USER'S MANUAL FOR WATEQ4F, WITH REVISED THERMODYNAMIC DATA BASE AND TEST CASES FOR CALCULATING SPECIATION OF MAJOR, TRACE, AND REDOX ELEMENTS IN NATURAL WATERS

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TABLES

CONVERSION FACTORS AND ABBREVIATIONS

Multiply	By	To obtain
cal (calorie)	0.003968	Btu (British thermal unit)
cm^2 (square centimeter)	0.1550	in^2 (square inch)
kg (kilogram)	2.200	lb (pound)
L (liter)	0.2642	gal (gallon)
mg (milligram)	3.520×10^{-5}	oz (ounce)

Explanation of abbreviations:

°C (degrees Celsius)
cu ft/sec (cubic feet per second)
kcal (kilocalories)
mg/L (milligrams per liter)
mol (molar, moles per liter)
μS (microSiemens, reciprocal megohms)

Running WATEQ4F

The WATEQ4F software package consists of 4 files or sets of files:

- WATEQ4F.EXE, the executable code for WATEQ4F.
- TABLE1 and TABLE2, the thermodynamic data tables.
- TABLE3, TABL3A, and TABLE4, the tables of reference numbers used to print the results.
- WQ4FINPT.EXE, a program to assist you with creating correctly formatted input data files for WATEQ4F.

To run WATEQ4F, first log in to directory WQ4F. Type:

cd \wq4f and press **Enter**

Then type:

wateq4f and press **Enter**

It does not matter whether you use upper case or lower case characters. WATEQ4F will prompt you for the names of your input (water analysis) and output files. The file containing the test cases that is shipped with the WATEQ4F software package is named TSTCASES.DAT. If there is no water analysis data file in the WQ4F directory, you will need to run program WQ4FINPT so you can create the file. To run WQ4FINPT, first log in to directory WQ4F, if necessary, according to the instructions above. Then type:

wq4finpt and press **Enter**

WQ4FINPT will prompt you for the necessary data items. For a description of the input data to WATEQ4F, please refer to page 10 of Open-File Report 91-183. Alternatively, you can create your own WATEQ4F input water analyis data sets by modifying a copy of file TSTCASES.DAT, using a line editor that saves files in ASCII format.

The README file on the distribution diskette contains information that is current for your copy of WATEQ4F. Please read this file, as it contains information unique to your version of the software that does not appear anywhere else. You may display it on your screen by logging into the floppy drive and typing:

help and pressing **Enter**

Alternatively, you may print this file on your printer. Consult your DOS manual or word processing software manual for procedures for printing files.

Installing WATEQ4F on your hard disk

The process for installing WATEQ4F on your hard disk consists of:

- Creating one main directory and one subdirectory on the hard disk.
- Copying the files required to run WATEQ4F and WQ4FINPT into the main directory.
- Optionally copying the FORTRAN source files into the subdirectory for later use, if you should want to modify the program in the future.

If you do not foresee ever wanting to modify the WATEQ4F program, or if space on your hard disk is limited, you may want to delete (or not install) the 19 FORTRAN files. Consult your DOS manual for the procedures for deleting files and directories.

The WATEQ4F installation diskette contains an Auto-Install batch program, called INSTALL.BAT, which helps you create the necessary directories on your hard disk, and copy the appropriate files to the directories. To run the Auto-Install program:

1. Start DOS on your computer.

2. Insert the WATEQ4F diskette containing the INSTALL.BAT program into your floppy drive.

3. Change the default drive to the floppy drive. For example, type a: and press Enter.

4. To install from floppy drive A: to hard drive C:, just type **install** and press Enter.

5. If your drives are not A: and C:, type

   install {from-drive} {to-drive} and press Enter

   where {from-drive} and {to-drive} are the floppy and hard drive letters, respectively, for your system (do NOT include colons or the braces). For example, to install from floppy drive B: to hard drive E:, type:

   install b e and press Enter.

6. Respond to the prompts as directed. If the prompt

   Insert disk with batch file
   Press any key to continue . . .

   appears, insert the WATEQ4F installation diskette in your floppy drive and press a key.

7. When the installation is complete, remove the diskette and store it in a safe place.

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ABSTRACT

A FORTRAN 77 version of the PL/1 computer program for the geochemical model WATEQ2, which computes major and trace element speciation and mineral saturation for natural waters, has been developed. The code WATEQ4F has been adapted to execute on an IBM PC[1] or compatible microcomputer with or without an 8087, 80287 or 80387 numeric coprocessor and, if recompilation is desired, a full-featured microcomputer FORTRAN compiler. The calculation procedure is identical to WATEQ2, which has been installed on many mainframes and minicomputers. Several data base revisions have been made that include the addition of Se (-II, 0, IV, VI) and U (III, IV, V, VI) species as well as the recently published values of Nordstrom and others (1990). A new set of redox options has been introduced so that all species that would exist in a disequilibrium system can be independently calculated, or selected species can be coupled, at the desire of the user. This report provides all the reactions and references for the complete data base, instructions for program operation, and an explanation of the input and output files. Attachments contain sample output from four water analyses used as test cases, and the complete source listings for WATEQ4F, its thermodynamic data base, input data preparation program WQ4FINPT, and a batch program to run WATEQ4F. The thermodynamic mass transfer program PHREEQE and the revised version of mass balance program BALANCE (BALN INPT) also have been adapted to execute on a personal microcomputer with the same specifications as those described above.

[1]The use of trade, brand, or product names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

INTRODUCTION

Background

WATEQ4F is a chemical speciation code for natural waters. It uses field measurements of temperature, pH, Eh, dissolved oxygen and alkalinity, and the chemical analysis of a water sample as input and calculates the distribution of aqueous species, ion activities, and mineral saturation indices that indicate the tendency of a water to dissolve or precipitate a set of minerals (see Drever, 1988; Nordstrom and Munoz, 1986). The model assumes homogeneous aqueous phase equilibria, except for redox species. Equilibrium with respect to mineral solubilities is not assumed. The program results are used primarily to examine the tendency of a water to reach mineral solubility equilibria as a constraint on interpreting the chemistry of natural waters. Results also may be used for reaction modeling with the programs BALANCE and PHREEQE.

The original computer program, WATEQ (Truesdell and Jones, 1973, 1974), written in PL/1, has been translated into FORTRAN IV (WATEQF, Plummer and others, 1976). Trace elements have been added (WATEQ2, Ball and others, 1979, 1980); uranium species added (WATEQ3, Ball and others, 1981); and WATEQ2 was translated from PL/1 into FORTRAN 77 (Ball and others, 1987). Additional recommendations for the data base have been made, primarily on the aqueous aluminum species and forms of gibbsite (Nordstrom and others, 1984; Nordstrom and May, 1989). The code described in this report includes the major update and revision of Nordstrom and others (1990). This report describes a revised version of the FORTRAN 77 code for WATEQ4F that has been adapted for operation on a personal microcomputer with or without a math coprocessor, and is named WATEQ4F, Version 2.0. This report replaces the reports of Ball and others (1980, 1981, 1987) as the primary reference and user's manual for program WATEQ4F. The entire library of reactions and thermodynamic data used in WATEQ4F is included in this report. The original translation of WATEQ2 into FORTRAN 77 was made by Zachmann and Baethge (written commun., January, 1985).

The geochemical simulation program PHREEQE (Parkhurst and others, 1980) and a revised version of the mass balance program BALANCE (Parkhurst and others, 1982), which is known as BALN INPT, have been adapted for operation on a personal microcomputer. The reader is referred to the reports of Parkhurst and others (1980, 1982) for full instructions on the operation of PHREEQE and BALANCE. Otherwise, similarly to WATEQ4F, the requirements are a suitably configured IBM PC or compatible with or without a math coprocessor, the PHREEQE or BALN INPT program, and, if recompilation is desired, with a full-featured microcomputer FORTRAN compiler.

Purpose and Scope

This report supersedes earlier Open-File Report 87-50 (Ball and others, 1987), and marks significant changes to the WATEQ4F source code and data base and correction of some errors in the text of Open-File Report 87-50. The present version is designated Version 2.0, and is compatible with Microsoft FORTRAN, Version 4.00 or later, or its equivalent. An executable code that does not use an 8087, 80287 or 80387 numeric coprocessor can be created by recompiling the source code using appropriate compiler options.

