNITS     DBL   Analytical input concentration                    |PRA 0150
C     DENS       DBL   Density                                           |PRA 0160
```

```
C     DUM       DBL   Array to hold results for printing                |PRA 0170
C     EXELT     DBL   Moles of components                                |PRA 0180
C     FD5       DBL   Number of Hydrogens in various activity ratios     |PRA 0190
C     GEOTH     INT   Flag to print geothermometers                      |PRA 0200
C     I         INT   Loop variable/pointer                              |PRA 0210
C     ID1       INT   Index of species to make ratios                    |PRA 0220
C     ID2       INT   Index of species to make ratios                    |PRA 0230
C     ID3       INT   Index of species to make ratios                    |PRA 0240
C     ID4       INT   Index of species to make ratios                    |PRA 0250
C     IPGLN     INT   Current line number of the output file             |PRA 0260
C     NMAX      INT   General array dimension to allow easy expansion    |PRA 0270
C     PCO2      DBL   Partial Pressure of Carbon Dioxide                 |PRA 0280
C     PF        DBL   Holds intermediate calculations                    |PRA 0290
C     PH        DBL   Measured pH of the solution                        |PRA 0300
C     PRESS     DBL   Total pressure                                     |PRA 0310
C     RATIO     INT   Flag for printing activity ratios of elements      |PRA 0320
C     RMG       DBL   Holds intermediate calculations                    |PRA 0330
C     RMGD      DBL   Holds intermediate calculations                    |PRA 0340
C     SUBT      DBL   Array to hold calculated geothermometers           |PRA 0350
C     TEMP      DBL   Temperature of the solution when pH was measured   |PRA 0360
C     TITLE     CHA   Name of the sample                                 |PRA 0370
C     TITMIX    CHA   TITLE for mixtures                                 |PRA 0380
C     TITR      DBL   Iteration array in DISTRB, used for guesses        |PRA 0390
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                   |PRA 0400
C     UNITS     CHA   Units of concentration                             |PRA 0410
C     UNO       INT   File unit assigned for output file                 |PRA 0420
C -------------------------------------------------------------------    |PRA 0430
                                                                         PRA 0440
      DOUBLE PRECISION CPUMIN                                            PRA 0450
      INTEGER NMAX, UNO                                                  PRA 0460
      PARAMETER (CPUMIN = 1.0D-35, UNO = 6)                              PRA 0470
      PARAMETER (NMAX = 340)                                             PRA 0480
                                                                         PRA 0490
      INTEGER I, ID1(10), ID2(10), ID3(10), ID4(6), IPAGE, IPGLN         PRA 0500
      INTEGER GEOTH, RATIO                                               PRA 0510
                                                                         PRA 0520
      CHARACTER *  1 TOF, CR                                             PRA 0530
      CHARACTER *  5 UNITS                                               PRA 0540
      CHARACTER * 40 TITMIX                                              PRA 0550
      CHARACTER * 80 TITLE                                               PRA 0560
                                                                         PRA 0570
      DOUBLE PRECISION A1, A2, A3, A4, ALFA(NMAX), ANALM(NMAX)           PRA 0580
      DOUBLE PRECISION CO, CO2F, CUNITS(NMAX)                            PRA 0590
      DOUBLE PRECISION DENS, DUM(10)                                     PRA 0600
      DOUBLE PRECISION HTOTI, EXELT(35), FD5(6), M(NMAX), OHTOTI         PRA 0610
      DOUBLE PRECISION PCO2, PF, PH, PRESS, RMG, RMGD, SUBT(21)          PRA 0620
      DOUBLE PRECISION TEMP, TITR(11), TOTEL(5)                          PRA 0630
                                                                         PRA 0640
      INTRINSIC DABS, DLOG10, DSQRT                                      PRA 0650
      EXTERNAL  PAGE                                                     PRA 0660
                                                                         PRA 0670
      COMMON /EXTOT / EXELT, TOTEL, TITR                                 PRA 0680
      COMMON /FMFD  / TOF, CR, TITMIX                                    PRA 0690
      COMMON /FORM  / IPAGE, IPGLN                                       PRA 0700
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                         PRA 0710
      COMMON /TOTALS/ CO2F, HTOTI, OHTOTI                                PRA 0720
                                                                         PRA 0730
      DATA ID1 /  1,  2, 3, 4, 14, 18,  6,  7,  1,  1/                   PRA 0740
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      DATA ID2 / 32, 22, 4, 2, 26, 15,  6,  7,  8, 16/                  PRA 0750
      DATA ID3 /  3,  3, 3, 1,  1,  1, 20, 20, 20, 20/                  PRA 0760
      DATA ID4 /  1,  2, 3, 4, 14, 18/                                  PRA 0770
      DATA FD5 / 2.0, 2.0, 1.0, 1.0, 3.0, 2.0/                          PRA 0780
                                                                        PRA 0790
C ======================================================================|PRA 0800
                                                                        PRA 0810
      DO 10 I = 1, 10                                                   PRA 0820
        DUM(I) = 0.0                                                    PRA 0830
   10 CONTINUE                                                          PRA 0840
                                                                        PRA 0850
      IF (RATIO .EQ. 1) THEN                                            PRA 0860
        CALL PAGE                                                       PRA 0870
        WRITE (UNO, 1000) TITLE, TEMP, TITMIX                           PRA 0880
        WRITE (UNO, 1010) CR                                            PRA 0890
        WRITE (UNO, 1020) CR                                            PRA 0900
                                                                        PRA 0910
        IF (EXELT(5) .GT. CPUMIN) THEN                                  PRA 0920
          DO 20 I = 1, 8                                                PRA 0930
            IF (ANALM(ID1(I)) .GT. CPUMIN) DUM(I) = EXELT(5) /          PRA 0940
                                                    ANALM(ID1(I))       PRA 0950
   20       CONTINUE                                                    PRA 0960
        END IF                                                          PRA 0970
                                                                        PRA 0980
        IF (ANALM(2) .GT. CPUMIN) THEN                                  PRA 0990
          DUM(9) = ANALM(1) / ANALM(2)                                  PRA 1000
          IF (ANALM(3) .GT. CPUMIN) DUM(10) = DSQRT(ANALM(1)) / ANALM(3)PRA 1010
        END IF                                                          PRA 1020
                                                                        PRA 1030
        WRITE (UNO, 1030) (DUM(I), I = 1, 10)                           PRA 1040
        WRITE (UNO, 1040)                                               PRA 1050
        WRITE (UNO, 1050) CR                                            PRA 1060
        IPGLN = IPGLN + 3                                               PRA 1070
                                                                        PRA 1080
        DO 25 I = 1, 10                                                 PRA 1090
          DUM(I) = 0.0D00                                               PRA 1100
   25   CONTINUE                                                        PRA 1110
                                                                        PRA 1120
        DO 30 I = 1, 6                                                  PRA 1130
          IF (ANALM(ID2(I)) .GT. CPUMIN .AND.                           PRA 1140
              ANALM(ID3(I)) .GT. CPUMIN)                                PRA 1150
                            DUM(I) = ANALM(ID2(I)) / ANALM(ID3(I))      PRA 1160
   30   CONTINUE                                                        PRA 1170
                                                                        PRA 1180
                                                                        PRA 1190
        IF (EXELT(5) .GT. CPUMIN) THEN                                  PRA 1200
          IF (ANALM(6) .GT. CPUMIN) DUM(7)  = ANALM(6)  / EXELT(5)      PRA 1210
          IF (ANALM(7) .GT. CPUMIN) DUM(8)  = ANALM(7)  / EXELT(5)      PRA 1220
          IF (EXELT(22).GT. CPUMIN) DUM(9)  = EXELT(22) / EXELT(5)      PRA 1230
          IF (EXELT(23).GT. CPUMIN) DUM(10) = EXELT(23) / EXELT(5)      PRA 1240
        END IF                                                          PRA 1250
                                                                        PRA 1260
        WRITE (UNO, 1060) (DUM(I), I = 1, 10)                           PRA 1270
        WRITE (UNO, 1070) CR                                            PRA 1280
        WRITE (UNO, 1080)                                               PRA 1290
        WRITE (UNO, 1090) CR                                            PRA 1300
        IPGLN = IPGLN + 7                                               PRA 1310
                                                                        PRA 1320
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      DO 40 I = 1, 6                                                    PRA 1330
        DUM(I) = 0.D0                                                   PRA 1340
        IF (ALFA(ID4(I)) .GT. CPUMIN) DUM(I) = DLOG10(ALFA(ID4(I)))     PRA 1350
                                              + (FD5(I) * PH)           PRA 1360
40    CONTINUE                                                          PRA 1370
                                                                        PRA 1380
      DUM(7) = 0.D0                                                     PRA 1390
      DUM(8) = 0.D0                                                     PRA 1400
                                                                        PRA 1410
      IF (ALFA(1) .GT. CPUMIN .AND. ALFA(2) .GT. CPUMIN)                PRA 1420
        DUM(7) = DLOG10(ALFA(1) / ALFA(2))                              PRA 1430
      IF (ALFA(3) .GT. CPUMIN .AND. ALFA(4) .GT. CPUMIN)                PRA 1440
        DUM(8) = DLOG10(ALFA(3) / ALFA(4))                              PRA 1450
                                                                        PRA 1460
      WRITE (UNO, 1100) (DUM(I), I = 1, 8)                             PRA 1470
      IPGLN = IPGLN + 1                                                 PRA 1480
    END IF                                                              PRA 1490
                                                                        PRA 1500
    IF (GEOTH .EQ. 1 .OR. RATIO .EQ. 1) THEN                            PRA 1510
      RMG  = 0.0D0                                                      PRA 1520
      RMGD = 0.0D0                                                      PRA 1530
      CO   = 0.0D0                                                      PRA 1540
      A1   = 0.0D0                                                      PRA 1550
      A2   = 0.0D0                                                      PRA 1560
      A3   = 0.0D0                                                      PRA 1570
      A4   = 0.0D0                                                      PRA 1580
                                                                        PRA 1590
      IF (ANALM(2) .GT. CPUMIN) RMG = ANALM(2) * 2 * 100 /              PRA 1600
         (ANALM(2) * 2 + ANALM(1) * 2 + ANALM(4))                       PRA 1610
      IF (ANALM(1) .GT. CPUMIN) A1 = DLOG10(ANALM(1))                   PRA 1620
      IF (ANALM(3) .GT. CPUMIN) A3 = DLOG10(ANALM(3))                   PRA 1630
      IF (ANALM(4) .GT. CPUMIN) A4 = DLOG10(ANALM(4))                   PRA 1640
                                                                        PRA 1650
      A1 = 0.5 * A1                                                     PRA 1660
      A2 = A1                                                           PRA 1670
                                                                        PRA 1680
      IF (DABS(A1) .GT. CPUMIN .OR. DABS(A3) .GT. CPUMIN                PRA 1690
                               .OR. DABS(A4) .GT. CPUMIN) THEN          PRA 1700
        A1 = A3 - A4 + (1.D0 / 3.D0) * (A1 - A3)                        PRA 1710
        A2 = A3 - A4 + (4.D0 / 3.D0) * (A2 - A3)                        PRA 1720
                                                                        PRA 1730
        IF (RATIO .EQ. 1) THEN                                          PRA 1740
          WRITE (UNO, 1110) A1, A2                                      PRA 1750
          IPGLN = IPGLN + 5                                             PRA 1760
        END IF                                                          PRA 1770
      END IF                                                            PRA 1780
    END IF                                                              PRA 1790
                                                                        PRA 1800
    A3   = 0.0D0                                                        PRA 1810
    A4   = 0.0D0                                                        PRA 1820
                                                                        PRA 1830
    IF (GEOTH .EQ. 1) THEN                                              PRA 1840
      IF (UNITS .EQ. 'MOL/L' .OR. UNITS .EQ. 'MOL/K') THEN              PRA 1850
        WRITE (UNO, 1120)                                               PRA 1860
        RETURN                                                          PRA 1870
      END IF                                                            PRA 1880
                                                                        PRA 1890
C -------------------------------------------------------------------|PRA 1900
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C     Calculation of the subsurface temperature "subt" of the sample   |PRA 1910
C     from the chemical data.                                          |PRA 1920
C -------------------------------------------------------------------|PRA 1930
                                                                       PRA 1940
      IF (RATIO .NE. 1) CALL PAGE                                      PRA 1950
                                                                       PRA 1960
      DO 50 I = 1, 21                                                  PRA 1970
        SUBT(I) = 0.D0                                                 PRA 1980
   50 CONTINUE                                                         PRA 1990
                                                                       PRA 2000
      IF (CUNITS(12) .LT. CPUMIN) GO TO 60                             PRA 2010
                                                                       PRA 2020
      IF      (UNITS .EQ. 'MG/L ') THEN                                PRA 2030
        CO = DLOG10(CUNITS(12) / DENS)                                 PRA 2040
      ELSE IF (UNITS .EQ. 'PPM  ') THEN                                PRA 2050
        CO = DLOG10(CUNITS(12))                                        PRA 2060
      END IF                                                           PRA 2070
                                                                       PRA 2080
      SUBT( 1) = 1.309D3 / (5.19D0 - CO) - 273.16D0                    PRA 2090
      SUBT( 2) = 1.522D3 / (5.75D0 - CO) - 273.16D0                    PRA 2100
      SUBT( 3) = 0.731D3 / (4.52D0 - CO) - 273.16D0                    PRA 2110
      SUBT( 8) = 1.032D3 / (4.69D0 - CO) - 273.16D0                    PRA 2120
      SUBT(10) = 1.000D3 / (4.78D0 - CO) - 273.16D0                    PRA 2130
                                                                       PRA 2140
      PF = 1.00 - 7.862D-5 * 2.718**(3.61D-3 * TEMP) * PRESS           PRA 2150
      CO = DLOG10(PF * ALFA(11) / ALFA(10)**2)                         PRA 2160
                                                                       PRA 2170
      SUBT(16) =  1309.0D00 / ( 0.41 - CO) - 273.16D0                  PRA 2180
      SUBT(17) =  1522.0D00 / ( 0.97 - CO) - 273.16D0                  PRA 2190
      SUBT(18) =  1032.0D00 / (-0.09 - CO) - 273.16D0                  PRA 2200
      SUBT(19) = -1000.0D00 / CO           - 273.16D0                  PRA 2210
                                                                       PRA 2220
      CO = PF * ALFA(11)                                               PRA 2230
      SUBT(21) =   731.0D00 / (-0.26 - DLOG10(CO)) - 273.16D0          PRA 2240
                                                                       PRA 2250
   60 CONTINUE                                                         PRA 2260
      IF (CUNITS(3) .GT. 0.0D0 .AND. CUNITS(4) .GT. 0.0D0)             PRA 2270
        SUBT(4) = 1.217D3 / (1.483D0 + DLOG10((CUNITS(3) /             PRA 2280
                  CUNITS(4)))) - 273.16D0                              PRA 2290
                                                                       PRA 2300
C -------------------------------------------------------------------|PRA 2310
C     Calculation of paces geothermometer.                             |PRA 2320
C -------------------------------------------------------------------|PRA 2330
                                                                       PRA 2340
      IF (PCO2 .GT. 1.0D-6) THEN                                       PRA 2350
        A4    = A2 - (-1.36 - 0.253 * DLOG10(PCO2))                    PRA 2360
        SUBT(12) = 1.647D3 / (2.24D0 + A4) - 273.16                    PRA 2370
      END IF                                                           PRA 2380
                                                                       PRA 2390
      IF (A1 .GT. CPUMIN .AND. A2 .GT. CPUMIN) THEN                    PRA 2400
        SUBT(5) = 1.647D3 / (2.240D0 + A1) - 273.16                    PRA 2410
        SUBT(6) = 1.647D3 / (2.240D0 + A2) - 273.16                    PRA 2420
      END IF                                                           PRA 2430
                                                                       PRA 2440
      IF (RMG .LT. 0.5) THEN                                           PRA 2450
        SUBT(14) = SUBT(5)                                             PRA 2460
        GO TO 70                                                       PRA 2470
      END IF                                                           PRA 2480
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                                                                      PRA 2490
      IF (RMG .GT. 50.0 .OR. SUBT(6) .LT. 70.0) GO TO 70              PRA 2500
                                                                      PRA 2510
      IF (SUBT(6) .LT. 100) THEN                                      PRA 2520
        RMGD = SUBT(6)                                                PRA 2530
      ELSE                                                            PRA 2540
        RMGD = SUBT(5)                                                PRA 2550
      END IF                                                          PRA 2560
                                                                      PRA 2570
      IF (RMG .LT. 5.0) THEN                                          PRA 2580
        SUBT(14) = RMGD - (-1.03 + 59.971 * DLOG10(RMG) + 145.05 *    PRA 2590
     .               (DLOG10(RMG))**2 - 36711 * (DLOG10(RMG))**2 /    PRA 2600
     .               (RMGD + 273.16D0) - 1.67D7 * DLOG10(RMG) /       PRA 2610
     .               (RMGD + 273.16D0)**2)                            PRA 2620
      ELSE                                                            PRA 2630
        SUBT(14) = RMGD - (10.66 - 4.74 * RMG + 325.87 *              PRA 2640
     .               DLOG10(RMG)**2 - (1.032D5 * DLOG10(RMG)**2) /    PRA 2650
     .               (RMGD + 273.16D0) - (1.968D7 * DLOG10(RMG)**2 /  PRA 2660
     .               (RMGD + 273.16D0)**2) + ((1.605D7 *              PRA 2670
     .               DLOG10(RMG)**3) / (RMGD + 273.16D0)**2))         PRA 2680
      END IF                                                          PRA 2690
                                                                      PRA 2700
   70 CONTINUE                                                        PRA 2710
      IF (CUNITS(2) .GT. CPUMIN .AND. CUNITS(22) .GT. CPUMIN) THEN    PRA 2720
        IF (UNITS .EQ. 'MG/L ') A3 = DSQRT(CUNITS(2)) / CUNITS(22)    PRA 2730
        IF (UNITS .EQ. 'PPM  ')                                       PRA 2740
     .    A3 = DSQRT(CUNITS(2) / DENS) / CUNITS(22)                   PRA 2750
        SUBT(7) = 2.2D3 / (5.47 + DLOG10(A3)) - 273.16D0              PRA 2760
      END IF                                                          PRA 2770
                                                                      PRA 2780
      IF (CUNITS(3) .GT. CPUMIN .AND. CUNITS(22) .GT. CPUMIN)         PRA 2790
     .  SUBT(9) = 1.59D3 / (DLOG10(CUNITS(3) / CUNITS(22)) + 0.779) - PRA 2800
     .            273.16D0                                           PRA 2810
                                                                      PRA 2820
      DO 80 I = 1, 21                                                 PRA 2830
        IF (SUBT(I) .LT. CPUMIN) SUBT(I) = 999.0                      PRA 2840
   80 CONTINUE                                                        PRA 2850
                                                                      PRA 2860
      WRITE (UNO, 1130) CR, CR                                        PRA 2870
      WRITE (UNO, 1140) SUBT(1), SUBT(16), SUBT(2),  SUBT(17)         PRA 2880
      WRITE (UNO, 1150) SUBT(8), SUBT(18), SUBT(10), SUBT(19)         PRA 2890
      WRITE (UNO, 1160) SUBT(3), SUBT(21), SUBT(4),  SUBT(5)          PRA 2900
      WRITE (UNO, 1170) SUBT(6), SUBT(12)                             PRA 2910
      WRITE (UNO, 1180) SUBT(14), SUBT(7), SUBT(9)                    PRA 2920
    END IF                                                            PRA 2930
                                                                      PRA 2940
    IF (GEOTH .EQ. 1) GEOTH = 2                                       PRA 2950
                                                                      PRA 2960
    RETURN                                                            PRA 2970
                                                                      PRA 2980
 1000 FORMAT (' SAMPLE IDENT - ', A80, 4X, 'TEMPERATURE = ', F8.2, /, PRA 2990
     .        20X, A40)                                               PRA 3000
 1010 FORMAT (//, ' MOLE RATIOS (USING ANALYTICAL MOLALITY)', /, A1,  PRA 3010
     .        39('_'), //, 8X, ' CL/CA', 8X, 'CL/MG', 8X, 'CL/NA',    PRA 3020
     .        8X, 'CL/K',   8X, 'CL/AL', 8X, 'CL/FE', 7X, 'CL/SO4',   PRA 3030
     .        6X, 'CL/HCO3', 5X, 'CA/MG', 7X, 'SQRT(CA)/NA')          PRA 3040
 1020 FORMAT (A1, 3(8X,'_____'), 8X, '____', 2(8X, '_____'),          PRA 3050
     .        7X, '______', 6X, '_______', 5X, '_____',               PRA 3060
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     .        7X, '__________')                                          PRA 3070
1030 FORMAT (1X, 10E13.4)                                               PRA 3080
1040 FORMAT (/, 8X, 'NH3/NA', 8X, 'LI/NA', 8X, 'K/NA', 8X, 'MG/CA',     PRA 3090
     .          8X, 'SR/CA', 8X, 'BA/CA', 8X, 'SO4/CL', 8X, 'HCO3/CL', PRA 3100
     .          8X, 'F/CL', 8X, 'B/CL')                                 PRA 3110
1050 FORMAT (A1, 8X, '______', 8X, '_____', 8X, '____', 8X, '_____',   PRA 3120
     .          8X, '_____', 8X, '_____', 8X, '______', 8X, '_______',PRA 3130
     .          8X, '____', 8X, '____')                                 PRA 3140
1060 FORMAT (2X, 6E13.4, 2E14.4, 2E12.4)                                PRA 3150
1070 FORMAT (///, ' LOG OF ACTIVITY RATIOS', /, A1, 22('_'))            PRA 3160
1080 FORMAT (8X, 'CA/H2', 8X, 'MG/H2', 9X, 'NA/H', 10X, 'K/H',          PRA 3170
     .        8X, 'AL/H3', 8X, 'FE/H2', 8X, 'CA/MG', 9X, 'NA/K', A1)   PRA 3180
1090 FORMAT (A1, 8X, '______', 8X, '_____', 9X, '____', 10X, '___',     PRA 3190
     .          8X, '_____', 8X, '_____', 8X, '_____', 9X, '____')     PRA 3200
1100 FORMAT (8E13.4)                                                    PRA 3210
1110 FORMAT (/, '  LOG(NA/K)+1/3(LOG(SQRT(CA)/NA)) =', E10.3, /,       PRA 3220
     .          '  LOG(NA/K)+4/3(LOG(SQRT(CA)/NA)) =', E10.3, //)     PRA 3230
1120 FORMAT (//, '  NO TEMP. DATA IN MOL/L')                            PRA 3240
1130 FORMAT (//, ' CHEMICAL GEOTHERMOMETER TEMPERATURES (IN DEGREES',   PRA 3250
     .          ' CENTIGRADE)', /, A1, 60('_'), /, 2X,                  PRA 3260
     .          '("999.0" INDICATES THAT A VALUE GREATER THAN 0.0 ',    PRA 3270
     .          'WAS NOT CALCULATED)', //, 45X,                         PRA 3280
     .          'TEMP. WITH PRESSURE', /, ' TEMPERATURE', 29X,          PRA 3290
     .          'AND/OR ACTIVITY CORRECTION', /, A1, 62('_'), /)        PRA 3300
1140 FORMAT (1X, F10.1,       ' : QUARTZ (CONDUCTIVE)          : ',     PRA 3310
     .        1X, F10.1, T70, ' A. IF THE WATER IS BOILING OR STEAM',  PRA 3320
     .                        ' IS LOST DURING', /,                    PRA 3330
     .        1X, F10.1,      ' : QUARTZ (ADIABATIC)           : ',     PRA 3340
     .        1X, F10.1, T70, '    THE SAMPLING OF GROUNDWATERS',      PRA 3350
     .                        ' THEN USE THE QUARTZ', /,               PRA 3360
     .                   T70, '    ADIABATIC TEMPERATURE.')            PRA 3370
1150 FORMAT (1X, F10.1,       ' : CHALCEDONY WITH SIO2         : ',     PRA 3380
     .        1X, F10.1, T70, ' B. IF THERE IS NO STEAM LOSS THEN',    PRA 3390
     .                        ' USE THE QUARTZ', /,                    PRA 3400
     .                   T70, '    CONDUCTIVE TEMPERATURE.', /,        PRA 3410
     .        1X, F10.1,      ' : ALFA CRISTOBALITE WITH SIO2 : ',     PRA 3420
     .        1X, F10.1, T70, ' C. The Amorphous Silica Temperature',  PRA 3430
     .                        ' Should Be Considered', /,              PRA 3440
     .                   T70, '    When The Sample Is Saturated With', PRA 3450
     .                        ' Amorphous Silica')                     PRA 3460
1160 FORMAT (1X, F10.1,       ' : Amorphous Silica With SiO2  : ',     PRA 3470
     .        1X, F10.1, T70, '    (THE DELTA G OF MINERAL NO. 275 IS', PRA 3480
     .                        ' POSITIVE).', /,                        PRA 3490
     .                   T70, ' D. IF THE IN SITU TEMPERATURE EXCEEDS', PRA 3500
     .                        ' 150 DEGREES', /,                       PRA 3510
     .                   T70, '    THEN THE NA/K TEMPERATURE MAY BE',  PRA 3520
     .                        ' USED.', /,                             PRA 3530
     .        1X, F10.1,      ' : LOG (NA/K)',                         PRA 3540
     .                   T70, ' E. ALTHOUGH THE 4/3 LOG TEMPERATURE IS',PRA 3550
     .                        ' GENERALLY USED', /,                    PRA 3560
     .        1X, F10.1,      ' : LOG (NA/K) + 1/3 LOG(SQRT(CA)/NA)',  PRA 3570
     .                   T70, '    WHEN THE TEMPERATURE IS LESS THAN', PRA 3580
     .                        ' 100 DEGREES IT IS')                    PRA 3590
1170 FORMAT (1X, F10.1,       ' : LOG (NA/K) + 4/3 LOG(SQRT(CA)/NA)',  PRA 3600
     .                   T70, '    CONSIDERED LESS RELIABLE THAN THE', PRA 3610
     .                        ' 1/3 LOG TEMPERATURE.', /,              PRA 3620
     .        1X, F10.1,      ' : LOG (NA/K) + 4/3 LOG(SQRT(CA)/NA)',  PRA 3630
     .                   T70, ' F. THE ACTIVITIES OF H4SIO4 AND',      PRA 3640
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     .                         ' WATER WILL BE COMPUTED', /,                  PRA 3650
     .       24X,              ' + 1.36+0.253*LOG(PCO2)',                     PRA 3660
     .                    T70, '    AT THE SURFACE TEMPERATURE ONLY IF',      PRA 3670
     .                         ' THE HITEMP',/,                               PRA 3680
     .                    T70, '    OPTION IS SELECTED.')                    PRA 3690
1180 FORMAT (1X, F10.1,        ' : MG CORRECTED 1/3 (NA-K-CA)',               PRA 3700
     .                    T70, ' G. THE ORDER OF RELIABILITY OF THE',        PRA 3710
     .                         ' CATION GEOTHERMOMETERS:', /,                 PRA 3720
     .                    T70, '    MG-LI>MG-CORRECTED NA-K-CA>NA-LI>',      PRA 3730
     .                        'OTHERS', /,                                    PRA 3740
     .        1X, F10.1,       ' : LOG (SQRT(MG)/LI)',                        PRA 3750
     .                    T70, ' H. DETAILS OF THE EQUATIONS AND',           PRA 3760
     .                         ' PARAMETERS CAN BE', /,                       PRA 3770
     .        1X, F10.1,       ' : LOG (NA/LI)',                              PRA 3780
     .                    T70, '    FOUND IN KHARAKA AND MARINER,',          PRA 3790
     .                        '1988).',/)                                     PRA 3800
                                                                             PRA 3810
      END                                                                    PRA 3820
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      SUBROUTINE PRINTR (TITLE, EHM, UNITS, DENS, PRESS, GFW, TEMP, Z,  PRI 0010
     .                   GAMMA, PH2O, PCO2, TDS, MU, MNACLD, SCO2,      PRI 0020
     .                   HTOT, OHTOT, MXSP)                             PRI 0030
C ==========================================================================|PRI 0040
C     This routine prints the results of the iterations and the            |PRI 0050
C     distribution of species.                                             |PRI 0060
C --------------------------------------------------------------------------|PRI 0070
C     ALFA      DBL   Activity of aqueous species i                        |PRI 0080
C     ALK1      DBL   Various forms of Alkalinity (different units)        |PRI 0090
C     ALK2      DBL                          "                             |PRI 0100
C     ALK3      DBL                          "                             |PRI 0110
C     ALK7      DBL                          "                             |PRI 0120
C     ANALM     DBL   Analyzed molality of species i                       |PRI 0130
C     C1        DBL                                                         PRI 0140
C     CAR1      DBL   Various forms of total/partial Carbon in solution    |PRI 0150
C     CAR4      DBL                          "                             |PRI 0160
C     CFLG      DBL                          "                             |PRI 0170
C     CPUMIN    DBL   Smallest positive real value program uses            |PRI 0180
C     CR        CHA   Inserts carriage returns in output                   |PRI 0190
C     CU        DBL   Conversion factor between units                      |PRI 0200
C     CUNITS    DBL   Analytical input concentration                       |PRI 0210
C     DENS      DBL   Density                                              |PRI 0220
C     DUM1      DBL   Dummy variable for printing/storage                  |PRI 0230
C     DUM2      DBL   Dummy variable for printing/storage                  |PRI 0240
C     DUM3      DBL   Dummy variable for printing/storage                  |PRI 0250
C     DUM4      DBL   Dummy variable for printing/storage                  |PRI 0260
C     EHM       DBL   Measured Eh in volts                                 |PRI 0270
C     EXELT     DBL   Moles of components                                  |PRI 0280
C     GAMMA     DBL   Activity coefficients                                |PRI 0290
C     GFW       DBL   Gram formula weight of aqueous species               |PRI 0300
C     HTOT      DBL   Sum of the hydronium in solution                     |PRI 0310
C     I         INT   Loop variable                                        |PRI 0320
C     IPGLN     INT   Current line number of the output file               |PRI 0330
C     M         DBL   Calculated molality of aqueous species               |PRI 0340
C     MNACLD    DBL   Sum of Molality * charge / 2                         |PRI 0350
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C     MU        DBL   Ionic strength of aqueous solution                    |PRI 0360
C     MXSP      INT   Total number of aqueous species                       |PRI 0370
C     NMAX      INT   General array dimension to allow easy expansion       |PRI 0380
C     OHTOT     DBL   Sum of OH in the solution                             |PRI 0390
C     PAGE1     CHA   Names of aqueous species                              |PRI 0400
C     PCH4      DBL   (Partial) pressure of CH4 .. calculated               |PRI 0410
C     PCO2      DBL   (Partial) pressure of CO2 .. calculated               |PRI 0420
C     PH        DBL   Measured pH of the solution                           |PRI 0430
C     PH2O      DBL   Pressure of H2O (saturation curve)                    |PRI 0440
C     PH2S      DBL   (Partial) pressure of H2S .. calculated               |PRI 0450
C     PNH3      DBL   (Partial) pressure of NH3 .. calculated               |PRI 0460
C     PRESS     DBL   Total pressure                                        |PRI 0470
C     PSS       DBL   Total Pressure for printing                           |PRI 0480
C     SCO2      DBL   TIC                                                   |PRI 0490
C     SUM2      DBL   Storage for printing                                  |PRI 0500
C     SUM3      DBL   Storage for printing                                  |PRI 0510
C     T         DBL   Temperature in K                                      |PRI 0520
C     TDS       DBL   Total Dissolved Solids   (UNITS = KG/L)               |PRI 0530
C     TEMP      DBL   Temperature of the solution when pH was measured      |PRI 0540
C     TITLE     CHA   Name of the sample                                    |PRI 0550
C     TITMIX    CHA   Title for mixing runs                                 |PRI 0560
C     TITR      DBL   Iteration array in DISTRB, used for guesses           |PRI 0570
C     TOTEL     DBL   Contains HTOT, OHTOT and Sum CO2                      |PRI 0580
C     UNITS     CHA   Units of concentration                                |PRI 0590
C     UNO       INT   File unit assigned for output file                    |PRI 0600
C     Z         INT   Charge of aqueous species                             |PRI 0610
C -------------------------------------------------------------------------|PRI 0620
                                                                           PRI 0630
      INTEGER NMAX, UNO                                                    PRI 0640
      DOUBLE PRECISION CPUMIN                                              PRI 0650
      PARAMETER (NMAX = 340, UNO = 6, CPUMIN = 1.0D-35)                    PRI 0660
                                                                           PRI 0670
      INTEGER I, IPAGE, IPGLN, MXSP, Z(NMAX)                               PRI 0680
                                                                           PRI 0690
      DOUBLE PRECISION GAMMA(NMAX), GFW(NMAX), T                           PRI 0700
                                                                           PRI 0710
      CHARACTER *  1 CR, TOF                                               PRI 0720
      CHARACTER *  5 UNITS                                                 PRI 0730
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                 PRI 0740
      CHARACTER * 40 TITMIX                                                PRI 0750
      CHARACTER * 80 TITLE                                                 PRI 0760
                                                                           PRI 0770
      DOUBLE PRECISION ALFA(NMAX), ALK1, ALK2, ALK3                        PRI 0780
      DOUBLE PRECISION ALK7, ANALM(NMAX), Cl                               PRI 0790
      DOUBLE PRECISION CAR1, CAR4, CFLG                                    PRI 0800
      DOUBLE PRECISION CU, CUNITS(NMAX), DENS                              PRI 0810
      DOUBLE PRECISION DUM1, DUM2, DUM3                                    PRI 0820
      DOUBLE PRECISION EHM, EXELT(35), HTOT                                PRI 0830
      DOUBLE PRECISION KHCH4, KHCO2, KHH2S, KHNH3, M(NMAX), MNACLD         PRI 0840
      DOUBLE PRECISION MU, OHTOT, PCO2, PCH4, PH, PH2O, PH2S, PNH3         PRI 0850
      DOUBLE PRECISION PRESS, PSS, SCO2, SUM2, SUM3                        PRI 0860
      DOUBLE PRECISION TDS, TEMP, TITR(11), TOTEL(5)                       PRI 0870
                                                                           PRI 0880
      EXTERNAL KHCO2, KHCH4, KHH2S, KHNH3, PAGE                            PRI 0890
                                                                           PRI 0900
      INTRINSIC DMAX1, DLOG10                                              PRI 0910
                                                                           PRI 0920
      COMMON /EXTOT / EXELT, TOTEL, TITR                                   PRI 0930
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      COMMON /FMFD  / TOF, CR, TITMIX                                    PRI 0940
      COMMON /FORM  / IPAGE, IPGLN                                       PRI 0950
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                         PRI 0960
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                PRI 0970
                                                                         PRI 0980
C ========================================================================|PRI 0990
                                                                         PRI 1000
      T = TEMP + 273.15                                                  PRI 1010
                                                                         PRI 1020
      TOTEL(1) = HTOT                                                    PRI 1030
      TOTEL(2) = OHTOT                                                   PRI 1040
      TOTEL(3) = SCO2                                                    PRI 1050
                                                                         PRI 1060
      CALL PAGE                                                          PRI 1070
      WRITE (UNO, 1060) TITLE, TITMIX                                    PRI 1080
      WRITE (UNO, 1070)                                                  PRI 1090
      WRITE (UNO, 1080) CR                                               PRI 1100
      IPGLN = IPGLN + 4                                                  PRI 1110
                                                                         PRI 1120
C -----------------------------------------------------------------------|PRI 1130
C     Calculation of analytical cation-anion balance.                    |PRI 1140
C     Printing of pH, Eh, temperature, and balance                       |PRI 1150
C -----------------------------------------------------------------------|PRI 1160
                                                                         PRI 1170
      DUM1 = 0.0D0                                                       PRI 1180
      DUM2 = 0.0D0                                                       PRI 1190
      DO 50 I = 1, MXSP + 44                                             PRI 1200
        IF (Z(I) .GT. 0) THEN                                            PRI 1210
          DUM1 = DUM1 + (Z(I) * ANALM(I))                                PRI 1220
        ELSE                                                             PRI 1230
          DUM2 = DUM2 - (Z(I) * ANALM(I))                                PRI 1240
        END IF                                                           PRI 1250
   50 CONTINUE                                                           PRI 1260
      DUM1 = DUM1 * (DENS - TDS) * 1.0D03                                PRI 1270
      DUM2 = DUM2 * (DENS - TDS) * 1.0D03                                PRI 1280
                                                                         PRI 1290
      WRITE (UNO,1090) PH, EHM, TEMP, DUM1, DUM2, (DUM1 - DUM2)          PRI 1300
      IPGLN = IPGLN + 1                                                  PRI 1310
                                                                         PRI 1320
C -----------------------------------------------------------------------|PRI 1330
C     Calculation of partial pressures                                   |PRI 1340
C -----------------------------------------------------------------------|PRI 1350
                                                                         PRI 1360
      PCO2 = 0.0D0                                                       PRI 1370
      PNH3 = 0.0D0                                                       PRI 1380
      PCH4 = 0.0D0                                                       PRI 1390
      PH2S = 0.0D0                                                       PRI 1400
                                                                         PRI 1410
      IF (M(97)  .GE. CPUMIN) PCO2 = M(97)  * KHCO2(T, MNACLD)           PRI 1420
      IF (M(33)  .GE. CPUMIN) PH2S = M(33)  * KHH2S(T, MNACLD)           PRI 1430
      IF (M(285) .GE. CPUMIN) PCH4 = M(285) * KHCH4(T, MNACLD, 1.0D00)   PRI 1440
      IF (M(147) .GE. CPUMIN) PNH3 = M(147) * KHNH3(T)                   PRI 1450
                                                                         PRI 1460
      PSS = DMAX1( 1.0D00, PH2O, PRESS)                                  PRI 1470
                                                                         PRI 1480
C -----------------------------------------------------------------------|PRI 1490
C     Recalculation of cation-anion balance.                             |PRI 1500
C -----------------------------------------------------------------------|PRI 1510
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                                                                      PRI 1520
      DUM1 = 0.0D0                                                    PRI 1530
      DUM2 = 0.0D0                                                    PRI 1540
                                                                      PRI 1550
      DO 10 I = 1, MXSP + 44                                          PRI 1560
        IF (M(I) .LT. CPUMIN) M(I) = 0.0                              PRI 1570
        IF (Z(I) .LT. 0.0) THEN                                       PRI 1580
          DUM2 = DUM2 - (Z(I) * M(I))                                 PRI 1590
        ELSE                                                          PRI 1600
          DUM1 = DUM1 + (Z(I) * M(I))                                 PRI 1610
        END IF                                                        PRI 1620
   10 CONTINUE                                                        PRI 1630
                                                                      PRI 1640
C -----------------------------------------------------------------|PRI 1650
C     Print total inorganic carbon as mg/l, ppm, and molality      |PRI 1660
C -----------------------------------------------------------------|PRI 1670
                                                                      PRI 1680
      DUM1 = DUM1 * (DENS - TDS) * 1.0D03                             PRI 1690
      DUM2 = DUM2 * (DENS - TDS) * 1.0D03                             PRI 1700
      WRITE (UNO, 1100) DUM1, DUM2,  (DUM1 - DUM2),                   PRI 1710
     .                  HTOT, OHTOT, (HTOT - OHTOT)                  PRI 1720
      WRITE (UNO, 1000)                                               PRI 1730
      WRITE (UNO, 1010)                                               PRI 1740
      WRITE (UNO, 1190) CR                                            PRI 1750
      WRITE (UNO, 1020) DENS, (TDS * 1.0D6), MU, ALFA(10), PSS,       PRI 1760
     .                  PH2O, PCO2, PH2S, PCH4, PNH3                 PRI 1770
      IPGLN = IPGLN + 5                                               PRI 1780
                                                                      PRI 1790
      SUM2 = M(7)  + M(52) + M(56)  + M(121) +  M(132) +  M(139)      PRI 1800
     .             + M(156)                                         PRI 1810
      SUM3 = M(98) + M(51)  + M(55)  + M(114) +  M(120) +  M(138)     PRI 1820
     .             + M(140) + M(155) + M(207) + 2*M(208) + 3*M(209)  PRI 1830
                                                                      PRI 1840
      DUM2 = SUM2 * 6.102D4 * (DENS - TDS)                            PRI 1850
      DUM3 = SUM3 * 6.001D4 * (DENS - TDS)                            PRI 1860
      DUM1 = DUM2 / DENS                                              PRI 1870
      ALK7 =       M(9)  +     M(28) + 3.0*M(29) +     M(38) +       PRI 1880
     .       2.0*M(39) + 4.0*M(40) +     M(48) + 3.0*M(50) +         PRI 1890
     .           M(53) +     M(57) +     M(69) +     M(75) +         PRI 1900
     .       2.0*M(76) +     M(77) +     M(85) + 2.0*M(86) +         PRI 1910
     .       3.0*M(87) + 4.0*M(88) +     M(89) + 2.0*M(90) +         PRI 1920
     .           M(91) + 2.0*M(92) + 2.0*M(93) +     M(94) +         PRI 1930
     .       2.0*M(99)                                              PRI 1940
      ALK7 = ALK7       +                                           PRI 1950
     .           M(100) +     M(101) + 2.0*M(102) +     M(103) +    PRI 1960
     .           M(118) +     M(123) +     M(135) +     M(147) +    PRI 1970
     .           M(154) +     M(165) + 2.0*M(166) +     M(170) +    PRI 1980
     .       2.0*M(171) + 3.0*M(172) + 4.0*M(173) + 5.0*M(174) +    PRI 1990
     .       2.0*M(182) + 4.0*M(183) + 6.0*M(184) + 8.0*M(185) +    PRI 2000
     .      15.0*M(188) +     M(189) + 2.0*M(190) + 2.0*M(191) +    PRI 2010
     .       5.0*M(192) + 7.0*M(193)                                PRI 2020
      ALK7 = ALK7       +                                           PRI 2030
     .           M(201) + 2.0*M(202) + 2.0*M(203) +     M(204) +    PRI 2040
     .       2.0*M(205) + 3.0*M(206) + 4.0*M(212) + 3.0*M(213) +    PRI 2050
     .       2.0*M(214) +     M(215) + 3.0*M(217) +     M(220) +    PRI 2060
     .           M(221) + 3.0*M(222) +     M(223) +     M(234) +    PRI 2070
     .           M(239) + 2.0*M(240) +     M(243) +     M(245) +    PRI 2080
     .           M(246) +    .M(250) +     M(258) + 2.0*M(259)      PRI 2090
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      ALK7 = ALK7        +                                                  PRI 2100
     .        2.0*M(265) +     M(266) +     M(269) +     M(289) +          PRI 2110
     .            M(293) + 2.0*M(294) +     M(295)                         PRI 2120
      ALK7 = ALK7        +     M(MXSP+34) +     M(MXSP+35) +               PRI 2130
     .        3.0*M(MXSP+36) + M(MXSP+38) + 2.0*M(MXSP+39) +               PRI 2140
     .        2.0*M(MXSP+41) + M(MXSP+40) + 2.0*M(MXSP+42)                 PRI 2150
                                                                           PRI 2160
      ALK7 = ALK7            +   SUM2     + 2.0*SUM3                      PRI 2170
                                                                           PRI 2180
      ALK1 = ALK7 *  61.02 * 1000.0 * (DENS - TDS)                         PRI 2190
      ALK2 = ALK7 *  60.01 *  500.0 * (DENS - TDS)                         PRI 2200
      ALK3 = ALK7 * 100.08 *  500.0 * (DENS - TDS)                         PRI 2210
                                                                           PRI 2220
      CAR1 = 12.011D03 * SCO2 * (DENS - TDS)                               PRI 2230
      CAR4 = M(97) * GFW(97) * 1000.0 * (DENS - TDS)                       PRI 2240
                                                                           PRI 2250
C -------------------------------------------------------------------------|PRI 2260
C     Print solute data.                                                   |PRI 2270
C -------------------------------------------------------------------------|PRI 2280
                                                                           PRI 2290
      WRITE (UNO, 1110)                                                    PRI 2300
      WRITE (UNO, 1120) CR                                                 PRI 2310
      WRITE (UNO, 1130)                                                    PRI 2320
      WRITE (UNO, 1140) CR                                                 PRI 2330
      WRITE (UNO, 1150)                                                    PRI 2340
                                                                           PRI 2350
      WRITE (UNO, 1160) ALK1,  ALK2, ALK3, CAR1, (DUM2 + 2.0*DUM3),        PRI 2360
                        CAR4,  DUM2, DUM3                                  PRI 2370
                                                                           PRI 2380
      ALK1 = ALK1 / DENS                                                   PRI 2390
      ALK2 = ALK2 / DENS                                                   PRI 2400
      ALK3 = ALK3 / DENS                                                   PRI 2410
      CAR1 = CAR1 / DENS                                                   PRI 2420
      CAR4 = CAR4 / DENS                                                   PRI 2430
      DUM3 = DUM3 / DENS                                                   PRI 2440
                                                                           PRI 2450
      WRITE (UNO, 1170) ALK1,  ALK2, ALK3, CAR1, (DUM1 + 2.0*DUM3),        PRI 2460
                        CAR4,  DUM1, DUM3                                  PRI 2470
                                                                           PRI 2480
      WRITE (UNO, 1180) ALK7,  (ALK7/2.0), (ALK7/2.0), SCO2,               PRI 2490
                       (SUM2 + 2.0*SUM3), M(97), SUM2, SUM3                PRI 2500
                                                                           PRI 2510
      IPGLN = IPGLN + 8                                                    PRI 2520
                                                                           PRI 2530
      WRITE (UNO, 1030)                                                    PRI 2540
      WRITE (UNO, 1200)                                                    PRI 2550
      WRITE (UNO, 1210) CR                                                 PRI 2560
      IPGLN = IPGLN + 4                                                    PRI 2570
                                                                           PRI 2580
      DO 20 I = 1, MXSP + 44                                               PRI 2590
        CFLG = CUNITS(I)                                                   PRI 2600
        IF (CFLG .LT. CPUMIN .AND. M(I) .LT. CPUMIN) GO TO 20              PRI 2610
        C1  = 0.0D0                                                        PRI 2620
        CU  = 0.0D0                                                        PRI 2630
        IF (ALFA(I) .GT. CPUMIN) C1 = -DLOG10(ALFA(I))                     PRI 2640
                                                                           PRI 2650
        IF (CFLG .GE. CPUMIN) THEN                                         PRI 2660
          IF      (UNITS .EQ. 'MG/L ') THEN                                PRI 2670
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          CU   = CFLG / DENS                                                PRI 2680
        ELSE IF (UNITS .EQ. 'PPM  ') THEN                                   PRI 2690
          CU   = CFLG                                                       PRI 2700
          CFLG = CFLG * DENS                                                PRI 2710
        ELSE                                                                PRI 2720
          CU   = 1.0E3 * ANALM(I) * GFW(I) * (DENS-TDS) / DENS              PRI 2730
          CFLG = CU   * DENS                                                PRI 2740
        END IF                                                              PRI 2750
      END IF                                                                PRI 2760
                                                                            PRI 2770
      DUM2 = 1.0E3 * M(I) * GFW(I) * (DENS-TDS)                             PRI 2780
      DUM1 = DUM2   / DENS                                                  PRI 2790
                                                                            PRI 2800
      IF (IPGLN .GT. 59) THEN                                               PRI 2810
        CALL PAGE                                                           PRI 2820
        WRITE (UNO, 1030)                                                   PRI 2830
        WRITE (UNO, 1200)                                                   PRI 2840
        WRITE (UNO, 1210) CR                                                PRI 2850
        IPGLN = IPGLN + 3                                                   PRI 2860
      END IF                                                                PRI 2870
                                                                            PRI 2880
      IF(I .EQ. 12 .OR. I .EQ. 32)  THEN                                    PRI 2890
        WRITE (UNO, 1040) I, PAGE1(I), CU, CFLG, ANALM(I)                   PRI 2900
      ELSE IF(ANALM(I) .GT. CPUMIN) THEN                                    PRI 2910
        WRITE (UNO, 1040) I, PAGE1(I), CU, CFLG, ANALM(I),                  PRI 2920
     .                    DUM1, DUM2, M(I), ALFA(I), GAMMA(I), C1          PRI 2930
      ELSE                                                                  PRI 2940
        WRITE (UNO, 1050) I, PAGE1(I), DUM1, DUM2, M(I), ALFA(I),           PRI 2950
     .                    GAMMA(I), C1                                      PRI 2960
      END IF                                                                PRI 2970
                                                                            PRI 2980
      IPGLN = IPGLN + 1                                                     PRI 2990
   20 CONTINUE                                                              PRI 3000
                                                                            PRI 3010
      RETURN                                                                PRI 3020
                                                                            PRI 3030
 1000 FORMAT (/, 58X, 28('-'), 'PRESSURE', 28('-'), /,                      PRI 3040
     .            2X, 'DENSITY AT',2X,'TOTAL DISSOLVED', 5X, 'IONIC',    PRI 3050
     .            7X, 'ACTIVITY', 4X, 'P TOTAL', 7X, 'PH2O', 7X,         PRI 3060
     .            'PCO2', 7X, 'PH2S', 7X, 'PCH4', 7X, 'PNH3')            PRI 3070
 1010 FORMAT (4X, 'INPUT T', 4X, 'SOLIDS (MG/L)', 5X, 'STRENGTH',          PRI 3080
     .        5X, 'OF WATER', 5X, '(BARS)', 6X, '(BARS)', 5X, '(BARS)',  PRI 3090
     .        5X, '(BARS)', 5X, '(BARS)', 5X, '(BARS)', A1)              PRI 3100
 1020 FORMAT (2X, F9.4, 5X, F12.2, F13.5, 2X, F11.4, 3X, F10.4,            PRI 3110
     .        3X, E10.4, 4(1X, E10.4))                                   PRI 3120
 1030 FORMAT (19X, '-----------------ANALYZED-----------',                 PRI 3130
     .         3X, '---------------CALCULATED-----------',                PRI 3140
     .        17X, 'ACTIVITY', 5X, '-LOG10')                             PRI 3150
 1040 FORMAT (2X, I3, 2X, A8, 1X, 2F13.4, 5E13.4, F12.4, F11.4)           PRI 3160
 1050 FORMAT (2X, I3, 2X, A8, 40X, 4E13.4, F12.4, F11.4)                  PRI 3170
 1060 FORMAT (' SAMPLE IDENT:- ', A80, /, 20X, A40)                       PRI 3180
 1070 FORMAT (/, 4X, 'PH', 9X, 'EH', 7X, 'TEMP', 18X, 'CATIONS',          PRI 3190
     .           6X, 'ANIONS', 2X, 'DIFFERENCE (MEQ/L)',                  PRI 3200
     .          12X, '--- H - OH BALANCE (MOLES) -------')                PRI 3210
 1080 FORMAT (A1, 2X, '____', 6X, '______', 5X, '_____', 13X,             PRI 3220
     .            '_____________________________________________')        PRI 3230
 1090 FORMAT (1X, F6.2,  2X, F10.4, 2X, F8.2,   8X, 'ANAL=', 1X,          PRI 3240
               F10.4, 2X, F10.4, 2X, F10.4, 20X, 'HTOT',  8X,           PRI 3250
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                'OHTOT', 5X, 'DIFFERENCE')                                      PRI 3260
 1100 FORMAT (37X, 'CALC=', 1X, F10.4, 2X, F10.4, 2X, F10.4,                    PRI 3270
     .                  18X, E10.4, 2X, E10.4, 2X, E10.4)                       PRI 3280
 1110 FORMAT (/,  72X, 'Dissolved Inorganic Carbon')                            PRI 3290
 1120 FORMAT (A1, 71X, '_____________________________')                         PRI 3300
 1130 FORMAT (21X, 'Total Alkalinity as', 20X, 'as', 8X, 'HCO3-',               PRI 3310
     .         7X, 'H2CO3', 5X, 'Sum of', 5X, 'Sum of')                        PRI 3320
 1140 FORMAT (A1, 20X, '____________________')                                  PRI 3330
 1150 FORMAT (17X, 'HCO3-', 5X, 'CO3=', 7X, 'CaCO3', 17X, 'TIC',               PRI 3340
     .         5X, 'Alkalinity', 3X, 'species', 5X, 'HCO3-', 6X,               PRI 3350
     .         'CO3=')                                                         PRI 3360
 1160 FORMAT (7X, '(MG/L)=',      3(E10.4,1X), 10X, 5(E10.4, 1X))               PRI 3370
 1170 FORMAT (8X, '(PPM)=',       3(E10.4,1X), 10X, 5(E10.4, 1X))               PRI 3380
 1180 FORMAT (3X, '(MOLALITY)=', 3(E10.4,1X), 10X, 5(E10.4, 1X))                PRI 3390
 1190 FORMAT (A1, 3X,'_______',  4X,'_____________', 5X,'________',             PRI 3400
     .            5X,'________', 3X,'___________', 2X,'___________',           PRI 3410
     .            4(1X,'_________'))                                           PRI 3420
 1200 FORMAT (7X, 'SPECIES', 9X, 'PPM', 9X, 'MG/L', 7X, 'MOLALITY',             PRI 3430
     .        8X, 'PPM', 9X, 'MG/L', 7X, 'MOLALITY', 5X, 'ACTIVITY',           PRI 3440
     .        7X, 'COEFF.', 3X, 'ACTIVITY')                                    PRI 3450
 1210 FORMAT (A1, 6X, '_______', 5X, '__________', 2X, '___________',           PRI 3460
     .            3X, '__________', 3X, '__________', 3X, '__________',       PRI 3470
     .            3X, '__________', 3X, '__________', 4X, '________',         PRI 3480
     .            3X, '________')                                              PRI 3490
                                                                                PRI 3500
      END                                                                       PRI 3510
```