The text of this report represents revision of Open-File Report 87-50 to reflect changes made in the code to adapt it to a more extensive variety of computer hardware and software. The primary changes made in the model are: 1) The addition of Se, U, five Fe, Mn, and Ba carbonate reactions, and the $FeCl^+$ and $SrSO_4^o$ complexes to the model calculations; 2) Revision of the user options for the control of redox calculations; 3) Significant revision of the thermodynamic data base, after

Nordstrom and others (1990); 4) Inclusion of the entire WATEQ4F data base in the report. Model results for the test cases in Attachment A have been revised to show use of the new code, and are similar to results using the previous version of WATEQ4F. Most of the changes made to WATEQ4F since publication of Open-File Report 87-50 are described in a comment section at the beginning of the FORTRAN source code, found in Attachment C.

Acknowledgments

The authors wish to gratefully acknowledge the contributions of Neil Dubrovsky (U.S. Geological Survey) for providing the analytical results for test problem number 3 for use in this report, and of Charles Alpers (McGill University, U.S. Geological Survey) for many helpful discussions and suggestions during development of this version of the WATEQ4F model.

SOLUTE SPECIATION CALCULATIONS

Program WATEQ4F solves a set of nonlinear mass action and mass balance equations using the mathematical method known as the continued fraction method (Wigley, 1977). The Davies equation (Davies, 1962) is used in most cases to calculate individual ion activity coefficients for the solute species, because the å parameter required for the Debye Hückel equation frequently cannot be estimated. The WATEQ Debye-Hückel equation developed by Truesdell and Jones (1974) and expanded by Plummer and Busenberg (1982) and Busenberg and others (1984) is used for the major cations and anions:

Ion	å	b
Ca^{2+}	5.0	0.165
Mg^{2+}	5.5	0.20
Na^{+}	4.0	0.075
K^{+}	3.5	0.015
Cl^{-}	3.5	0.015
SO_4^{2-}	5.0	-0.04
HCO_3^{-}	5.4	0.0
CO_3^{2-}	5.4	0.0
$H_2CO_3^{\circ}$	0.0	0.0
Sr^{2+}	5.26	0.121

The extended Debye-Hückel equation is used for the following species because it forms an integral part of the thermodynamic data used for the species (Plummer and Busenberg, 1982; Busenberg and others, 1984; Cloke, 1963a):

Ion	å
H^{+}	9.0
$SrHCO3^{+}$	5.4
$SrOH^{+}$	5.0
$SrCO_3^{\circ}$	0.0
$Cu(S_4)_2^{3-}$	23.0
$CuS_4S_5^{3-}$	25.0
S_2^{2-}	6.5
S_3^{2-}	8.0

S_4^{2-}	10.0
S_5^{2-}	12.0
S_6^{2-}	14.0
$Ag(S_4)_2^{3-}$	22.0
$AgS_4S_5^{3-}$	24.0
$Ag(HS)S_4^{2-}$	15.0

SATURATION INDICES

The main objective of program WATEQ4F is to calculate saturation indices. As expressed so elegantly by Truesdell and Jones (1974):

> A water sample when collected is usually no longer in contact with mineral phases, and these phases may not be accessible to observation. It is of interest then to determine with what mineral phases the water is saturated or nearly so. The calculated activities of the dissolved ions in a water may be combined to produce the appropriate activity product which may be compared with the solubility equilibrium constant to show the degree of saturation of the water with each mineral considered.

The saturation index, (SI) [= $\log_{10}$ (IAP/$K_{sp(T)}$)], is approximately equal to zero when a water is at equilibrium. When the SI is above zero the water is supersaturated with that mineral, and the mineral would tend to precipitate. When the SI is less than zero the water is undersaturated with respect to the mineral, and the mineral would tend to be dissolved by the water. Because of thermodynamic and analytical errors there will be a range of uncertainty for the SI that must be taken into account. This uncertainty will vary according to both the complexity of the mineral stoichiometry and input data errors. Users must be aware of these problems when interpreting output.

LIMITS

The temperature range over which WATEQ4F can be used is 0 to 100 degrees Celsius. However, users are cautioned that uncertainties increase when there are large departures from 25°C. The effect of pressure is not calculated in WATEQ4F because for the majority of natural waters it can be neglected (Truesdell and Jones, 1974; Nordstrom and Munoz, 1986).

Speciation calculations show reliable results up to the ionic strength of seawater (0.72), although saturation indices frequently agree well with calculations using the Pitzer (1979) model at ionic strengths slightly greater than seawater. The discrepancies between the ion association model as calculated by WATEQ4F and the Pitzer specific ion interaction model depend upon the charge on the ions and the degree of certainty with which the equilibrium constants are known.

Charge imbalance is calculated using the following formula:

$$\Delta\% = \frac{\text{(Sum of Cation Species - Sum of Anion Species)*100}}{\text{(Sum of Cation Species + Sum of Anion Species)/2}} \quad (1)$$

Thus, the maximum value of the result of this calculation is ±200 percent. This means that a value for Δ% of zero denotes exact electrical balance, whereas departures of more than 10 percent suggest errors in the analytical input values. This charge imbalance calculation is twice the charge

imbalance normally computed. However, it is more appropriate to compare the cation/anion imbalance with the average of the cations and anions than with their sum.

THERMODYNAMIC DATA

The number assigned to the specific chemical reaction used in the computer code, the reaction, selected reaction enthalpy (ΔH_r°) and equilibrium reaction constant (log K_r°) values, and the sources of the thermodynamic data are given in table 2. Because of its length, table 2 follows the References in the text of this report. The most precise and internally consistent sets of data available for the solubility product constants and ion association constants in the $CaCO_3$-CO_2-H_2O system and in the $SrCO_3$-CO_2-H_2O system are those of Plummer and Busenberg (1982) and Busenberg and others (1984), respectively. These data are included in WATEQ4F. Two errors in Nordstrom and others (1990) are corrected in this report. They are the enthalpy and log K values for the $AlSO_4^+$ and $Al(SO_4)_2^-$ aqueous species, reactions 87 and 88 in table 2, respectively. Thermodynamic data revisions for gypsum, talc, sepiolite, muscovite, and chlorite were made but the use of solubility product constants (K_{sp}) for smectites, illites, chlorites, micas, feldspars, amphiboles, pyroxenes and pyrophyllites is not recommended at this time, because these phases have not demonstrated reversible, equilibrium solubility behavior (Nordstrom and others, 1990). Bisulfate ion association constants are given or estimated for Fe^{2+}, Fe^{3+}, Ca^{2+}, and Al^{3+} because of their importance in very acid waters such as some mine waters issuing from oxidizing ore deposits. Data for uranium reactions are from Grenthe and others (1990) where available. Data for aqueous uranium (IV) phosphate complexes are not given. These complexes are known to exist, but reliable data are not available at this time (Grenthe and others, 1990). The number of significant figures given in table 2 is not consistent because uncertainties in thermodynamic data are reaction-specific.

PROGRAM OPERATION

System Requirements

Program WATEQ4F is written in FORTRAN 77, and requires a minimum configuration of an IBM PC or full compatible with at least 512 kilobytes (KB, 1KB=1024 bytes, or characters) of random access memory (RAM). The packed executable code and supporting files occupy about 350KB of disk storage. The FORTRAN source code occupies about 200KB of disk storage. The program described in this report has been compiled, linked, and executed correctly on an IBM PC/AT with 640KB of RAM, an 80287 numeric coprocessor, and a 20MB hard disk, using Microsoft FORTRAN, Version 4.00. It also has been compiled, linked, and executed correctly on several similarly configured 8088, 80286 and 80386 based IBM PC compatibles with and without numeric coprocessor, and using other full-featured microcomputer FORTRAN compilers. For linking of the object code, the linker supplied with the compiler should be used. It was found by experiment that substitute linkers produced object codes that would not execute.