```
      SUBROUTINE PRNTAB (TITLE, TEMP, MXAQK)                                    PRN 0010
C ================================================================================|PRN 0020
C     Print out of tables.                                                        |PRN 0030
C --------------------------------------------------------------------------------|PRN 0040
C     I         INT   Loop variable                                             |PRN 0050
C     LOGKT1    DBL   Log K for aqueous species at specified temp.              |PRN 0060
C     MXAQK     INT   Total number of aqueous log k values                      |PRN 0070
C     NMAX      INT   General array dimension to allow easy expansion           |PRN 0080
C     PAGE1     CHA   Names of aqueous species                                  |PRN 0090
C     PAGE2     CHA   Names of equilibrium constants                            |PRN 0100
C     TEMP      DBL   Temperature of the solution when pH was measured          |PRN 0110
C     TITLE     CHA   Name of the sample                                        |PRN 0120
C     TOF       CHA   Places a form feed in output file                         |PRN 0130
C     UNO       INT   File unit assigned for output file                        |PRN 0140
C --------------------------------------------------------------------------------|PRN 0150
                                                                                PRN 0160
      INTEGER NMAX, UNO                                                         PRN 0170
      PARAMETER (NMAX = 340, UNO = 6)                                           PRN 0180
                                                                                PRN 0190
      INTEGER I, IPAGE, IPGLN, J, MXAQK                                         PRN 0200
                                                                                PRN 0210
      CHARACTER *  1 TOF, CR                                                    PRN 0220
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                      PRN 0230
      CHARACTER * 40 TITMIX                                                     PRN 0240
      CHARACTER * 80 TITLE                                                      PRN 0250
                                                                                PRN 0260
      DOUBLE PRECISION LOGKT1(NMAX), LOGKT2(NMAX)                               PRN 0270
```