The test cases were solved on the PC/AT in an average time of less than 20 seconds each, including output of the results to a disk file. This should represent an upper limit of execution time for this class of computer with a numeric coprocessor, since the first test case in particular contains a fairly comprehensive array of constituents and output options. The size of the output file varies as a function of the complexity of the input and the print options selected, but will occupy approximately 25-50KB of disk storage per data set. The results obtained using the PC are virtually identical to those obtained using the U.S. Geological Survey Prime 850 minicomputer, exhibiting

minor differences in the fifth or greater significant digit for less than one percent of the calculated results.

Executing WATEQ4F

To execute WATEQ4F, initiate execution of batch program WQ4F.BAT by typing WQ4F and pressing Enter. To initiate execution of WATEQ4F external to WQ4F.BAT, verify that the input data file you want to process is named WATEQ4F.DAT, then type WATEQ4F and press Enter. To initiate execution of the BASIC version of WQ4FINPT external to WQ4F.BAT, type the command you normally use to invoke your BASIC language program, followed by a space and WQ4FINPT, and press Enter. For IBM PC DOS, the BASIC program should be named BASICA. For MS DOS, the name should be GWBASIC. Program WQ4F.BAT uses the BASICA command. If your BASIC language program is a name other than BASICA, you may either use a line editor to edit WQ4F.BAT so that the invoking command matches the name of your BASIC language program or copy or rename your BASIC program file to BASICA.EXE. If you do not have a BASIC language interpreter, you will have to use the FORTRAN version of WQ4FINPT. To modify WQ4F.BAT to execute the FORTRAN version, use a line editor to remove the "BASICA" from the beginning of the line that invokes WQ4FINPT. To initiate execution of the FORTRAN version external to WQ4F.BAT, type WQ4FINPT and press Enter.

Input

The data base for the calculation of mineral and solute reactions and their accompanying thermodynamic data is read initially, from two separate files named TABLE1 and TABLE2. The use of two separate files facilitates future expansion of the data base, in that species are just appended to their respective file, rather than the file having to be expanded in the middle for insertion of data. Files TABLE3, TABL3A, and TABLE4 contain index numbers of all mineral phases, index numbers of a subset of mineral phases selected by the authors, and index numbers of all solute species, respectively.

User-supplied input of water analyses to WATEQ4F is read from a disk file that must be named WATEQ4F.DAT. The input format has been modified extensively to conform to constraints in the FORTRAN language, as compared with PL/1. The number of records per input data set is not fixed. To facilitate preparation of input data sets, a separate computer program, called WQ4FINPT, is included in this report. The interpreted BASIC source code for this program is found in Attachment D, and the source code for a FORTRAN version of WQ4FINPT is found in Attachment E. Batch program WQ4F.BAT, the code for which is found in Attachment F, has been written to facilitate formatting input data sets, running the program and producing printed output.

Expanded sets of printing (PRNT) and redox (EHOPT) options have been added to WATEQ4F. Generation of a printable disk file of the thermodynamic data base may be specified in addition to suppression of printing of some of the output. The CORALK, PRNT and PUNCH options are as follows:

CORALK	0 =	alkalinity input has NOT been corrected for noncarbonate alkalinity
	1 =	alkalinity input HAS been corrected for noncarbonate alkalinity
	2 =	alkalinity input is in terms of total inorganic carbon
PRNT	0 =	print minimum output (aqueous species ≥ 1% of master species input, selected subset of mineral saturation indices, no mole ratios)
	1 =	include complete aqueous speciation and mineral solubility listing

2 = include mole ratios page
3 = 1 plus 2
4 = 0 plus generate thermodynamic data table
5 = 1 plus generate thermodynamic data table
6 = 2 plus generate thermodynamic data table
7 = 3 plus generate thermodynamic data table

PUNCH 0 = generate a disk file of selected parameters for input to plotting program
1 = omit generation of the disk file

Redox Options

To allow greater flexibility in the use of the various redox values calculated by WATEQ4F, a user now may specify in the input data set which one of 14 input or calculated Eh values known to WATEQ4F is to be used in 9 separate areas of the program where redox calculations are done. The areas of calculation using the above redox parameters are:

EHOPT id
1 = Fe species distribution
2 = Mn species with a valence other than +2
3 = Cu species having a valence of +1
4 = As species distribution
5 = Se species distribution
6 = Ion activity product calculations
7 = Calculation of the partial pressure of atmospheric O_2
8 = Calculation of the activity of H_2S from input SO_4, pH and Eh
9 = U species distribution

The 14 possible Eh values that can be specified as an EHOPT parameter are:

Eh index #
0 = Measured Eh
1 = Eh calculated from the Fe^{2+}/Fe^{3+} activity ratio
2 = Eh calculated from the O_2/H_2O_2 activity ratio using the Sato relation
3 = Eh calculated from the O_2/H_2O activity ratio using the classical relation
4 = Eh calculated from the NH_4/NO_3 activity ratio
5 = Eh calculated from the $S^{=}/SO_4$ activity ratio
6 = Eh calculated from the NO_2/NO_3 activity ratio
7 = Eh calculated from the $S^{=}/S(s)$ activity ratio
8 = Eh calculated from the As^{3+}/As^{5+} activity ratio
9 = Eh calculated from the $As(s)/As^{3+}$ activity ratio
10= Eh calculated from the Se^{4+}/Se^{6+} activity ratio
11= Eh calculated from the $Se(s)/Se^{4+}$ activity ratio
12= Eh calculated from the $Se^{2-}/Se(s)$ activity ratio
13= Eh calculated from the U^{4+}/UO_2^{2+} activity ratio

Input concentrations of the members of the couples must be supplied for a selected option to have any effect. It must be emphasized that the above species are the only ones for which redox calculations are done. Note specifically that redox distributions of S and N species are not performed, with the exception of the calculation of the activity of H_2S from input SO_4, pH and Eh. As an example of the use of the Eh options, suppose you have a water analysis that includes analytical values for Fe(II) and Fe(III) and dissolved oxygen, but has no measured Eh value. Now, suppose

further that you want to use the Eh calculated from the activities of Fe^{2+} and Fe^{3+} to perform redox distribution of Mn and As and to calculate ion activity products of minerals, and to use the pe calculated from dissolved oxygen using the classical relation to perform redox distribution of Cu and to calculate the partial pressure of atmospheric O_2, but to use the pe calculated from dissolved oxygen using the Sato relation to calculate the activity of H_2S. You would set the EHOPT values as follows:

EHOPT(1) = 0 (would have no effect since the presence of redox species analysis takes precedence over the EHOPT settings)
EHOPT(2) = 1 = Eh calculated from the Fe^{2+}/Fe^{3+} activity ratio
EHOPT(3) = 3 = Eh calculated from the O_2/H_2O activity ratio using the classical relation
EHOPT(4) = 1 = Eh calculated from the Fe^{2+}/Fe^{3+} activity ratio
EHOPT(5) = 0 (no Se to distribute)
EHOPT(6) = 1 = Eh calculated from the Fe^{2+}/Fe^{3+} activity ratio
EHOPT(7) = 3 = Eh calculated from the O_2/H_2O activity ratio using the classical relation
EHOPT(8) = 2 = Eh calculated from the O_2/H_2O_2 activity ratio using the Sato relation
EHOPT(9) = 0 (no U to distribute)

As a second example of Eh option usage, suppose you have a set of samples with complete water analyses, but no analytical redox species, no dissolved oxygen measurement and no measured Eh value. You will have available the Eh calculations from NH_4/NO_3, NO_2/NO_3, and H_2S/SO_4, but you know from your previous experiences with geochemical modeling that Eh calculated from H_2S/SO_4 is seldom reflective of solution Eh, and that the two species hardly ever exist at thermodynamic equilibrium in solution in measurable quantities. Furthermore, you know that at least one of the nitrogen species is usually present at a concentration near the detection limit, hence that its determination frequently is subject to large uncertainties. Unfortunately, which species this applies to varies from sample to sample. You decide that you want to test both of these calculated Eh values as fully as possible in each sample, so you can decide which one to use in each sample for all the calculations, in a subseqent run of WATEQ4F. You decide to set the Eh options as follows:

EHOPT(1) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
EHOPT(2) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
EHOPT(3) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
EHOPT(4) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
EHOPT(5) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
EHOPT(6) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
EHOPT(7) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
EHOPT(8) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
EHOPT(9) = 4 = Eh calculated from the NH_4/NO_3 activity ratio

As a final precautionary summary for geochemical modeling of oxidation-reduction reactions, the user should always remember the following:

1. There is no such thing as an "Eh" or "pe" of a natural water (Thorstenson, 1984; Hostettler, 1984).
2. Redox couples do not tend to reach equilibrium with each other in natural waters. Redox disequilibrium is the general rule (see, for example, Lindberg and Runnells, 1984).
3. Only dissolved iron, dissolved sulfide and possibly dissolved uranium and vanadium are likely to give reversible potential measurements for a platinum electrode, and then only when the concentrations are high enough.