```
      DOUBLE PRECISION TEMP                                                  PRN 0280
                                                                             PRN 0290
      EXTERNAL PAGE                                                          PRN 0300
                                                                             PRN 0310
      COMMON /ALOGK / LOGKT1, LOGKT2                                         PRN 0320
      COMMON /FMFD  / TOF, CR, TITMIX                                        PRN 0330
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                    PRN 0340
      COMMON /FORM  / IPAGE, IPGLN                                           PRN 0350
                                                                             PRN 0360
C ============================================================================|PRN 0370
                                                                             PRN 0380
      J = ((MXAQK - 1) / 3) + 1                                              PRN 0390
                                                                             PRN 0400
      DO 10 I = 1, J                                                         PRN 0410
        IF (I .EQ. 1 .OR. IPGLN .GT. 57) THEN                                PRN 0420
          CALL PAGE                                                          PRN 0430
          WRITE (UNO, 110) TITLE, TEMP                                       PRN 0440
          WRITE (UNO, 120)                                                   PRN 0450
          WRITE (UNO, 130)                                                   PRN 0460
          IPGLN = IPGLN + 9                                                  PRN 0470
        END IF                                                               PRN 0480
        IPGLN = IPGLN + 1                                                    PRN 0490
                                                                             PRN 0500
        IF ((I+J+J) .LE. MXAQK) THEN                                         PRN 0510
          WRITE (UNO, 140) I,     PAGE2(I),     LOGKT1(I),                   PRN 0520
                           I+J,   PAGE2(I+J),   LOGKT1(I+J),                 PRN 0530
                           I+J+J, PAGE2(I+J+J), LOGKT1(I+J+J)                PRN 0540
        ELSE IF ((I+J) .LE. (MXAQK - (J - 1))) THEN                          PRN 0550
          WRITE (UNO, 140) I,     PAGE2(I),     LOGKT1(I),                   PRN 0560
                           I+J,   PAGE2(I+J),   LOGKT1(I+J)                  PRN 0570
        ELSE                                                                 PRN 0580
          WRITE (UNO, 140) I,     PAGE2(I),     LOGKT1(I)                    PRN 0590
        END IF                                                               PRN 0600
                                                                             PRN 0610
   10 CONTINUE                                                               PRN 0620
                                                                             PRN 0630
      RETURN                                                                 PRN 0640
                                                                             PRN 0650
  110 FORMAT (' SAMPLE IDENT:- ', A80, /, '  TEMPERATURE = ',F6.2,' C')      PRN 0660
  120 FORMAT (//,5X,'**TABLE OF LOG(KT) FOR THE AQUEOUS COMPLEXES**',/)      PRN 0670
  130 FORMAT (/, 3(3X, 'I  ','SPECIES', 11X, 'LOG K ',10X),/)                PRN 0680
  140 FORMAT (1X,3(I3, 2X, A8, 3X, F12.4, 12X))                              PRN 0690
                                                                             PRN 0700
      END                                                                    PRN 0710
```

```
      SUBROUTINE PSAT (TC, PS)                                               PSA 0010
C ============================================================================|PSA 0020
C     Calculates the saturation pressure for water                           |PSA 0030
C     (Keenan and others, 1969)                                              |PSA 0040
C ----------------------------------------------------------------------------|PSA 0050
C     F         DBL     Fit Coefficients                                     |PSA 0060
C     I         INT     Loop index                                           |PSA 0070
C     PCRT      DBL     Critical pressure (bars)                             |PSA 0080
C     PS        DBL     Saturation pressure                                  |PSA 0090
```

```
C     S          DBL     Temperary storage                                    |PSA 0100
C     TC         DBL     Temperature in deg. C                                |PSA 0110
C     TCRT       DBL     Critical Temperature (deg C)                         |PSA 0120
C     TR         DBL     1.0 / Termperature in deg K                          |PSA 0130
C -------------------------------------------------------------------------|PSA 0140
                                                                             PSA 0150
      INTEGER I                                                              PSA 0160
                                                                             PSA 0170
      DOUBLE PRECISION F(8), PCRT, PS, S, TC, TCRT, TR                       PSA 0180
                                                                             PSA 0190
      INTRINSIC DEXP                                                         PSA 0200
                                                                             PSA 0210
      PARAMETER (TCRT=374.136D00, PCRT=220.88D00)                            PSA 0220
                                                                             PSA 0230
      DATA F /-741.9242D0, -29.721D0, -11.55286D0, -8.685635D-1,             PSA 0240
               1.094098D-1, 4.3999D-1, 2.520658D-1, 5.218684D-2/             PSA 0250
                                                                             PSA 0260
C =========================================================================|PSA 0270
                                                                             PSA 0280
      TR = 1.0D03 / (TC + 273.15D00)                                         PSA 0290
                                                                             PSA 0300
      S  = 0.0D0                                                             PSA 0310
      DO 10 I = 1, 8                                                         PSA 0320
        S = S + F(I) * (0.65 - 0.01 * TC)**(I-1)                             PSA 0330
   10 CONTINUE                                                               PSA 0340
                                                                             PSA 0350
      PS = PCRT * DEXP(1.0D-5 * TR * (TCRT - TC) * S)                        PSA 0360
                                                                             PSA 0370
      RETURN                                                                 PSA 0380
      END                                                                    PSA 0390
```

```
      SUBROUTINE PTZINT (TEMP, TEMP1, B0, B00, B1, B11, CP, CPP, THTC,  PTZ 0010
                         THTCC, THTA, THTAA, PSIC, PSICC, PSIA, PSIAA)  PTZ 0020
C =========================================================================|PTZ 0030
C     This routine calculates the interpolated values of the               |PTZ 0040
C     pitzer coeffiencients for routine pitzer.  It uses the               |PTZ 0050
C     routine tluv to calculate the actual value.                          |PTZ 0060
C -------------------------------------------------------------------------|PTZ 0070
C     Future Modifications                                                 |PTZ 0080
C ------------------------                                                 |PTZ 0090
C     If and when more cation and anion data are incorporated into         |PTZ 0100
C     the data tables the values of the parameters ncat and nani will      |PTZ 0110
C     need to be increased.                                                |PTZ 0120
C -------------------------------------------------------------------------|PTZ 0130
C     History                                                              |PTZ 0140
C -----------                                                              |PTZ 0150
C     J.D. DeBraal           06/87     Initial Coding                      |PTZ 0160
C -------------------------------------------------------------------------|PTZ 0170
C     Local Constants                                                      |PTZ 0180
C -------------------                                                      |PTZ 0190
C     NANI               INT    Number of Anions                          |PTZ 0200
C     NCAT               INT    Number of Cations                         |PTZ 0210
C     NTEM               INT    Number of Temperatures                    |PTZ 0220
C -------------------------------------------------------------------------|PTZ 0230
```