4. Arsenic and Se, and probably all oxyanions, do not give reversible potentials at a platinum electrode (Runnells and Lindberg, 1990; Runnells and Skoda, 1990).
5. Redox reactions usually are kinetically controlled and many are microbially mediated. Hence, individual redox species must be analytically determined. The WATEQ4F program was designed for this contingency.
6. A useful general classification and guide for describing redox environments is presented by Berner (1981).

Description of Input Variables

A list of all the optional analytical input constituents and their assigned reference numbers is in table 1. The required input is as follows:

Record	Variable Name	Variable	FORTRAN Format	Comments
1	CHECK	start-of-data-set record	A4	four asterisks
2	CARD1	sample description	A80	
3	CARD2	Physical and chemical parameters carried through to plot program:		
		conductivity	F5.0	$\mu S/cm^2$ at 25°C
		total dissolved solids	F6.0,1X	parts per million
		date, year, month, day	F6.0	yymmdd
		discharge	F8.0	cu ft/sec
		dissolved organic carbon	F8.0	mg/L
		salinity	F8.0	parts per thousand
		Cr, Co, Mo, V	4F8.0	
4		dummy record	A80	ignored by program
5	TEMP	temperature	F8.2,1X	°C, 0 to 100 only
	PH	pH, measured in field	F8.2,1X	
	EHM	Eh, measured in field	F8.2,1X	volts
	DOC	dissolved organic carbon	F8.2,1X	mg/L
	DOX	dissolved oxygen	F8.2,1X	mg/L
	CORALK	alkalinity correction flag	I8	0, 1 or 2
6		dummy record	A80	ignored by program
7	FLG	units in which remaining concentrations are expressed	A4	options: MQ/L, MG/L, PPM, MMOL, MOL
	DENS	density	F11.5	
	PRNT	print option	I6	0 through 7
	PUNCH	punch option	I6,6X	0 or 1
	EHOPT(1)	Eh option for Fe redox species	I3	0 through 13
	EHOPT(2)	Eh option for Mn redox species	I3	0 through 13
	EHOPT(3)	Eh option for Cu redox species	I3	0 through 13
	EHOPT(4)	Eh option for As redox species	I3	0 through 13
	EHOPT(5)	Eh option for Se redox species	I3	0 through 13
	EHOPT(6)	Eh option for IAP calculations	I3	0 through 13
	EHOPT(7)	Eh option for pO_2 calculations	I3	0 through 13
	EHOPT(8)	Eh option for H_2S calculation	I3	0 through 13
	EHOPT(9)	Eh option for U redox species	I3	0 through 13
8		dummy record	A80	ignored by program
9	ITDS	analytical TDS	8X,F8.2,1X	parts per million
	COND	specific conductance	F8.2,1X	$\mu S/cm^2$ at 25°C
	SIGMDO	dissolved oxygen sigma	F12.4	
	SIGMEH	Eh sigma	F12.4	
	SIGMPH	pH sigma	F12.4	
10		dummy record	A80	ignored by program
11	CUNITS(I)	Ca, Mg, Na, K, Cl, SO_4	6F12.4	in FLG units
12		dummy record	A80	ignored by program
13	CUNITS(I)	HCO_3, Fe^{tot}, H_2S, CO_3, SiO_2^{tot}, NH_4	6F12.4	in FLG units
14		dummy record	A80	ignored by program
15	CUNITS(I)	B^{tot}, PO_4, Al, F, NO_3	5F12.4	in FLG units
16		dummy record	A80	ignored by program
17 to n-1, where n=# of records in the data set	WORD J CUNITS(J), SIGMA(J), LOGKTO(J)	additional concentration values, sigma values, or replacement $\log_{10}K_r^o$ values: record type identifier subscript concentration, sigma, or log K values	A4,1X I3,1X F12.5	'CUN','SIGM','LOKT' 0 to 653 numerical value for referenced quantity
n		blank-final record in a data set		REQUIRED

Table 1. Reference Numbers for Optional Analytical Input Constituents

Number	Ionic Constituent	Charge	Number	Ionic Constituent	Charge
7	Fe	2	204	Ni	2
8	Fe	3	212	Ag	1
48	Cs	1	249	As total	0
80	Li	1	261	As^3 tot	0
87	Sr	2	262	As^5 tot	0
89	Ba	2	284	Fulvate	-2
94	Rb	1	285	Humate	-2
96	I	-1	298	Se total	0
97	Br	-1	299	H_2Se	0
109	Mn	2	300	Se^4 tot	0
130	Cu	2	301	Se^6 tot	0
145	Zn	2	316	U total	0
160	Cd	2	317	U	4
182	Pb	2	359	U^6 tot	0
202	NO_2	-1			

Output

For the water analysis data, output is placed in a disk file named WATEQ4F.OUT. First, a listing of the input data is written, which includes the species name, index number, and input concentration of each species, as well as the values of all other parameters entered. Results of the anion mass balance calculations follow in the form: CO_2, SO_4, F, PO_4, Cl, H_2S, fulvic, and humic. When mass balance convergence to within 0.1 percent is obtained (or 40 iterations have been done), a table of distribution of aqueous species is written. If convergence to 0.1 percent or better is not obtained after 40 iterations, a warning message is printed and execution continues as though convergence were obtained. Both the sums of analytical and calculated milliequivalents per kilogram cation and anion values, and analytical and calculated specific conductance are listed for comparison. The percentage differences in the input and calculated charge balances are computed and displayed. The total (based on the input data) and the effective (calculated after speciation) ionic strengths are displayed for comparison. Numerous input and calculated solution parameters also are listed, including temperature, pH, and Eh and pe calculated using various redox couples.

The concentration of each aqueous species with a value greater than one mole percent of the input concentration of its master species, or all species greater than $1X10^{-78}$ molal, as selected by user option, is listed in parts per million, molality, mole percent of master species, and activity, as well as the individual ion activity coefficient and the negative log activity of each species. This is followed by a table of analytical molality ratios and log activity ratios, if selected by user option. A table follows of the mineral equilibrium calculations for a selected subset of, or all (as selected by user option) solid phases for which an activity product has been calculated, printed in the following order: the reaction number, the name of the solid phase, the computed saturation index [$\log_{10}(IAP/K_{sp(T)})$], the $\log_{10}(IAP)$, the analytical propagated standard deviation in the $\log_{10}$ of the ion activity product,

$\log_{10}(K_{sp(T)})$, and the uncertainty in the $\log_{10}$ of the equilibrium constant. The lists of solute and mineral species have been arranged in alphabetical order for convenience in locating species of interest. All the above is written to the disk file WATEQ4F.OUT for subsequent printing.

By specifying a value for PRNT of 4, 5, 6 or 7 in an input data set, WATEQ4F can be directed to produce a disk file containing the permanent data base in tabular form, followed by a table of the analytical expressions for the temperature dependence of selected equilibrium constants, and by a listing of the names and reference numbers of all possible analytical input constituents. This information is written into a separate file, named TABLES.OUT, on the default disk drive, for later printing at the user's convenience.

TEST CASES AND PROGRAM LISTINGS

Attachment A contains a listing of the output from WATEQ4F of calculations for four test problems. The first two test cases appear in Ball and others (1980, 1987), and are from Nordstrom and others (1979). The third test case is the analysis of a well water containing measurable concentrations of Se (IV), Se (VI) and total As. The fourth test case is the U test case of Ball and others (1981), taken from Potter and others (1979). Test case 1 is a seawater analysis, which contains concentrations for virtually every species available for consideration by WATEQ4F, and is of relatively high (0.7) ionic strength. Test case 2 is a surface water analysis and is much more dilute, but also contains a fairly complete array of analytical values. These two test cases are described in more detail by Nordstrom and others (1979). Test case 2 demonstrates the capability of the model for computing independent Eh (pe) values based on analytical determinations of Fe (II/III), dissolved oxygen, NO_3, NO_2, NH_3, and S (VI/-II). Test case 3 is a real analysis that demonstrates the model's capability for computing Eh (pe) values based on total As plus measured Eh, and on Se (IV/VI) determinations. These analyses were provided to us by Neil Dubrovsky of the California District Office, Water Resources Division, U.S. Geological Survey. Test case 4 is a real analysis of a U-containing water which demonstrates the capabilities of WATEQ4F for U speciation and mineral equilibrium calculations.

Users are cautioned that the Davies and Debye-Hückel equations are used in WATEQ4F to calculate the activity coefficients of all charged species except Ca, Mg, Na, K, Cl, SO_4, HCO_3, CO_3, H_2CO_3 and Sr. The ion-association models on which these two equations are based become less valid as ionic strengths increase above the seawater value of 0.7. Hence, results obtained for solutions of ionic strengths significantly higher than 0.7 always should be interpreted with caution.

Attachment B gives a listing of the TABLE1 and TABLE2 permanent data base files used by WATEQ4F. Attachment C gives a listing of the Version 2.0 FORTRAN source code. Attachment D gives the interpreted BASIC source code for WQ4FINPT, and the source code for a FORTRAN version of this program is given in Attachment E. The listing for batch program WQ4F.BAT is found in Attachment F.

PROGRAM PHREEQE

PHREEQE (Parkhurst and others, 1980) is a FORTRAN 77 computer program designed to model geochemical reactions, and is, like WATEQ4F, based on an ion pairing aqueous model. This program can calculate pH, redox potential, and mass transfer (amounts of solid or gaseous phases entering or leaving the aqueous phase) as a function of reaction progress, and can calculate the

composition of solutions in equilibrium with multiple phases. PHREEQE is an attractive alternative tool for the interpretation and investigation of geochemical processes, and is well-suited to adaptation for execution on a microcomputer. Thus, PHREEQE was modified to be run on an IBM PC or compatible with or without an 8087, 80287 or 80387 numeric coprocessor, using the report of Parkhurst and others (1980) as a source of program documentation and running instructions.

PROGRAM BALANCE

PC BALN INPT (Prestemon, E. C., written commun., 1989) is a FORTRAN 77 computer program adapted from the mainframe version of BALN INPT, which is a revision of program BALANCE (Parkhurst and others, 1982). BALN INPT calculates the mass transfer necessary to account for the observed change in composition between two solutions. The program also can help to define and quantify chemical reactions that take place between ground water and minerals. BALN INPT also is particularly well-suited for execution on a microcomputer. Program documentation and running instructions can be found in Parkhurst and others (1982).

SUMMARY

The WATEQ2 geochemical model by Ball and others has been translated into FORTRAN 77, and Se and U have been added to the model. This WATEQ version is called WATEQ4F, Version 2.0. WATEQ4F, the PHREEQE geochemical reaction simulation program by Parkhurst and others, and the BALN INPT mass transfer calculation program by Parkhurst and others have been adapted for operation on an IBM or compatible personal microcomputer with or without an 8087, 80287 or 80387 math coprocessor or FORTRAN compiler. The codes are known to execute correctly on an IBM PC/AT with 20MB hard disk and 640KB RAM, and on many similarly configured 8088, 80286 and 80386 microcomputers. For WATEQ4F, the data base and computer code have been extensively revised from WATEQ2, and many changes have been made in the calculation options and in the appearance of the output. This program has been used for a wide variety of natural waters, including many types of ground waters, acid mine waters, river waters and lake waters that occur in a wide variety of host rocks. WATEQ4F can be very useful as one of several tools used for the interpretation of the chemistry of natural waters.

The source code and documentation for WATEQ4F, PC PHREEQE and PC BALN INPT may be obtained by contacting:

U.S. Geological Survey
Water Resources Division
437 National Center
12201 Sunrise Valley Drive
Reston, Virginia 22092

Attn: Robin Sevin

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Table 2. Thermodynamic Data

ΔH_r^o is enthalpy of reaction; Log K_r^o is equilibrium constant for the reaction; kcal/mol is kilocalories per mole; 1σ is the uncertainty in the listed value.

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
0	kFe +3	$Fe^{2+} = Fe^{3+} + e^-$	9.68±0.5	47	-13.02±0.01	47
1	kFeOH +2	$Fe^{3+} + H_2O = FeOH^{2+} + H^+$	10.4±0.2	47	-2.19±0.02	47
2	kFeOH +	$Fe^{2+} + H_2O = FeOH^+ + H^+$	13.2±1.6	3	-9.5±0.1	3
3	kFe(OH)3 -	$Fe^{2+} + 3H_2O = Fe(OH)_3^- + 3H^+$	30.3±3.6	3	-31.0±1.5	3
4	kFeSO4 +	$Fe^{3+} + SO_4^{2-} = FeSO_4^+$	3.91	47	4.04	47
5	kFeCl +2	$Fe^{3+} + Cl^- = FeCl^{2+}$	5.6	69	1.48	69
6	kFeCl2 +	$Fe^{3+} + 2Cl^- = FeCl_2^+$	---[2]	---[2]	2.13	69
7	kFeCl3 aq	$Fe^{3+} + 3Cl^- = FeCl_3^o$	---[2]	---[2]	1.13	79
8	kFeSO4 aq	$Fe^{2+} + SO_4^{2-} = FeSO_4^o$	3.23	4,45	2.25	4,45,69
9	Siderite (d)[3]	$FeCO_3 = Fe^{2+} + CO_3^{2-}$	---[2]	---[2]	-10.45	47
10	Magnesite	$MgCO_3 = Mg^{2+} + CO_3^{2-}$	-6.169	64	-8.029	32
11	Dolomite (d)	$CaMg(CO_3)_2 = Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	-11.09	47	-16.54	47
12	Calcite	$CaCO_3 = Ca^{2+} + CO_3^{2-}$	-2.297±0.3[4]	53	-8.48±0.02	53
		$\log K_r = -171.9065-0.077993T+2839.319/T+71.595\log_{10}T$				
13	kH3SiO4 -	$H_4SiO_4^o = H^+ + H_3SiO_4^-$	6.12[4]	47	-9.83	47
		$\log K_r = -302.3724-0.050698T+15669.69/T-1.119669*10^6/T^2+108.18466\log_{10}T$				
14	kH2SiO4 -2	$H_4SiO_4^o = 2H^+ + H_2SiO_4^{2-}$	17.6[4]	47	-23.0	47
		$\log K_r = -294.0184-0.07265T+11204.49/T-1.119669*10^6/T^2+108.18466\log_{10}T$				
15	kHPO4 -2	$H + PO_4^{3-} = HPO_4^{2-}$	-3.49±0.9	21	12.5±0.03	21
16	kH2PO4 -	$2H^+ + PO_4^{3-} = H_2PO_4^-$	-4.35±1.1	21	19.56±0.03	21
17	Anhydrite	$CaSO_4 = Ca^{2+} + SO_4^{2-}$	-1.71[4]	47	-4.36	47
		$\log K_r = 197.52-8669.8/T-69.835\log_{10}T$				
18	Gypsum	$CaSO_4 \cdot 2H_2O = Ca^{2+} + SO_4^{2-} + 2H_2O$	-0.109[4]	47	-4.58±0.02	47
		$\log K_r = 68.2401-3221.51/T-25.0627\log_{10}T$				
19	Brucite	$Mg(OH)_2 + 2H^+ = Mg^{2+} + 2H_2O$	-27.1	47	16.84	47
20	Chrysotile	$Mg_3Si_2O_5(OH)_4+6H^+ = 3Mg^{2+}+2H_4SiO_4^o+H_2O$	-46.8[4]	47	32.20	47
		$\log K_r = 13.248+10217.1/T-6.1894\log_{10}T$				