```
C     Declare Constants                                                    |PTZ 0240
C     --------------------                                                 |PTZ 0250
      INTEGER      NANI,     NCAT,      NTEM                               PTZ 0260
      PARAMETER   (NANI = 5, NCAT = 10, NTEM = 11)                         PTZ 0270
C     -------------------------------------------------------------------|PTZ 0280
C     Local Variables                                                      |PTZ 0290
C     -------------------                                                  |PTZ 0300
C     B0      (i,k)      DBL    Beta zero parameter for current temp       |PTZ 0310
C     B00     (i,k,t)    DBL    Array of B0 for all temps                  |PTZ 0320
C     B1      (i,k)      DBL    Beta one parameter for current temp        |PTZ 0330
C     B11     (i,k,t)    DBL    Array of B1 for all temps                  |PTZ 0340
C     CP      (i,k)      DBL    C super phi parameter for current temp     |PTZ 0350
C     CPP     (i,k,t)    DBL    Array of CP for all temps                  |PTZ 0360
C     I                  INT    Cation 1 loop variable                     |PTZ 0370
C     J                  INT    Cation 2 loop variable                     |PTZ 0380
C     K                  INT    Anion 1 loop variable                      |PTZ 0390
C     L                  INT    Anion 2 loop variable                      |PTZ 0400
C     OK                 INT    Error flag used in LAGINT                  |PTZ 0410
C     PSIA    (k,l,i)    DBL    PSI anion-anion-cation parameter           |PTZ 0420
C     PSIAA   (k,l,i,t)  DBL    Array of PSIA for all temps                |PTZ 0430
C     PSIC    (i,j,k)    DBL    PSI cation-cation-anion parameter          |PTZ 0440
C     PSICC   (i,j,k,t)  DBL    Array of PSIC for all temps                |PTZ 0450
C     TB0     (k,t)      DBL    Temporary B0 array with cation constant    |PTZ 0460
C     TB1     (k,t)      DBL    Temporary B1 array with cation constant    |PTZ 0470
C     TCP     (k,t)      DBL    Temporary CP array with cation constant    |PTZ 0480
C     TEMP    (t)        DBL    Array of 11 temperatures                   |PTZ 0490
C     TEMP1              DBL    Temperature of interest                    |PTZ 0500
C     THTA    (i,k)      DBL    Pitzer theta anion parameter               |PTZ 0510
C     THTAA   (i,k,t)    DBL    Array of THTA for all temps                |PTZ 0520
C     THTC    (i,k)      DBL    Pitzer theta cation parameter              |PTZ 0530
C     THTCC   (i,k,t)    DBL    Array of THTC for all temps                |PTZ 0540
C     TMP     (t)        DBL    Interpolated value from LAGINT             |PTZ 0550
C     TP                 INT    Temperature loop variable                  |PTZ 0560
C     TPSIA   (i,t)      DBL    Temporary PSIA with anions constant        |PTZ 0570
C     TPSIC   (k,t)      DBL    Temporary PSIC with cations constant       |PTZ 0580
C     TTHTA   (l,t)      DBL    Temporary THTA with anion 1 constant       |PTZ 0590
C     TTHTC   (j,t)      DBL    Temporary THTC with cation 1 constant      |PTZ 0600
C     -------------------------------------------------------------------|PTZ 0610
C     Declare Variables                                                    |PTZ 0620
C     --------------------                                                 |PTZ 0630
      INTEGER I, J, K, L, OK, TP                                           PTZ 0640
                                                                           PTZ 0650
      DOUBLE PRECISION B0(NCAT,NANI), B00(NCAT,NANI,NTEM)                  PTZ 0660
      DOUBLE PRECISION B1(NCAT,NANI), B11(NCAT,NANI,NTEM)                  PTZ 0670
      DOUBLE PRECISION CP(NCAT,NANI), CPP(NCAT,NANI,NTEM)                  PTZ 0680
      DOUBLE PRECISION PSIA(NANI,NANI,NCAT), PSIAA(NANI,NANI,NCAT,NTEM)    PTZ 0690
      DOUBLE PRECISION PSIC(NCAT,NCAT,NANI), PSICC(NCAT,NCAT,NANI,NTEM)    PTZ 0700
      DOUBLE PRECISION TB0(NANI,NTEM), TB1(NANI,NTEM), TCP(NANI,NTEM)      PTZ 0710
      DOUBLE PRECISION TEMP(NTEM), TEMP1                                   PTZ 0720
      DOUBLE PRECISION THTA(NANI,NANI), THTAA(NANI,NANI,NTEM)              PTZ 0730
      DOUBLE PRECISION THTC(NCAT,NCAT), THTCC(NCAT,NCAT,NTEM)              PTZ 0740
      DOUBLE PRECISION TMP(NCAT)                                           PTZ 0750
      DOUBLE PRECISION TPSIA(NCAT,NTEM), TPSIC(NANI,NTEM)                  PTZ 0760
      DOUBLE PRECISION TTHTA(NANI,NTEM), TTHTC(NCAT,NTEM)                  PTZ 0770
C     -------------------------------------------------------------------|PTZ 0780
C     Routines                                                             |PTZ 0790
C     -------------------------------------------------------------------|PTZ 0800
C     LAGINT             SUB    Calculate a Value for Desired Temp        |PTZ 0810
```

```
C ------------------------------------------------------------------|PTZ 0820
      EXTERNAL LAGINT                                                PTZ 0830
C ------------------------------------------------------------------|PTZ 0840
C     Initialize Variables                                           |PTZ 0850
C ------------------------                                          |PTZ 0860
      DATA TMP /NCAT*0.0/                                            PTZ 0870
C ==================================================================|PTZ 0880
                                                                     PTZ 0890
      DO 40 I = 1, NCAT                                              PTZ 0900
        DO 20 K = 1, NANI                                            PTZ 0910
          DO 10 TP = 1, NTEM                                         PTZ 0920
            TB0(K,TP) = B00(I,K,TP)                                  PTZ 0930
   10     CONTINUE                                                   PTZ 0940
   20   CONTINUE                                                     PTZ 0950
                                                                     PTZ 0960
        CALL LAGINT (TEMP, TB0, TEMP1, TMP, NANI, NANI, OK)          PTZ 0970
                                                                     PTZ 0980
        DO 30 K = 1, NANI                                            PTZ 0990
          B0(I,K) = TMP(K)                                           PTZ 1000
   30   CONTINUE                                                     PTZ 1010
   40 CONTINUE                                                       PTZ 1020
                                                                     PTZ 1030
      DO 80 I = 1, NCAT                                              PTZ 1040
        DO 60 K = 1, NANI                                            PTZ 1050
          DO 50 TP = 1, NTEM                                         PTZ 1060
            TB1(K,TP) = B11(I,K,TP)                                  PTZ 1070
   50     CONTINUE                                                   PTZ 1080
   60   CONTINUE                                                     PTZ 1090
                                                                     PTZ 1100
        CALL LAGINT (TEMP, TB1, TEMP1, TMP, NANI, NANI, OK)          PTZ 1110
                                                                     PTZ 1120
        DO 70 K = 1, NANI                                            PTZ 1130
          B1(I,K) = TMP(K)                                           PTZ 1140
   70   CONTINUE                                                     PTZ 1150
   80 CONTINUE                                                       PTZ 1160
                                                                     PTZ 1170
      DO 120 I = 1, NCAT                                             PTZ 1180
        DO 100 K = 1, NANI                                           PTZ 1190
          DO 90 TP = 1, NTEM                                         PTZ 1200
            TCP(K,TP) = CPP(I,K,TP)                                  PTZ 1210
   90     CONTINUE                                                   PTZ 1220
  100   CONTINUE                                                     PTZ 1230
                                                                     PTZ 1240
        CALL LAGINT (TEMP, TCP, TEMP1, TMP, NANI, NANI, OK)          PTZ 1250
                                                                     PTZ 1260
        DO 110 K = 1, NANI                                           PTZ 1270
          CP(I,K) = TMP(K)                                           PTZ 1280
  110   CONTINUE                                                     PTZ 1290
  120 CONTINUE                                                       PTZ 1300
                                                                     PTZ 1310
      DO 160 I = 1, NCAT                                             PTZ 1320
        DO 140 J = 1, NCAT                                           PTZ 1330
          DO 130 TP = 1, NTEM                                        PTZ 1340
            TTHTC(J,TP) = THTCC(I,J,TP)                              PTZ 1350
  130     CONTINUE                                                   PTZ 1360
  140   CONTINUE                                                     PTZ 1370
                                                                     PTZ 1380
        CALL LAGINT (TEMP, TTHTC, TEMP1, TMP, NCAT, NCAT, OK)        PTZ 1390
```

```
                                                                      PTZ 1400
      DO 150 J = 1, NCAT                                              PTZ 1410
        THTC(I,J) = TMP(J)                                            PTZ 1420
150   CONTINUE                                                        PTZ 1430
160 CONTINUE                                                          PTZ 1440
                                                                      PTZ 1450
    DO 200 K = 1, NANI                                                PTZ 1460
      DO 180 L = 1, NANI                                              PTZ 1470
        DO 170 TP = 1, NTEM                                           PTZ 1480
          TTHTA(L,TP) = THTAA(K,L,TP)                                 PTZ 1490
170     CONTINUE                                                      PTZ 1500
180   CONTINUE                                                        PTZ 1510
                                                                      PTZ 1520
      CALL LAGINT (TEMP, TTHTA, TEMP1, TMP, NCAT, NCAT, OK)           PTZ 1530
                                                                      PTZ 1540
      DO 190 L = 1, NANI                                              PTZ 1550
        THTA(K,L) = TMP(L)                                            PTZ 1560
190   CONTINUE                                                        PTZ 1570
200 CONTINUE                                                          PTZ 1580
                                                                      PTZ 1590
    DO 250 I = 1, NCAT                                                PTZ 1600
      DO 240 J = 1, NCAT                                              PTZ 1610
        DO 220 K = 1, NANI                                            PTZ 1620
          DO 210 TP = 1, NTEM                                         PTZ 1630
            TPSIC(K,TP) = PSICC(I,J,K,TP)                             PTZ 1640
210       CONTINUE                                                    PTZ 1650
220     CONTINUE                                                      PTZ 1660
                                                                      PTZ 1670
        CALL LAGINT (TEMP, TPSIC, TEMP1, TMP, NANI, NANI, OK)         PTZ 1680
                                                                      PTZ 1690
        DO 230 K = 1, NANI                                            PTZ 1700
          PSIC(I,J,K) = TMP(K)                                        PTZ 1710
230     CONTINUE                                                      PTZ 1720
240   CONTINUE                                                        PTZ 1730
250 CONTINUE                                                          PTZ 1740
                                                                      PTZ 1750
    DO 300 K = 1, NANI                                                PTZ 1760
      DO 290 L = 1, NANI                                              PTZ 1770
        DO 270 I = 1, NCAT                                            PTZ 1780
          DO 260 TP = 1, NTEM                                         PTZ 1790
            TPSIA(I,TP) = PSIAA(K,L,I,TP)                             PTZ 1800
260       CONTINUE                                                    PTZ 1810
270     CONTINUE                                                      PTZ 1820
                                                                      PTZ 1830
        CALL LAGINT (TEMP, TPSIA, TEMP1, TMP, NCAT, NCAT, OK)         PTZ 1840
                                                                      PTZ 1850
        DO 280 I = 1, NCAT                                            PTZ 1860
          PSIA(K,L,I) = TMP(K)                                        PTZ 1870
280     CONTINUE                                                      PTZ 1880
290   CONTINUE                                                        PTZ 1890
300 CONTINUE                                                          PTZ 1900
                                                                      PTZ 1910
    RETURN                                                            PTZ 1920
    END                                                               PTZ 1930
```

```
      DOUBLE PRECISION FUNCTION SEXP10 (X)                                SEX 0010
C ================================================================================|SEX 0020
C     If a number is too small to be raised to the power of ten,            |SEX 0030
C       return zero, else raise it.                                         |SEX 0040
C --------------------------------------------------------------------------|SEX 0050
                                                                            SEX 0060
      DOUBLE PRECISION X, CPUMIN, CPUMAX                                    SEX 0070
      PARAMETER (CPUMIN = 1.0D-35, CPUMAX = 1.0D+35)                        SEX 0080
      INTRINSIC DLOG10                                                      SEX 0090
                                                                            SEX 0100
C ================================================================================|SEX 0110
                                                                            SEX 0120
      IF (X .GT. DLOG10(CPUMIN) .AND. X .LT. DLOG10(CPUMAX)) THEN           SEX 0130
          SEXP10 = 10.0D00**X                                               SEX 0140
      ELSE                                                                  SEX 0150
          SEXP10 = 0.0D00                                                   SEX 0160
      END IF                                                                SEX 0170
                                                                            SEX 0180
      RETURN                                                                SEX 0190
      END                                                                   SEX 0200
```

```
      DOUBLE PRECISION FUNCTION SLOG10(X)                                 SLO 0010
C ================================================================================|SLO 0020
C     If a number is too small to have it's log taken, return -999          |SLO 0030
C --------------------------------------------------------------------------|SLO 0040
                                                                            SLO 0050
      DOUBLE PRECISION X, CPUMIN                                            SLO 0060
      PARAMETER (CPUMIN = 1.0D-35)                                          SLO 0070
      INTRINSIC DLOG10                                                      SLO 0080
                                                                            SLO 0090
C ================================================================================|SLO 0100
                                                                            SLO 0110
      IF (X .GT. CPUMIN) THEN                                               SLO 0120
          SLOG10 = DLOG10(X)                                                SLO 0130
      ELSE                                                                  SLO 0140
          SLOG10 = -999.9D00                                                SLO 0150
      END IF                                                                SLO 0160
                                                                            SLO 0170
      RETURN                                                                SLO 0180
      END                                                                   SLO 0190
```

```
      SUBROUTINE SORTA (A, B, INUM, IPOINT)                               SOR 0010
C ================================================================================|SOR 0020
C     A utility routine to sort arrays before using GUESS                   |SOR 0030
C --------------------------------------------------------------------------|SOR 0040
C     A          DBL   Array to be sorted based on matching value in B     |SOR 0050
C     B          DBL   Sort this array (smallest to largest)               |SOR 0060
C     I          INT   Index counter                                       |SOR 0070
C     INUM       INT   Number of points to sort                            |SOR 0080
C     IPOINT     INT   Pointer to specific entry ... return                |SOR 0090
```

```
C                       new position                                    |SOR 0100
C     J         INT   Index counter                                     |SOR 0110
C     X         DBL   Temporary storage                                 |SOR 0120
C -------------------------------------------------------------------- |SOR 0130
                                                                        SOR 0140
      INTEGER INUM, IPOINT, I, J                                        SOR 0150
      DOUBLE PRECISION A(*), B(*), X                                    SOR 0160
                                                                        SOR 0170
C ==================================================================== |SOR 0180
                                                                        SOR 0190
      IF (INUM .LE. 1) RETURN                                           SOR 0200
                                                                        SOR 0210
      DO 200 I = 1, (INUM-1)                                            SOR 0220
        DO 100 J = (I+1), INUM                                          SOR 0230
          IF (B(I) .GT. B(J)) THEN                                      SOR 0240
            X    = A(J)                                                 SOR 0250
            A(J) = A(I)                                                 SOR 0260
            A(I) = X                                                    SOR 0270
            X    = B(J)                                                 SOR 0280
            B(J) = B(I)                                                 SOR 0290
            B(I) = X                                                    SOR 0300
            IF (IPOINT .EQ. I) THEN                                     SOR 0310
              IPOINT = J                                                SOR 0320
            ELSE IF (IPOINT .EQ. J) THEN                                SOR 0330
              IPOINT = I                                                SOR 0340
            END IF                                                      SOR 0350
          END IF                                                        SOR 0360
  100   CONTINUE                                                        SOR 0370
  200 CONTINUE                                                          SOR 0380
                                                                        SOR 0390
      RETURN                                                            SOR 0400
      END                                                               SOR 0410
```

```
      SUBROUTINE STORE (TEMP, HITEMP)                                   STO 0010
C ==================================================================== |STO 0020
C     Writes out current data values to create a restart file           |STO 0030
C -------------------------------------------------------------------- |STO 0040
C     ADEX      INT   Flag for surface chemistry option                 |STO 0050
C     ALFA      DBL   Activity of aqueous species i                     |STO 0060
C     ALK       INT   Flag for distribution of carbonate species        |STO 0070
C     AMOL      DBL   Molality of aqueous/mineral species added         |STO 0080
C     ANALM     DBL   Analyzed molality of species i                    |STO 0090
C     ANS1      INT   Number of complexes for added anion #1            |STO 0100
C     ANS2      INT   Number of complexes for added anion #2            |STO 0110
C     CEC       DBL   Cation exchange capacity                          |STO 0120
C     COEF      DBL   Stoichiometric coefficient and Id number          |STO 0130
C     CONV1     DBL   Tolerance factor for convergence of anions        |STO 0140
C     CONV2     DBL   Tolerance factor for hydronium mass-balance       |STO 0150
C     CPUMIN    DBL   Smallest positive real value program uses         |STO 0160
C     CUNITS    DBL   Analytical input concentration                    |STO 0170
C     DCH4      DBL   Concentration of CH4 lost up annulas              |STO 0180
C     DDCH4     DBL   Concentration of CH4 lost before pH measurement   |STO 0190
C     DCO2      DBL   Concentration of CO2 lost up annulas              |STO 0200
C     DDCO2     DBL   Concentration of CO2 lost before pH measurement   |STO 0210
```