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
21	Aragonite	$CaCO_3 = Ca^{2+} + CO_3^{2-}$	-2.589±0.3[4]	53	-8.336±0.020	53
		log K_r= -171.9773-0.077993T+2903.293/T+71.595Log_{10}T				
22	kMgF +	$Mg^{2+} + F^- = MgF^+$	3.2	47	1.82	47
23	kCaSO4 aq	$Ca^{2+} + SO_4^{2-} = CaSO_4^\circ$	1.65	47	2.30	47
24	kMgOH +	$Mg^{2+} + H_2O = MgOH^+ + H^+$	15.952[5]	39	-11.44±0.05	47
25	kH3BO3 aq	$H_3BO_3^\circ = H^+ + H_2BO_3^-$	3.224	40	-9.240	40
26	kNH3 aq	$NH_4^+ = NH_3^\circ + H^+$	12.48	44	-9.252	44
27	Forsterite	$Mg_2SiO_4 + 4H^+ = 2Mg^{2+} + H_4SiO_4^\circ$	-48.578[5]	64	28.306[5]	64
28	Diopside	$CaMgSi_2O_6 + 4H^+ + 2H_2O = Ca^{2+} + Mg^{2+} + 2H_4SiO_4^\circ$	-32.348[5]	64	19.894[5]	64
29	Clinoenstatite	$MgSiO_3 + 2H^+ + H_2O = Mg^{2+} + H_4SiO_4^\circ$	-20.049[5]	64	11.342[5]	64
30	kNaHPO4 -	$Na^+ + HPO_4^{2-} = NaHPO_4^-$	---[2]	---[2]	0.29	54
31	Tremolite	$Ca_2Mg_5Si_8O_{22}(OH)_2+14H^+ +8H_2O = 2Ca^{2+}+5Mg^{2+}+8H_4SiO_4^\circ$	-96.853[5]	64	56.574[5]	64
32	kKHPO4 -	$K^+ + HPO_4^{2-} = KHPO_4^-$	---[2]	---[2]	0.29	54
33	kMgHPO4 aq	$Mg^{+2} + HPO_4^{2-} = MgHPO_4^\circ$	3.3	15	2.870	67
34	kCaHPO4 aq	$Ca^{+2} + HPO_4^{2-} = CaHPO_4^\circ$	3.3	15	2.739	15
35	kH2CO3 aq	$HCO_3^- + H^+ = H_2CO_3^\circ$	-2.247[4]	53	6.351±0.01	53
		log K_r= 356.3094+0.0609196T-21834.37/T-126.8339Log_{10}T+1684915/T^2				
36	Sepiolite(c)	$Mg_2Si_3O_{7.5}OH\cdot 3H_2O+0.5H_2O+4H^+ = 2Mg^{2+}+3H_4SiO_4^\circ$	-10.7	47	15.76	47
37	Talc	$Mg_3Si_4O_{10}(OH)_2+4H_2O+6H^+=3Mg^{2+}+4H_4SiO_4^\circ$	-46.352	63	21.399±2.0	63
38	Hydromagnesite	$Mg_5(CO_3)_4(OH)_2\cdot 4H_2O + 2H^+ = 5Mg^{2+} + 4CO_3^{2-} + 6H_2O$	-52.244[5]	62	-8.762[5]	62
39	Adularia	$KAlSi_3O_8 + 8H_2O = K^+ + Al(OH)_4^- + 3H_4SiO_4^\circ$	30.82	64	-20.573	64
40	Albite	$NaAlSi_3O_8 + 8H_2O = Na^+ + Al(OH)_4^- + 3H_4SiO_4^\circ$	25.896	64	-18.002	64
41	Anorthite	$CaAl_2Si_2O_8 + 8H_2O = Ca^{2+} + 2Al(OH)_4^- + 2H_4SiO_4^\circ$	11.58	44	-19.714	44
42	Analcime	$NaAlSi_2O_6\cdot H_2O + 5H_2O = Na^+ + Al(OH)_4^- + 2H_4SiO_4^\circ$	18.206	64	-12.701	64
43	Kmica	$KAl_3Si_3O_{10}(OH)_2+10H^+=K^++3Al^{3+}+3H_4SiO_4^\circ$	-59.376	63	12.703±1.3	63
44	Phlogopite	$KMg_3AlSi_3O_{10}(OH)_2 + 10H^+ = K^+ + 3Mg^{2+} + Al^{3+} + 3H_4SiO_4^\circ$	-42.3±4.0	42,63[6]	43.3±3.0	7,42[6]
45	Illite	$K_{0.6}Mg_{0.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 11.2H_2O = 0.6K^+$ $+0.25Mg^{+2} + 2.3Al(OH)_4^- + 3.5H_4SiO_4^\circ + 1.2H^+$	54.684	22	-40.267	22
46	Kaolinite	$Al_2Si_2O_5(OH)_4 + 6H^+ = 2Al^{3+} + 2H_4SiO_4^\circ + H_2O$	-35.3	47	7.435	47

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
47	Halloysite	$Al_2Si_2O_5(OH)_4 + 6H^+ = 2Al^{3+} + 2H_4SiO_4^\circ + H_2O$	-39.82[5]	64	12.498[5]	64
48	Beidellite	$(Na,K,1/2Mg)_{0.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O =$ $0.33(Na,K,1/2Mg)^+ + 2.33Al(OH)_4^- + 3.67H_4SiO_4^\circ + 2H^+$	60.355	22	-45.272	22
49	Chlorite 14A	$Mg_5Al_2Si_3O_{10}(OH)_8+16H^+ = 5Mg^{2+}+2Al^{3+}+3H_4SiO_4^\circ+6H_2O$	-151.494	23	68.380±6.0	23
50	Alunite	$KAl_3(SO_4)_2(OH)_6 = K^+ + 3Al^{3+} + 2SO_4^{2-} + 6OH^-$	-50.25	47	-1.4	47
51	Gibbsite (c)	$Al(OH)_3 + 3H^+ = Al^{3+} + 3H_2O$	-22.8	47	8.11±0.2	47
52	Boehmite	$AlOOH + 3H^+ = Al^{+3} + 2H_2O$	-28.181[5]	64	8.584[5]	64
53	Pyrophyllite	$Al_2Si_4O_{10}(OH)_2 + 12H_2O = 2Al(OH)_4^- + 4H_4SiO_4^\circ + 2H^+$	---[2]	---[2]	-48.314	59
54	Phillipsite	$Na_{0.5}K_{0.5}AlSi_3O_8 \cdot H_2O+7H_2O = 0.5Na^+ + 0.5K^+ + Al(OH)_4^- + 3H_4SiO_4^\circ$	---[2]	---[2]	-19.874	26
55	Erionite	$NaAlSi_{3.5}O_9 \cdot 3H_2O + 6H_2O = Na^+ + Al(OH)_4^- + 3.5H_4SiO_4^\circ$	---[2]	---[2]	---[2]	---[2]
56	Clinoptilolite	$(K,Na)AlSi_5O_{12} \cdot 3.5H_2O+8.5H_2O = (K,Na)^+ + Al(OH)_4^- + 5H_4SiO_4^\circ$	---[2]	---[2]	---[2]	---[2]
57	Mordenite	$(Na,K)AlSi_{4.5}O_{11} \cdot 3H_2O+8H_2O = (Na,K)^+ + Al(OH)_4^- + 4.5H_4SiO_4^\circ$	---[2]	---[2]	---[2]	---[2]
58	Nahcolite	$NaHCO_3 = Na^+ + HCO_3^-$	3.72	34	-0.548	34
59	Trona	$NaHCO_3 \cdot Na_2CO_3 \cdot 2H_2O = 2H_2O + 3Na^+ + CO_3^{2-} + HCO_3^-$	-18.0	34,35,74	-0.795	34,35,74
60	Natron	$Na_2CO_3 \cdot 10H_2O = 2Na^+ + CO_3^{2-} + 10H_2O$	15.745	74,77	-1.311	74,77
61	Thermonatrite	$Na_2CO_3 \cdot H_2O = 2Na^+ CO_3^{2-} + H_2O$	-2.802	34,77	0.125	34,77
62	Fluorite	$CaF_2 = Ca^{2+} + 2F^-$	4.69[4]	47	-10.6±0.02	47
		$\log K_r = 66.348-4298.2/T-25.271\log_{10}T$				
63	Montmorillonite (Ca)	$Ca_{0.17}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O = 0.17Ca^{+2} + 2.33Al(OH)_4^- + 3.67H_4SiO_4^\circ + 2H^+$	58.373	22	-45.027	22
64	Halite	$NaCl = Na^+ + Cl^-$	0.918	64	1.582	64
65	Thenardite	$Na_2SO_4 = 2Na^+ SO_4^{2-}$	-0.572	64	-0.179	64
66	Mirabilite	$Na_2SO_4 \cdot 10H_2O = 2Na^+ + SO_4^{2-} + 10H_2O$	18.987	64	-1.114	64
67	Mackinawite	$FeS + H^+ = Fe^{2+} + HS^-$	---[2]	---[2]	-4.648	5
68	kHCO3 -	$H^+ + CO_3^{2-} = HCO_3^-$	-3.167[4]	53	10.33±0.01	53
		$\log K_r = 107.8871+0.03252849T-5151.79/T-38.92561\log_{10}T+563713.9/T^2$				
69	kNaCO3 -	$Na^+ + CO_3^{2-} = NaCO_3^-$	8.91	47	1.27	47
70	NaHCO3 aq	$Na^+ + HCO_3^- = NaHCO_3^\circ$	---[2]	---[2]	-0.250	20