```
C     DH2S      DBL   Concentration of H2S lost up annulas                |STO 0220
C     DDH2S     DBL   Concentration of H2S lost before pH measurement     |STO 0230
C     DNH3      DBL   Concentration of NH3 lost up annulas                |STO 0240
C     DDNH3     DBL   Concentration of NH3 lost before pH measurement     |STO 0250
C     DENS      DBL   Density                                             |STO 0260
C     DFRAC1    DBL   Smallest fraction of soln 1 mixed with soln 2       |STO 0270
C     DHA       DBL   Ion size parameter                                  |STO 0280
C     DINC      DBL   Increment of solution 1 to be added                 |STO 0290
C     DP        DBL   Dissolution/precipitation switch                    |STO 0300
C     DSEP      DBL   Density of oil at 15 degree C                       |STO 0310
C     EHM       DBL   Measured Eh in volts                                |STO 0320
C     EHMC      DBL   Measured Eh using the Calomel electrode             |STO 0330
C     EMFZSC    DBL   Measured Eh using the Zobell's solution             |STO 0340
C     EXELT     DBL   Moles of components                                 |STO 0350
C     FBOIL     DBL   Fraction of solution boiled-off as steam            |STO 0360
C     FCCSAT    DBL   Tolerance factor for pH and CO2 options             |STO 0370
C     FIXIT     DBL   Fixing value in the CO2 option                      |STO 0380
C     FLAGS     INT   Selection flags for calculation of redox equil.     |STO 0390
C     GEOTH     INT   Flag to select geothermometer                       |STO 0400
C     GFW       DBL   Gram formula weight of aqueous species              |STO 0410
C     HITEMP    DBL   In-situ temperature                                 |STO 0420
C     I         INT   Loop counting variable                              |STO 0430
C     IBMIX     INT   Switch for mixing option                            |STO 0440
C     ICCSAT    INT   Switch for pH option                                |STO 0450
C     IDDP      INT   Id number of the mineral to be dissolved/ppt        |STO 0460
C     IDMIX     INT   Id number of the aqueous species to be added        |STO 0470
C     IDN       INT   Id numbers of the ISCOMP components adsorption      |STO 0480
C     IDSAT     INT   Id number of the mineral to be equilibrated         |STO 0490
C     IMCO3     INT   Selects CO2 option                                  |STO 0500
C     IMIX      INT   Switch used in MIXER routines                       |STO 0510
C     INFORM    INT   Flag to print all the log K values in data base     |STO 0520
C     INMIX     INT   Total number of mixtures of two solution mixed      |STO 0530
C     INSP      INT   Total number of surface sites for adsorption        |STO 0540
C     IOPT      INT   Switch for co2/h option                             |STO 0550
C     IPAGE     INT   Current page number of output file                  |STO 0560
C     IPGLN     INT   Current line number of the output file              |STO 0570
C     IPHASE    INT   Switch for oil/water/gas calculations               |STO 0580
C     IPIT      INT   Flag to use pitzer activity coefficients            |STO 0590
C     IPRIN1    INT   Flag for printing iteration of anions               |STO 0600
C     IPRIN2    INT   Flag for printing hydronium balance                 |STO 0610
C     IRXDP     INT   Id number of the aqueous species to be added        |STO 0620
C     ISCHG     INT   Charge of each surface site for adsorption          |STO 0630
C     ISCOMP    INT   Total number of components in dissociation          |STO 0640
C     ITIC      INT   Hitemp distribution of carbonate species            |STO 0650
C     ITMIX     INT   Switch for the mineral saturation option            |STO 0660
C     ITT       INT   Number of aqueous species to add/sub with water     |STO 0670
C     J         INT   Loop counting variable                              |STO 0680
C     KCH4OL    DBL   Henry's law coefficient for CH4 in oil              |STO 0690
C     KCO2OL    DBL   Henry's law coefficient for CO2 in oil              |STO 0700
C     KH2SOL    DBL   Henry's law coefficient for H2S in oil              |STO 0710
C     KRXN      DBL   K for dissociation reaction of surface species      |STO 0720
C     MBASE     DBL   Equivalence Mole Fraction (initial) on surface      |STO 0730
C     MINCO     DBL   Stoichiometric coefficient for added minerals       |STO 0740
C     MININD    INT   Index number of the added mineral                   |STO 0750
C     MINLOG    DBL   Log K values for added minerals                     |STO 0760
C     MXMNK     INT   Total number of mineral log k values                |STO 0770
C     MXSP      INT   Total number of aqueous species                     |STO 0780
C     NDUM      INT   Id of mineral/aqueous complex with K(T) changed     |STO 0790
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C     NMAX       INT   General array dimension to allow easy expansion  |STO 0800
C     NUFLAG     INT   Sets the activity coefficients of neutral species|STO 0810
C     NUMCOM     INT   Number of complex the ion is associated with     |STO 0820
C     NUMINS     INT   Number of minerals added                         |STO 0830
C     ODUM       CHA   Switch to indicate a mineral/aqueous complex     |STO 0840
C     OUTIN      CHA   Name of restart file name                        |STO 0850
C     PAGE1      CHA   Names of aqueous species                         |STO 0860
C     PAGE3      CHA   Names of solubility constants                    |STO 0870
C     PH         DBL   Measured pH of the solution                      |STO 0880
C     PRESS      DBL   Total pressure                                   |STO 0890
C     PTR        INT   Points to index number of the analytical species |STO 0900
C     RATIO      INT   Flag for printing activity ratios of elements    |STO 0910
C     RXDP       DBL   Molal amount of the aqueous species added        |STO 0920
C     SAREA      DBL   Total surface area per kilogram of solvent       |STO 0930
C     SPN        CHA   Name of each surface species adsorption          |STO 0940
C     TAREA      DBL   Site density per unit area adsorption            |STO 0950
C     TCH4M      DBL   Moles CH4 distributed between oil, water, vapor  |STO 0960
C     TCO2M      DBL   Moles CO2 distributed between oil, water, vapor  |STO 0970
C     TEMP       DBL   Temperature of the solution when pH was measured |STO 0980
C     TH2SM      DBL   Moles H2S distributed between oil, water, vapor  |STO 0990
C     TIC        DBL   Concentration of total inorganic carbon          |STO 1000
C     TITLE      CHA   Name of the sample                               |STO 1010
C     TITR       DBL   Iteration array in DISTRB, used for guesses      |STO 1020
C     TOTEL      DBL   Contains HTOT, OHTOT and Sum CO2                 |STO 1030
C     UN         INT   File unit assigned for output file               |STO 1040
C     UNITS      CHA   Units of concentration                           |STO 1050
C     WROIL      DBL   Oil to water weight ratio                        |STO 1060
C     XD         DBL   Holds Log K's for additional anions & cations    |STO 1070
C     XDUM       DBL   New log K(T) value                               |STO 1080
C     Z          INT   Charge of aqueous species                        |STO 1090
C ---------------------------------------------------------------------|STO 1100
      INTEGER NMAX                                                      STO 1110
      DOUBLE PRECISION CPUMIN                                           STO 1120
      PARAMETER (CPUMIN = 1.0D-35, NMAX = 340)                          STO 1130
                                                                        STO 1140
      INTEGER ALK, ANS1, ANS2, FLAGS(6), GEOTH, GETUNT, I               STO 1150
      INTEGER IBMIX, ICCSAT, IDDP, IDMIX(50)                            STO 1160
      INTEGER IDN(10,10), IDSAT, IMCO3, IMIX                            STO 1170
      INTEGER INFORM, INMIX, INSP, IOPT, IPHASE, IPIT                   STO 1180
      INTEGER IPRIN1, IPRIN2, IRXDP(10), ISCHG(10)                      STO 1190
      INTEGER ISCOMP(10), ITIC, ITMIX, ITT, J                           STO 1200
      INTEGER MININD(8,5), MXSP, MXMNK, NDUM(12), NUFLAG                STO 1210
      INTEGER NUMCOM, NUMINS, PTR(33), RATIO, UN, Z(NMAX)               STO 1220
                                                                        STO 1230
      CHARACTER *  1 ADEX, ODUM(12)                                     STO 1240
      CHARACTER *  5 UNITS                                              STO 1250
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)              STO 1260
      CHARACTER * 10 SPN(10)                                            STO 1270
      CHARACTER * 80 MIXFLE, OUTIN, TITLE                               STO 1280
                                                                        STO 1290
      DOUBLE PRECISION ALFA(NMAX), AMOL(50), ANALM(NMAX), CEC           STO 1300
      DOUBLE PRECISION COEF(10,10), CONV1, CONV2                        STO 1310
      DOUBLE PRECISION CUNITS(NMAX), DCH4, DCO2, DH2S, DNH3             STO 1320
      DOUBLE PRECISION DDCH4, DDCO2, DDH2S, DDNH3                       STO 1330
      DOUBLE PRECISION DENS, DFRAC1, DHA(NMAX), DINC                    STO 1340
      DOUBLE PRECISION DP, DSEP, EHM, EHMC, EXELT(35)                   STO 1350
      DOUBLE PRECISION EMFZSC, FBOIL, FCCSAT, FIXIT                     STO 1360
      DOUBLE PRECISION GFW(NMAX), HITEMP                                STO 1370
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      DOUBLE PRECISION KCH4OL, KCO2OL, KH2SOL                           STO 1380
      DOUBLE PRECISION KRXN(10), M(NMAX), MBASE(10), MINCO(9,5)         STO 1390
      DOUBLE PRECISION MINLOG(2,5), PH, PRESS                           STO 1400
      DOUBLE PRECISION RXDP(10), SAREA, TAREA, TCH4M                    STO 1410
      DOUBLE PRECISION TCO2M, TEMP, TH2SM, TITR(11), TOTEL(5), TIC      STO 1420
      DOUBLE PRECISION WROIL, XD(2,45), XDUM(12)                        STO 1430
                                                                        STO 1440
      INTRINSIC DABS                                                    STO 1450
                                                                        STO 1460
      EXTERNAL GETUNT                                                   STO 1470
                                                                        STO 1480
                                                                        STO 1490
      COMMON /AL    / NDUM, XDUM                                        STO 1500
      COMMON /AMM   / IDMIX, AMOL, ITMIX, INMIX, DFRAC1, DINC, FBOIL    STO 1510
      COMMON /BASIC / DENS, PRESS, EHM, EHMC, EMFZSC, TIC, FCCSAT, XD,  STO 1520
     .                NUMCOM, NUMINS, MINLOG, MINCO, MININD, CONV1,     STO 1530
     .                CONV2                                             STO 1540
      COMMON /CH    / ODUM                                              STO 1550
      COMMON /DIST  / TCO2M, TCH4M, TH2SM, WROIL, KCH4OL, KCO2OL,       STO 1560
     &                KH2SOL, IPHASE, DSEP                              STO 1570
      COMMON /EXCHAN/ COEF, MBASE, KRXN, CEC, TAREA, SAREA, IDN,        STO 1580
     &                ISCHG, ISCOMP, INSP                               STO 1590
      COMMON /EXTOT / EXELT, TOTEL, TITR                                STO 1600
      COMMON /FLAGCM/ ALK, ITIC, ICCSAT, IMCO3, ITT, ANS1, ANS2,        STO 1610
     .                NUFLAG, IPIT, FLAGS, INFORM, RATIO, GEOTH,        STO 1620
     .                IPRIN1, IPRIN2                                    STO 1630
      COMMON /GAS   / DCO2, DDCO2, DH2S, DDH2S, DNH3, DDNH3,            STO 1640
     &                DCH4, DDCH4, IOPT, FIXIT                          STO 1650
      COMMON /IMM   / IBMIX, IMIX                                       STO 1660
      COMMON /MOLS  / PH, ANALM, M, ALFA, CUNITS                        STO 1670
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                               STO 1680
      COMMON /NAMES2/ SPN                                               STO 1690
      COMMON /NAMES3/ MIXFLE, OUTIN, TITLE, UNITS, ADEX                 STO 1700
      COMMON /SAT   / IDDP, IDSAT, DP, RXDP, IRXDP                      STO 1710
      COMMON /TABCOM/ MXSP, MXMNK, GFW, Z, DHA                          STO 1720
                                                                        STO 1730
      DATA PTR /3, 4, 22, 1, 2, 18, 14, 12, 5, 6, 33, 7, 98, 30, 29,    STO 1740
     &          136, 32, 31, 26, 15, 25, 27, 16, 23, 21, 13, 28, 169,  STO 1750
     &          210, 48, 246, 265, 285/                                 STO 1760
                                                                        STO 1770
C ======================================================================STO 1780
                                                                        STO 1790
      IF (OUTIN .EQ. ' ') THEN                                          STO 1800
        RETURN                                                          STO 1810
      ELSE                                                              STO 1820
        UN = GETUNT (OUTIN)                                             STO 1830
      END IF                                                            STO 1840
                                                                        STO 1850
      UNITS = 'MOL/K'                                                   STO 1860
                                                                        STO 1870
      TIC   = TOTEL(3)                                                  STO 1880
      IF (TIC .GT. CPUMIN) THEN                                         STO 1890
        ANALM(7)  = 0.0D00                                              STO 1900
        ANALM(98) = 0.0D00                                              STO 1910
      ELSE                                                              STO 1920
        TIC = 0.0D00                                                    STO 1930
      END IF                                                            STO 1940
                                                                        STO 1950
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      WRITE (UN, 9010) TITLE                                            STO 1960
      WRITE (UN, 9030) TEMP, HITEMP, DENS, PRESS                        STO 1970
      WRITE (UN, 9030) PH, EHM, EHMC, EMFZSC, UNITS                     STO 1980
      WRITE (UN, 9080) (ANALM(PTR(I)), I =  1,  7)                      STO 1990
      WRITE (UN, 9080) (ANALM(PTR(I)), I =  8, 13), TIC                 STO 2000
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 14, 20)                      STO 2010
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 21, 26)                      STO 2020
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 27, 29)                      STO 2030
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 30, 33)                      STO 2040
      WRITE (UN, 9100) ALK, ITIC                                        STO 2050
      WRITE (UN, 9080) DCO2, DH2S, DNH3, DCH4                           STO 2060
      WRITE (UN, 9100) ICCSAT, IMCO3, FIXIT, FCCSAT                     STO 2070
      WRITE (UN, 9080) TCO2M, TCH4M, TH2SM, WROIL,                      STO 2080
     &                 KCO2OL, KCH4OL, KH2SOL, DSEP                     STO 2090
                                                                        STO 2100
      WRITE (UN, 9160) ADEX                                             STO 2110
      IF (ADEX .EQ. 'A' .OR. ADEX .EQ. 'E') THEN                        STO 2120
        WRITE (UN, 9150) CEC, TAREA, SAREA, INSP                        STO 2130
        DO 30 I = 1, INSP                                               STO 2140
          WRITE (UN, 9200) ISCHG(I), MBASE(I), SPN(I)                   STO 2150
          WRITE (UN, 9210) KRXN(I), ISCOMP(I), (COEF(I,J),              STO 2160
     &                     IDN(I,J), J = 1, ISCOMP(I))                  STO 2170
30    CONTINUE                                                          STO 2180
      END IF                                                            STO 2190
                                                                        STO 2200
      I = 0                                                             STO 2210
      WRITE (UN, 9100) I, I                                             STO 2220
                                                                        STO 2230
      WRITE (UN, 9180) (ODUM(I), NDUM(I), XDUM(I), I = 1,  6)           STO 2240
      WRITE (UN, 9180) (ODUM(I), NDUM(I), XDUM(I), I = 7, 12)           STO 2250
                                                                        STO 2260
      WRITE (UN, 9290) ANS1, ANS2                                       STO 2270
      IF (ANS1 .GT. 0) THEN                                             STO 2280
        WRITE (UN, 9350) ANALM(MXSP+1), GFW(MXSP+1), Z(MXSP+1),         STO 2290
     &                   DHA(MXSP+1), PAGE1(MXSP+1)                     STO 2300
        DO 60 I = 2, 15                                                 STO 2310
          IF (DABS(XD(1,I)) .GT. CPUMIN .OR.                            STO 2320
     &        DABS(XD(2,I)) .GT. CPUMIN) THEN                           STO 2330
            WRITE (UN, 9360) I, DHA(MXSP+I), XD(1,I), XD(2,I),          STO 2340
     &                       PAGE1(MXSP+I)                              STO 2350
          END IF                                                        STO 2360
60    CONTINUE                                                          STO 2370
      END IF                                                            STO 2380
      IF (ANS2 .GT. 0) THEN                                             STO 2390
        WRITE (UN, 9350) ANALM(MXSP+16), GFW(MXSP+16), Z(MXSP+16),      STO 2400
     &                   DHA(MXSP+16), PAGE1(MXSP+16)                   STO 2410
        DO 70 I = 2, 15                                                 STO 2420
          IF (DABS(XD(1,I+15)) .GT. CPUMIN .OR.                         STO 2430
     &        DABS(XD(2,I+15)) .GT. CPUMIN) THEN                        STO 2440
            WRITE (UN, 9360) I+15, DHA(MXSP+I+15), XD(1,I+15),          STO 2450
     &                       XD(2,I+15), PAGE1(MXSP+15+I)               STO 2460
          END IF                                                        STO 2470
70    CONTINUE                                                          STO 2480
      END IF                                                            STO 2490
                                                                        STO 2500
      IF (NUMCOM .GT. 0) THEN                                           STO 2510
        WRITE (UN, 9500) NUMCOM, Z(MXSP+31), DHA(MXSP+31),              STO 2520
     &                   GFW(MXSP+31), ANALM(MXSP+31), PAGE1(MXSP+31)   STO 2530
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      DO 80 I = 2, 14                                                    STO 2540
        IF (DABS(XD(1,I+30)) .GT. CPUMIN .OR.                            STO 2550
     &      DABS(XD(2,I+30)) .GT. CPUMIN) THEN                           STO 2560
          WRITE (UN, 9360) I+30, DHA(MXSP+I+30), XD(1,I+30),             STO 2570
     &                     XD(2,I+30), PAGE1(MXSP+30+I)                  STO 2580
        END IF                                                           STO 2590
   80   CONTINUE                                                         STO 2600
      ELSE                                                               STO 2610
        WRITE (UN, 9500) NUMCOM                                          STO 2620
      END IF                                                             STO 2630
                                                                         STO 2640
      WRITE (UN, 9360) NUMINS                                            STO 2650
      DO 90 I = 1, NUMINS                                                STO 2660
        IF (DABS(MINLOG(1,I)) .GT. CPUMIN .OR. DABS(MINLOG(2,I))         STO 2670
     .     .GT. CPUMIN) THEN                                             STO 2680
          WRITE (UN, 9560) MINLOG(1,I), MINLOG(2,I),                     STO 2690
     .                     MINCO(9,I), PAGE3(MXMNK+I)                    STO 2700
          WRITE (UN, 9210) (MINCO(J,I), MININD(J,I), J = 1, 8)           STO 2710
        END IF                                                           STO 2720
   90 CONTINUE                                                           STO 2730
                                                                         STO 2740
      WRITE (UN, 9290) NUFLAG, IPIT, (FLAGS(I), I = 1, 6)               STO 2750
      IF (GEOTH .GT. 0) GEOTH = 1                                        STO 2760
      WRITE (UN, 9300) INFORM, RATIO, GEOTH, IPRIN1, IPRIN2              STO 2770
      WRITE (UN, 9080) CONV1, CONV2                                      STO 2780
                                                                         STO 2790
      RETURN                                                             STO 2800
                                                                         STO 2810
C -----------------------------------------------------------------------|STO 2820
C     Format Statements                                                  |STO 2830
C ---------------------                                                  |STO 2840
                                                                         STO 2850
 9010 FORMAT (A80)                                                       STO 2860
 9030 FORMAT (4E10.4, A5)                                                STO 2870
 9080 FORMAT (8E10.4)                                                    STO 2880
 9100 FORMAT (2I2, 2E10.4)                                               STO 2890
 9150 FORMAT (3E10.4, I3)                                                STO 2900
 9160 FORMAT (A1)                                                        STO 2910
 9180 FORMAT (6(A1, I4, E10.4))                                          STO 2920
 9200 FORMAT (I4, E10.4, A10)                                            STO 2930
 9210 FORMAT (11(E10.4, I3))                                             STO 2940
 9270 FORMAT (2I4, E10.4)                                                STO 2950
 9280 FORMAT (I4, 2E10.4)                                                STO 2960
 9290 FORMAT (8I2)                                                       STO 2970
 9300 FORMAT (5I2, A80)                                                  STO 2980
 9350 FORMAT (2E10.4, I2, E10.4, A8)                                     STO 2990
 9360 FORMAT (I2, 3E10.4, A8)                                            STO 3000
 9500 FORMAT (2I2, 3E10.4, A8)                                           STO 3010
 9560 FORMAT (5E10.4, A8)                                                STO 3020
                                                                         STO 3030
      END                                                                STO 3040