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
71	kNaSO4 -	$Na^+ + SO_4^{2-} = NaSO_4^-$	1.12	45	0.70±0.05	45
72	kKSO4 -	$K^+ + SO_4^{2-} = KSO_4^-$	2.25±1.0	45	0.85±0.05	45
73	kMgCO3 aq	$Mg^{2+} + CO_3^{2-} = MgCO_3^o$	2.713[4]	47	2.98±0.03	47
		$\log K_r = 0.9910 + 0.00667T$				
74	kMgHCO3 +	$Mg^{2+} + HCO_3^- = MgHCO_3^+$	0.79[4]	47	1.07±0.03	47
		$\log K_r = -59.215+2537.455/T+20.92298Log_{10}T$				
75	kMgSO4 aq	$Mg^{2+} + SO_4^{2-} = MgSO_4^o$	4.55	47	2.37±0.02	47
76	kCaOH +	$Ca^{2+} + H_2O = CaOH^+ + H^+$	---[2]	---[2]	-12.78	47
77	kCaHCO3 +	$Ca^{2+} + HCO_3^- = CaHCO_3^+$	5.410[4]	53	1.11±0.07	53
		$\log K_r = 1209.12+0.31294T-34765.05/T-478.782Log_{10}T$				
78	kCaCO3 aq	$Ca^{2+} + CO_3^{2-} = CaCO_3^o$	4.030[4]	53	3.22±0.14	53
		$\log K_r = -1228.732-0.299444T+35512.75/T+485.818Log_{10}T$				
79	kSrHCO3 +	$Sr^{2+} + HCO_3^- = SrHCO_3^+$	6.047[4]	11	1.18	11
		$\log K_r = -3.248 + 0.014867T$				
80	kAlOH +2	$Al^{3+} + H_2O = AlOH^{2+} + H^+$	11.49[4]	47	-5.00±0.02	47
		$\log K_r = -38.253-656.27/T+14.327Log_{10}T$				
81	kAl(OH)2 +	$Al^{3+} + 2H_2O = Al(OH)_2^+ + 2H^+$	26.90[4]	47	-10.1±0.2	47
		$\log K_r = 88.5-9391.6/T-27.121Log_{10}T$				
82	kAl(OH)4 -	$Al^{3+} + 4H_2O = Al(OH)_4^- + 4H^+$	42.30[4]	47	-22.7±0.3	47
		$\log K_r = 51.578-11168.9/T-14.865Log_{10}T$				
83	kAlF +2	$Al^{3+} + F^- = AlF^{2+}$	1.06	47	7.0	47
84	kAlF2 +	$Al^{3+} + 2F^- = AlF_2^+$	1.98	47	12.7	47
85	kAlF3 aq	$Al^{3+} + 3F^- = AlF_3^o$	2.16	47	16.8	47
86	kAlF4 -	$Al^{3+} + 4F^- = AlF_4^-$	2.20	47	19.4	47
87	kAlSO4 +	$Al^{3+} + SO_4^{2-} = AlSO_4^+$	2.29	47	3.5	47
88	kAl(SO4)2 -	$Al^{3+} + 2SO_4^{2-} = Al(SO_4)_2^-$	3.11	47	5.0	47
89	kHSO4 -	$H^+ + SO_4^{2-} = HSO_4^-$	3.85[4]	47	1.988	47
		$\log K_r = -56.889+0.006473T+2307.9/T+19.8858Log_{10}T$				
90	kH2S/SO4	$SO_4^{2-} + 10H^+ + 8e^- = H_2S^o + 4H_2O$	-65.440	44	40.644	44

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
91	kH2S aq	$H_2S = H^+ + HS^-$	5.300	44	-6.994	44
92	kHS -	$HS^- = H^+ + S^{2-}$	12.100	44	-12.918	44
93	koxy	$0.5H_2O = 0.25O_2(g) + H^+ + e^-$	34.158	17	-20.769	17
94	Siderite (c)	$FeCO_3 = Fe^{2+} + CO_3^{2-}$	-2.48	47	-10.89	47
95	Hydroxyapatite	$Ca_5(PO_4)_3OH + 4H^+ = 5Ca^{2+} + 3HPO_4^{2-} + H_2O$	-36.223[5]	64	-3.421[5]	10
96	Fluorapatite	$Ca_5(PO_4)_3F + 3H^+ = 5Ca^{2+} + 3HPO_4^{2-} + F^-$	-20.07	13,38	-17.6	13,38
97	Chalcedony	$SiO_2 + 2H_2O = H_4SiO_4^\circ$	4.72[4]	47	-3.55	47
		$\log K_r = -0.09-1032/T$				
98	Magadiite	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O = Na^+ + 7H_4SiO_4^\circ$	---[2]	---[2]	-14.300	9
99	Cristobalite	$SiO_2 + 2H_2O = H_4SiO_4^\circ$	5.500	64	-3.587	64
100	Silica gel	$SiO_2 + 2H_2O = H_4SiO_4^\circ$	4.440	64	-3.018	64
101	Quartz	$SiO_2 + 2H_2O = H_4SiO_4^\circ$	5.99[4]	47	-3.98	47
		$\log K_r = 0.41-1309/T$				
102	kFe(OH)2 +	$Fe^{3+} + 2H_2O = Fe(OH)_2^+ + 2H^+$	17.1	47	-5.67±0.1	47
103	kFe(OH)3 aq	$Fe^{3+} + 3H_2O = Fe(OH)_3^\circ + 3H^+$	24.8	47	-12.56	47
104	kFe(OH)4 -	$Fe^{3+} + 4H_2O = Fe(OH)_4^- + 4H^+$	31.9	47	-21.6±0.2	47
105	Fe(OH)2 aq	$Fe^{+2} + 2H_2O = Fe(OH)_2^\circ + 2H^+$	28.6±2.9	3	-20.5±1.0	3
106	Vivianite	$Fe_3(PO_4)_2 \cdot 8H_2O = 3Fe^{2+} + 2PO_4^{3-} + 8H_2O$	---[2]	---[2]	-36.000	50
107	Magnetite	$Fe_3O_4 + 8H^+ = 2Fe^{3+} + Fe^{2+} + 4H_2O$	-50.460	64	3.737	64
108	Hematite	$Fe_2O_3 + 6H^+ = 2Fe^{3+} + 3H_2O$	-30.845	64	-4.008	64
109	Maghemite	$Fe_2O_3 + 6H^+ = 2Fe^{3+} + 3H_2O$	---[2]	---[2]	6.386	32
110	Goethite	$FeOOH + 3H^+ = Fe^{3+} + 2H_2O$	-14.48[5]	64	-1.0±0.8	47
111	Greenalite	$Fe_3Si_2O_5(OH)_4 + 6H^+ = 3Fe^{2+} + 2\,H_4SiO_4^\circ + H_2O$	---[2]	---[2]	20.81[5]	54
112	Ferrihydrite	$Fe(OH)_3 + 3H^+ = Fe^{3+} + 3H_2O$	---[2]	---[2]	4.891	32
113	Annite	$KFe_3AlSi_3O_{10}(OH)_2 + 10H_2O = K^+ + 3Fe^{2+} + Al(OH)_4^- + 3H_4SiO_4^\circ$	62.480	22	-85.645	22
114	Pyrite	$FeS_2 + 2H^+ + 2e^- = Fe^{2+} + 2HS^-$	11.300	64	-18.479	64
115	Montmorillonite	$(H,Na,K)_{0.28}Mg_{0.29}Fe^{3+}_{0.23}Al_{1.58}Si_{3.93}O_{10}(OH)_2 + 10.04H_2O =$	---[2]	---[2]	-34.913	30
	Belle Fourche	$0.28(H,Na,K)^+ + 0.29Mg^{2+} + 0.23Fe^{3+} + 1.58Al(OH)_4^- + 3.93H_4SiO_4^\circ$				