      SUBROUTINE TABLES (MXAQK, BDAT, TK, TCO2, MXPC)                    TAB 0010
C ===================================================================== |TAB 0020
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C     This routine reads in all required tables.                          |TAB 0030
C ------------------------------------------------------------------------|TAB 0040
C     AHI        DBL   Pressure correction fit parameter                  |TAB 0050
C     ALOW       DBL   Pressure correction fit parameter                  |TAB 0060
C     BDAT       DBL   B-dot as a function of temperature                 |TAB 0070
C     BHI        DBL   Pressure correction fit parameter                  |TAB 0080
C     BLOW       DBL   Pressure correction fit parameter                  |TAB 0090
C     CHI        DBL   Pressure correction fit parameter                  |TAB 0100
C     CLOW       DBL   Pressure correction fit parameter                  |TAB 0110
C     DELVR      DBL   Change in volume at 25 degrees                     |TAB 0120
C     DHA        DBL   Ion size parameter                                 |TAB 0130
C     GFW        DBL   Gram formula weight of aqueous species             |TAB 0140
C     I          INT   Loop variable                                      |TAB 0150
C     J          INT   Loop variable                                      |TAB 0160
C     LKT1       DBL   Log K for aqueous species with temperature         |TAB 0170
C     LKT2       DBL   Log K for minerals with temperature                |TAB 0180
C     MXAQK      INT   Total number of aqueous log k values               |TAB 0190
C     MXMNK      INT   Total number of mineral log k values               |TAB 0200
C     MXPC       INT   Total number of mineral pressure constants         |TAB 0210
C     MXSP       INT   Total number of aqueous species                    |TAB 0220
C     N          INT   Index number                                       |TAB 0230
C     NH2O       DBL   Number of water ionization reactions               |TAB 0240
C     NMAX       INT   General array dimension to allow easy expansion    |TAB 0250
C     PAGE1      CHA   Names of aqueous species                           |TAB 0260
C     PAGE2      CHA   Names of equilibrium constants                     |TAB 0270
C     PAGE3      CHA   Names of solubility constants                      |TAB 0280
C     TCO2       DBL   Activity coefficients of CO2 with temperature      |TAB 0290
C     TK         DBL   Temperature steps used by program                  |TAB 0300
C     TOF        CHA   Places a form feed in output file                  |TAB 0310
C     UND        INT   File unit assigned for data tables                 |TAB 0320
C     UNO        INT   File unit assigned for output file                 |TAB 0330
C     Z          INT   Charge of aqueous species                          |TAB 0340
C ------------------------------------------------------------------------|TAB 0350
                                                                           TAB 0360
      INTEGER NMAX, UND, UNO                                               TAB 0370
      PARAMETER (NMAX = 340, UND = 10, UNO = 6)                            TAB 0380
                                                                           TAB 0390
      INTEGER I, J, N, MXSP, MXAQK, MXMNK, MXPC, Z(NMAX)                   TAB 0400
                                                                           TAB 0410
      CHARACTER *  1 TOF, CR                                               TAB 0420
      CHARACTER *  8 PAGE1(NMAX), PAGE2(NMAX), PAGE3(NMAX)                 TAB 0430
      CHARACTER * 40 TITMIX                                                TAB 0440
                                                                           TAB 0450
      DOUBLE PRECISION AHI(200), ALOW(200), BDAT(10), BHI(200)             TAB 0460
      DOUBLE PRECISION BLOW(200), CHI(200), CLOW(200), DELVR(NMAX)         TAB 0470
      DOUBLE PRECISION DHA(NMAX), GFW(NMAX)                                TAB 0480
      DOUBLE PRECISION LKT1(NMAX,11), LKT2(NMAX,11), NH2O(NMAX)            TAB 0490
      DOUBLE PRECISION TCO2(10), TK(11)                                    TAB 0500
                                                                           TAB 0510
      COMMON /FMFD  / TOF, CR, TITMIX                                      TAB 0520
      COMMON /KK    / LKT1, LKT2                                           TAB 0530
      COMMON /NAMES1/ PAGE1, PAGE2, PAGE3                                  TAB 0540
      COMMON /PTK   / DELVR, NH2O, ALOW, BLOW, CLOW, AHI, BHI, CHI         TAB 0550
      COMMON /TABCOM/ MXSP, MXMNK, GFW, Z, DHA                             TAB 0560
                                                                           TAB 0570
C ========================================================================|TAB 0580
                                                                           TAB 0590
      OPEN (UND, FILE = 'DATA.TBL', STATUS = 'OLD')                        TAB 0600
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C      OPEN (UND, STATUS = 'OLD', shared, readonly)                    TAB 0610
                                                                       TAB 0620
       READ (UND, 1000) MXSP, MXAQK, MXMNK, MXPC                       TAB 0630
                                                                       TAB 0640
       DO 10 I = 1, MXSP                                               TAB 0650
         READ (UND, 1010, END = 70) N, PAGE1(I), Z(I), DHA(I), GFW(I)  TAB 0660
    10 CONTINUE                                                        TAB 0670
                                                                       TAB 0680
       DO 20 I = 1, MXAQK                                              TAB 0690
         READ (UND, 1020, END = 80) N, PAGE2(I), (LKT1(I,J), J = 1, 11) TAB 0700
    20 CONTINUE                                                        TAB 0710
                                                                       TAB 0720
       DO 30 I = 1, MXMNK                                              TAB 0730
         READ (UND, 1020, END = 90) N, PAGE3(I), (LKT2(I,J), J = 1, 11) TAB 0740
    30 CONTINUE                                                        TAB 0750
                                                                       TAB 0760
       READ (UND, 1030, END = 100) (BDAT(I), I = 1, 10)                TAB 0770
                                                                       TAB 0780
       READ (UND, 1040, END = 110) (TK(I), I = 1, 11)                  TAB 0790
                                                                       TAB 0800
       READ (UND, 1050, END = 120) (TCO2(I), I = 1, 10)                TAB 0810
                                                                       TAB 0820
       DO 40 I = 1, MXPC                                               TAB 0830
         READ (UND, 1060, END = 130) ALOW(I), BLOW(I), CLOW(I),        TAB 0840
                                     AHI(I),  BHI(I),  CHI(I)          TAB 0850
         BLOW(I) = BLOW(I) * 1.0D-4                                    TAB 0860
         BHI(I)  = BHI(I)  * 1.0D-4                                    TAB 0870
         CLOW(I) = CLOW(I) * 1.0D-16                                   TAB 0880
         CHI(I)  = CHI(I)  * 1.0D-16                                   TAB 0890
    40 CONTINUE                                                        TAB 0900
                                                                       TAB 0910
       DO 50 I = 1, MXAQK                                              TAB 0920
         DELVR(I) = 0.0D0                                              TAB 0930
         NH2O(I) = 0.0D0                                               TAB 0940
         READ (UND, 1070, ERR = 140, END = 60) J, DELVR(J), NH2O(J)    TAB 0950
    50 CONTINUE                                                        TAB 0960
                                                                       TAB 0970
    60 CONTINUE                                                        TAB 0980
       CLOSE (UND)                                                     TAB 0990
       RETURN                                                          TAB 1000
                                                                       TAB 1010
C ======================================================================TAB 1020
                                                                       TAB 1030
    70 CONTINUE                                                        TAB 1040
       WRITE (UNO, 1080) TOF                                           TAB 1050
       WRITE (UNO, 1090)                                               TAB 1060
       STOP                                                            TAB 1070
                                                                       TAB 1080
    80 CONTINUE                                                        TAB 1090
       WRITE (UNO, 1080) TOF                                           TAB 1100
       WRITE (UNO, 1100)                                               TAB 1110
       STOP                                                            TAB 1120
                                                                       TAB 1130
    90 CONTINUE                                                        TAB 1140
       WRITE (UNO, 1080) TOF                                           TAB 1150
       WRITE (UNO, 1110)                                               TAB 1160
       STOP                                                            TAB 1170
                                                                       TAB 1180
```

```
  100 CONTINUE                                                          TAB 1190
      WRITE (UNO, 1080) TOF                                             TAB 1200
      WRITE (UNO, 1120)                                                 TAB 1210
      STOP                                                              TAB 1220
                                                                        TAB 1230
  110 CONTINUE                                                          TAB 1240
      WRITE (UNO, 1080) TOF                                             TAB 1250
      WRITE (UNO, 1130)                                                 TAB 1260
      STOP                                                              TAB 1270
                                                                        TAB 1280
  120 CONTINUE                                                          TAB 1290
      WRITE (UNO, 1080) TOF                                             TAB 1300
      WRITE (UNO, 1140)                                                 TAB 1310
      STOP                                                              TAB 1320
                                                                        TAB 1330
  130 CONTINUE                                                          TAB 1340
      WRITE (UNO, 1080) TOF                                             TAB 1350
      WRITE (UNO, 1150)                                                 TAB 1360
      STOP                                                              TAB 1370
                                                                        TAB 1380
  140 CONTINUE                                                          TAB 1390
      WRITE (UNO, 1160) TOF                                             TAB 1400
      STOP                                                              TAB 1410
                                                                        TAB 1420
 1000 FORMAT (4I4)                                                      TAB 1430
 1010 FORMAT (I3, 1X, A8, 1X, I2, 1X, F3.1, 1X, F8.3)                   TAB 1440
 1020 FORMAT (I3, 1X, A8, 7(1X, F7.2) / 13X, 4(F7.2, 1X))               TAB 1450
 1030 FORMAT (10(F5.3, 1X))                                             TAB 1460
 1040 FORMAT (F3.1, 3(1X, F4.1), 7(1X, F5.1))                           TAB 1470
 1050 FORMAT (F3.1, 2(1X, F4.1), 7(1X, F5.1))                           TAB 1480
 1060 FORMAT (5(F8.3, 1X), F8.3)                                        TAB 1490
 1070 FORMAT (I4, 2F8.3)                                                TAB 1500
 1080 FORMAT (A1)                                                       TAB 1510
 1090 FORMAT (5X,'ERROR IN READING TABLE-PAGE1', /, '   Program Stop')  TAB 1520
 1100 FORMAT (5X,'ERROR IN READING TABLE-PAGE2', /, '   Program Stop')  TAB 1530
 1110 FORMAT (5X,'ERROR IN READING TABLE-PAGE3', /, '   Program Stop')  TAB 1540
 1120 FORMAT (5X,'ERROR IN READING TABLE-BDAT ', /, '   Program Stop')  TAB 1550
 1130 FORMAT (5X,'ERROR IN READING TABLE-TK   ', /, '   Program Stop')  TAB 1560
 1140 FORMAT (5X,'ERROR IN READING TABLE-TCO2 ', /, '   Program Stop')  TAB 1570
 1150 FORMAT (5X,'ERROR IN READING TABLE-PRESS', /, '   Program Stop')  TAB 1580
 1160 FORMAT (A1, 5X, 'ERROR IN READING TABLE-PRESS (IONS) ', /,        TAB 1590
                    ' Program Stop')                                    TAB 1600
                                                                        TAB 1610
      END                                                               TAB 1620
```

```
      SUBROUTINE WAPVT (TC, X, P, BETA, G, ALPHA)                       WAP 0010
C ======================================================================|WAP 0020
C     Routine to calculate the properties of pure water                 |WAP 0030
C     from the steam tables of keenan et al (1969)                      |WAP 0040
C ----------------------------------------------------------------------|WAP 0050
C     A          DBL   Fit coefficents A(i,j)                           |WAP 0060
C     AF         DBL   Helmholtz free energy as a function of rho and T |WAP 0070
C     AF0        DBL   Intermediate storage variable                    |WAP 0080
C     ALPHA      DBL   Coefficient of thermal expansion                 |WAP 0090
```

```
C     BETA       DBL   Coefficient of compressibility                        |WAP 0100
C     C          DBL   Fit coefficients C(i)                                 |WAP 0110
C     DIDX       DBL   First derivative of SI with respect to density        |WAP 0120
C     DIDX2      DBL   Second derivative of SI with respect to density       |WAP 0130
C     DKDX       DBL   First derivative of SK with respect to density        |WAP 0140
C     DKDX2      DBL   Second derivative of SK with respect to density       |WAP 0150
C     DPDT       DBL   Derivative of pressure with respect to temp.          |WAP 0160
C     DPDTR      DBL   Derivative of Q by tau with constant rho              |WAP 0170
C     DPDX       DBL   Derivative of pressure by density at constant T       |WAP 0180
C     DQDTR      DBL   Intermediate storage variable                         |WAP 0190
C     DQDX       DBL   First derivative of Q by density at constant T        |WAP 0200
C     DQDX2      DBL   Second derivative of Q by density at constant T       |WAP 0210
C     DTDTR      DBL   First derivative of TJ with respect to Tau            |WAP 0220
C     DTRDT      DBL   Derivative of TR with respect to temperature          |WAP 0230
C     E          DBL   Fit constant                                          |WAP 0240
C     FK         DBL   Intermediate storage variable                         |WAP 0250
C     G          DBL   Gibbs Free Energy in joules per mole                  |WAP 0260
C     I          INT   Loop variable                                         |WAP 0270
C     J          INT   Loop variable                                         |WAP 0280
C     MW         DBL   Molecular weight of water                             |WAP 0290
C     P          DBL   Pressure (bar)                                        |WAP 0300
C     Q          DBL   Intermediate storage variable                         |WAP 0310
C     RC         DBL   R in j/ g K                                           |WAP 0320
C     RP         DBL   R in bar cm(3)/g K                                    |WAP 0330
C     SC         DBL   Intermediate storage variable                         |WAP 0340
C     SI         DBL   Sum of A(i,j) * TI(i), i=1,8  in Q                    |WAP 035c
C     SK         DBL   Sum of A(i,j), i=9,10  in Q                           |WAP 0360
C     T          DBL   Temperature in deg K                                  |WAP 0370
C     TC         DBL   Temperature in deg C                                  |WAP 0380
C     TCR        DBL   1000 / critical temperature of water in kelvin        |WAP 0390
C     TF         DBL   Intermediate storage variable                         |WAP 0400
C     TI         DBL   Array of XTs to the (i-1)th power                     |WAP 0410
C     TJ         DBL   Intermediate storage variable                         |WAP 0420
C     TP         DBL   Tau(a,j)                                              |WAP 0430
C     TR         DBL   1000 / current temperature of water in kelvin         |WAP 0440
C     TT         DBL   Intermediate storage variable                         |WAP 0450
C     X          DBL   Density (g/cm3)                                       |WAP 0460
C     XP         DBL   Density(a,j)                                          |WAP 0470
C     XT         DBL   Intermediate storage variable                         |WAP 0480
C ------------------------------------------------------------------------- |WAP 0490
      DOUBLE PRECISION MW                                                     WAP 0500
      PARAMETER (MW = 18.0153D00)                                             WAP 0510
                                                                              WAP 0520
      INTEGER I, J                                                            WAP 0530
                                                                              WAP 0540
      DOUBLE PRECISION A(10,7), AF, AF0, ALPHA, BETA, C(8)                    WAP 0550
      DOUBLE PRECISION DIDX, DIDX2, DKDX, DKDX2, DPDT, DPDTR, DPDX            WAP 0560
      DOUBLE PRECISION DQDTR, DQDX, DQDX2, DTDTR, DTRDT                       WAP 0570
      DOUBLE PRECISION E, FK, G, P, Q                                         WAP 0580
      DOUBLE PRECISION RC, RP, SC, SI, SK                                     WAP 0590
      DOUBLE PRECISION T, TC, TCR, TF, TI(8), TJ, TP, TR, TT                  WAP 0600
      DOUBLE PRECISION X, XP, XT                                              WAP 0610
                                                                              WAP 0620
      INTRINSIC DEXP, DLOG                                                    WAP 0630
                                                                              WAP 0640
      DATA TCR, E, RP/ 1.544912D+0, 4.8D+0, 4.6151D+0/                        WAP 0650
      DATA C /1.857065D+3,   3.22912D+3,  -4.19465D+2,    3.66649D+1,        WAP 0660
             -2.05516D+1,    4.85233D+0,   4.6D+1,       -1.011249D+3/       WAP 0670
```

```
                                                                      WAP 0680
      DATA A /2.9492937D+1, -1.3213917D+2, 2.7464632D+2, -3.6093828D+2, WAP 0690
     .        3.4218431D+2, -2.4450042D+2, 1.5518535D+2,  5.9728487D+0, WAP 0700
     .       -4.1030848D+2, -4.1605860D+2,-5.1985860D+0,  7.7779182D+0, WAP 0710
     .       -3.3301902D+1, -1.6254622D+1,-1.7731074D+2,  1.2748742D+2, WAP 0720
     .        1.3746153D+2,  1.5597836D+2, 3.3731180D+2, -2.0988866D+2, WAP 0730
     .        6.8335354D+0, -2.6149751D+1, 6.5326396D+1, -2.6181978D+1, WAP 0740
     .        0.0D+0,        0.0D+0,       0.0D+0,        0.0D+0,       WAP 0750
     .       -1.3746618D+2, -7.3396848D+2,-1.564104D-1,  -7.2546108D-1, WAP 0760
     .       -9.2734289D+0,  4.3125840D+0, 0.0D+0,        0.0D+0,       WAP 0770
     .        0.0D+0,        0.0D+0,       6.7874983D+0,  1.0401717D+1, WAP 0780
     .       -6.3972405D+0,  2.6409282D+1,-4.7740374D+1,  5.6323130D+1, WAP 0790
     .        0.0D+0,        0.0D+0,       0.0D+0,        0.0D+0,       WAP 0800
     .        1.3687317D+2,  6.4581880D+2,-3.9661401D+0,  1.5453061D+1, WAP 0810
     .       -2.9142470D+1,  2.9568796D+1, 0.0D+0,        0.0D+0,       WAP 0820
     .        0.0D+0,        0.0D+0,       7.9847970D+1,  3.9917570D+2, WAP 0830
     .       -6.9048554D-1,  2.7407416D+0,-5.1028070D+0,  3.9636085D+0, WAP 0840
     .        0.0D+0,        0.0D+0,       0.0D+0,        0.0D+0,       WAP 0850
     .        1.3041253D+1,  7.1531353D+1/                              WAP 0860
                                                                      WAP 0870
C ======================================================================|WAP 0880
                                                                      WAP 0890
      RC = RP / 10.0D+0                                               WAP 0900
      T  = TC + 273.15D00                                             WAP 0910
      TR = 1.0D+3 / T                                                 WAP 0920
      TF = TR - TCR                                                   WAP 0930
      FK = DEXP(-E * X)                                               WAP 0940
      SC = 0.0D+0                                                     WAP 0950
                                                                      WAP 0960
C -----------------------------------------------------------------------|WAP 0970
C     Calculate psi sub 0                                              |WAP 0980
C -----------------------------------------------------------------------|WAP 0990
                                                                      WAP 1000
      DO 10 I = 1, 6                                                  WAP 1010
        SC = SC + C(I) / TR**(I-1)                                    WAP 1020
   10 CONTINUE                                                        WAP 1030
                                                                      WAP 1040
      AF0   = SC + C(7) * DLOG(T) + C(8) * DLOG(T / TR)               WAP 1050
                                                                      WAP 1060
C -----------------------------------------------------------------------|WAP 1070
C     Calculate Q term by term                                         |WAP 1080
C -----------------------------------------------------------------------|WAP 1090
                                                                      WAP 1100
      Q     = 0.0D+0                                                  WAP 1110
      DQDX  = 0.0D+0                                                  WAP 1120
      DQDX2 = 0.0D+0                                                  WAP 1130
      DPDTR = 0.0D+0                                                  WAP 1140
      DQDTR = 0.0D+0                                                  WAP 1150
                                                                      WAP 1160
      DO 50 J = 1, 7                                                  WAP 1170
        IF (J .GT. 1) THEN                                            WAP 1180
          TP = 2.5D+0                                                 WAP 1190
          XP = 1.0D+0                                                 WAP 1200
        ELSE                                                          WAP 1210
          TP = TCR                                                    WAP 1220
          XP = 0.634D+0                                               WAP 1230
        END IF                                                        WAP 1240
                                                                      WAP 1250
```

```
30    CONTINUE                                                                WAP 1260
      XT = X - XP                                                             WAP 1270
      TT = TR - TP                                                            WAP 1280
      TI(1) = 1.0D+0                                                          WAP 1290
                                                                              WAP 1300
      DO 40 I = 2, 8                                                          WAP 1310
        TI(I) = TI(I-1) * XT                                                  WAP 1320
40    CONTINUE                                                                WAP 1330
                                                                              WAP 1340
      SI = A(1,J) + A(2,J) * TI(2) + A(3,J) * TI(3) + A(4,J) * TI(4) +WAP 1350
     .             A(5,J) * TI(5) + A(6,J) * TI(6) + A(7,J) * TI(7) +WAP 1360
     .             A(8,J) * TI(8)                                             WAP 1370
      DIDX = A(2,J) + 2.0*A(3,J) * TI(2) + 3.0*A(4,J) * TI(3) +               WAP 1380
     .               4.0*A(5,J) * TI(4) + 5.0*A(6,J) * TI(5) +               WAP 1390
     .               6.0*A(7,J) * TI(6) + 7.0*A(8,J) * TI(7)                 WAP 1400
      DIDX2 = 2.0*A(3,J) + 6.0*A(4,J) * TI(2) + 12.0*A(5,J) * TI(3) + WAP 1410
     .                    20.0*A(6,J) * TI(4) + 30.0*A(7,J) * TI(5) + WAP 1420
     .                    42.0*A(8,J) * TI(6)                                WAP 1430
                                                                              WAP 1440
      SK = FK * (A(9,J) + A(10,J) * X)                                        WAP 1450
      DKDX = FK * A(10,J) - E * SK                                            WAP 1460
      DKDX2 = -E * FK * A(10,J) - E * DKDX                                    WAP 1470
                                                                              WAP 1480
      TJ = TT**(J-2)                                                          WAP 1490
      DTDTR = (J-2) * TT**(J-3)                                               WAP 1500
                                                                              WAP 1510
      Q = Q + TJ * (SI + SK)                                                  WAP 1520
      DQDX  = DQDX  + TJ * (DIDX  + DKDX)                                     WAP 1530
      DQDX2 = DQDX2 + TJ * (DIDX2 + DKDX2)                                    WAP 1540
      DPDTR = DPDTR + DTDTR * (SI + SK)                                       WAP 1550
      DQDTR = DQDTR + DTDTR * (DIDX + DKDX)                                   WAP 1560
50  CONTINUE                                                                  WAP 1570
                                                                              WAP 1580
    DPDTR = Q + TF * DPDTR                                                    WAP 1590
    DQDTR = DQDX + TF * DQDTR                                                 WAP 1600
    Q = TF * Q                                                                WAP 1610
    DQDX  = TF * DQDX                                                         WAP 1620
    DQDX2 = TF * DQDX2                                                        WAP 1630
    DTRDT = -1.0D+3 / T**2                                                    WAP 1640
    DPDT  = DTRDT * (DPDTR + DQDTR * X)                                       WAP 1650
                                                                              WAP 1660
    AF = AF0 + RC * T * (DLOG(X) + X * Q)                                     WAP 1670
                                                                              WAP 1680
    P = X * RP * T * (1.0D+0 + X * Q + X**2 * DQDX)                           WAP 1690
                                                                              WAP 1700
    DPDX = P / X + X * RP * T * (Q + 3.0 * X * DQDX + X**2 * DQDX2)           WAP 1710
                                                                              WAP 1720
    BETA = 1.0 / (X * DPDX)                                                   WAP 1730
                                                                              WAP 1740
    ALPHA = BETA * (P / T + T * RP * DPDT * X**2)                             WAP 1750
                                                                              WAP 1760
    G  = (AF + (P / X) * (RC / RP)) * MW                                      WAP 1770
                                                                              WAP 1780
    RETURN                                                                    WAP 1790
    END                                                                       WAP 1800
```

```
      SUBROUTINE WDBP (TC, P, DC, DCDT)                                 WDB 0010
C ================================================================== |WDB 0020
C     Routine to calculate the dielectric constant of water          |WDB 0030
C     based on eq (1) of Bradley and Pitzer (1979)                   |WDB 0040
C     This equation is only valid for temperatures of 0-350 C        |WDB 0050
C      and pressures up to 2000 bar at 70 C and lower and up to      |WDB 0060
C      5000 bar greater than 70 C                                    |WDB 0070
C ------------------------------------------------------------------ |WDB 0080
C     B          DBL   Intermediate storage variable                 |WDB 0090
C     C          DBL   Intermediate storage variable                 |WDB 0100
C     DC         DBL   Dielectric constant of water                  |WDB 0110
C     DCDT       DBL   Derivative of dielectic constant wrt T        |WDB 0120
C     DCO        DBL   Intermediate storage variable                 |WDB 0130
C     DT1        DBL   Intermediate storage variable                 |WDB 0140
C     DT2        DBL   Intermediate storage variable                 |WDB 0150
C     DT3        DBL   Intermediate storage variable                 |WDB 0160
C     P          DBL   Pressure in bars                              |WDB 0170
C     T          DBL   Temperature in deg k                          |WDB 0180
C     TC         DBL   Temperature in deg c                          |WDB 0190
C     U          DBL   Fit constants                                 |WDB 0200
C ------------------------------------------------------------------ |WDB 0210
                                                                      WDB 0220
      DOUBLE PRECISION B, C, DC, DCDT, DCO, DT1, DT2, DT3           WDB 0230
      DOUBLE PRECISION P, T, TC, U(9)                               WDB 0240
                                                                    WDB 0250
      INTRINSIC DEXP, DLOG                                          WDB 0260
                                                                    WDB 0270
      DATA U/ 3.4279D+2, -5.0866D-3,  9.4690D-7, -2.0525D+0,        WDB 0280
     .        3.1159D+3, -1.8289D+2, -8.0325D+3,  4.2142D+6,        WDB 0290
     .        2.1417D+0 /                                           WDB 0300
                                                                    WDB 0310
C ================================================================== |WDB 0320
                                                                    WDB 0330
      T    = TC + 273.15D+00                                        WDB 0340
      DCO  = U(1) * DEXP(U(2)*T + U(3)*T**2)                        WDB 0350
      C    = U(4) + (U(5) / (U(6) + T))                             WDB 0360
      B    = U(7) + (U(8) / T) + (U(9) * T)                         WDB 0370
      DC   = DCO  + (C * DLOG((B + P) / (B + 1.0D+3)))              WDB 0380
      DT1  = U(1) * (U(2) + (2.0 * U(3) * T))                       WDB 0390
     .            * (DEXP((U(2) * T) + (U(3) * T**2)))             WDB 0400
      DT2  = (U(5) / (U(6) + T)**2) * DLOG((B+P) / (B + 1.0D+3))    WDB 0410
      DT3  = (C * (1.0D+3 - P) * (U(9) - (U(8)/T**2)))              WDB 0420
     .       / ((B + P) * (B + 1.0D+3))                             WDB 0430
      DCDT = DT1 - DT2 + DT3                                        WDB 0440
                                                                    WDB 0450
      RETURN                                                        WDB 0460
      END                                                           WDB 0470
```

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