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
116	Montmorillonite	$(H,Na,K)_{0.42}Mg_{0.45}Fe^{3+}_{0.34}Al_{1.47}Si_{3.82}O_{10}(OH)_2+9.16H_2O+$	---[2]	---[2]	-29.688	31
	Aberdeen	$0.84H^+ = 0.42(H,Na,K)^+ + 0.45Mg^{2+} + 0.34Fe^{3+} + 1.47Al(OH)_4^- + 3.82H_4SiO_4^o$				
117	Huntite	$CaMg_3(CO_3)_4 = 3Mg^{2+} + Ca^{2+} + 4CO_3^{2-}$	-25.760	25	-29.968	25
118	Greigite	$Fe_3S_4 + 4H^+ = 2Fe^{3+} + Fe^{2+} + 4HS^-$	---[2]	---[2]	-45.035[7]	54
119	FeS ppt	$FeS + H^+ = Fe^{2+} + HS^-$	---[2]	---[2]	-3.915	5
120	kFeH2PO4 +	$Fe^{2+} + H_2PO_4^- = FeH_2PO_4^+$	---[2]	---[2]	2.700	50
121	kCaPO4 -	$Ca^{2+} + PO_4^{3-} = CaPO_4^-$	3.100	15	6.459	15
122	kCaH2PO4 +	$Ca^{2+} + H_2PO_4^- = CaH_2PO_4^+$	3.400	15	1.408	15
123	kMgPO4 -	$Mg^{2+} + PO_4^{3-} = MgPO_4^-$	3.100	74	6.589	74
124	kMgH2PO4 +	$Mg^{2+} + H_2PO_4^- = MgH_2PO_4^+$	3.400	74	1.513	74
125	Chlorite 7A	$Mg_5Al_2Si_3O_{10}(OH)_8+16H^+ = 5Mg^{2+}+2Al^{3+}+3H_4SiO_4^o+6H_2O$	-155.261	23	71.752±6.0	23
126	kLiSO4 -	$Li^+ + SO_4^{2-} = LiSO_4^-$	---[2]	---[2]	0.640	67
127	kNH4/NO3	$NH_4^+ + 3H_2O = NO_3^- + 10H^+ + 8e^-$	187.055[8]	44	-119.077[8]	44
128	Laumontite	$CaAl_2Si_4O_{12}\cdot 4H_2O + 8H_2O = Ca^{2+} + 2Al(OH)_4^- + 4H_4SiO_4^o$	---[2]	---[2]	-30.96	54
129	kSrOH +	$Sr^{2+} + H_2O = SrOH^+ + H^+$	---[2]	---[2]	-13.29	47
130	kBaOH +	$Ba^{2+} + H_2O = BaOH^+ + H^+$	---[2]	---[2]	-13.47	47
131	kNH4SO4 -	$NH^+ + SO_4^{2-} = NH_4SO_4^-$	---[2]	---[2]	1.110	67
132	Blank		---[9]	---[9]	---[9]	---[9]
133	Jarosite(ss)	$[K_{0.77}Na_{0.03}(H_3O)_{0.2}]Fe_3(SO_4)_2(OH)_6+5.8H^+ =$	---[2]	---[2]	-9.83	2
		$0.77K^+ + 0.03Na^+ + 3Fe^{3+} + 2SO_4^{2-} + 6.2H_2O$				
134	Mn2(SO4)3	$Mn_2(SO_4)_3 = 2Mn^{3+} + 3SO_4^{2-}$	-39.06	54	-5.711	54
135	kSrCO3 aq	$Sr^{2+} + CO_3^{2-} = SrCO_3^o$	5.217[4]	11	2.81	11
		$\log K_r = -1.019+0.012826T$				
136	kO2 Sato	$0.5H_2O = 0.25O_2(aq) + H^+ + e^-$	---[2]	---[2]	-11.748	27
137	kCO2 aq	$CO_2\ (g) + H_2O = H_2CO_3^o$	-4.776[4]	47	-1.468	47
		$\log K_r = 108.3865+0.01985076T-6919.53/T-6.69365*10^5/T^2-40.45154Log_{10}T$				
138	kFeHPO4 aq	$Fe^{2+} + HPO_4^{2-} = FeHPO_4^o$	---[2]	---[2]	3.600	50
139	kFeHPO4 +	$Fe^{3+} + HPO_4^{2-} = FeHPO_4^+$	5.76	43	5.43	48
140	Al(OH)3 (a)	$Al(OH)_3 + 3H^+ = Al^{3+} + 3H_2O$	-26.5	47	10.8	47

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
141	Prehnite	$Ca_2Al_2Si_3O_{10}(OH)_2+8H_2O+2H^+ = 2Ca^{+2}+2Al(OH)_4^-+3H_4SiO_4^\circ$	10.39	80	-11.695	80
142	Strontianite	$SrCO_3 = Sr^{2+} + CO_3^{2-}$	-0.401[4]	11	-9.271±0.02	11
		log K_r= 155.0305-7239.594/T-56.58638Log_{10}T				
143	Celestite	$SrSO_4 = Sr^{2+} + SO_4^{2-}$	-1.037[4]	47	-6.63	47
		log K_r= -14805.9622-2.4660924T+756968.533/T-4.05536*$10^7/T^2$+5436.3588Log_{10}T				
144	Barite	$BaSO_4 = Ba^{2+} + SO_4^{2-}$	6.35[4]	47	-9.97±0.02	47
		log K_r= 136.035-7680.41/T-48.595Log_{10}T				
145	Witherite	$BaCO_3 = Ba^{2+} + CO_3^{2-}$	0.703[4]	47	-8.562	47
		log K_r= 607.642+0.121098T-20011.25/T-236.4948Log_{10}T				
146	Strengite	$FePO_4 \cdot 2H_2O = Fe^{3+} + PO_4^{3-} + 2H_2O$	-2.030	64	-26.400	49
147	Leonhardite	$Ca_2Al_4Si_8O_{24} \cdot 7H_2O + 17H_2O = 2Ca^{+2} + 4Al(OH)_4^- + 8H_4SiO_4^\circ$	90.070	64	-69.756	64
148	kFeHSO4 +	$Fe^{2+} + HSO_4^- = FeHSO_4^+$	---[2]	---[2]	1.08	37
149	Nesquehonite	$MgCO_3 \cdot 3H_2O = Mg^{2+} + CO_3^{2-} + 3H_2O$	-5.789	29	-5.621	44
150	Artinite	$MgCO_3 \cdot Mg(OH)_2 \cdot 3H_2O + 2H^+ = 2Mg^{2+} + CO_3^{2-} + 5H_2O$	-28.742	29	9.6[5]	54
151	kO2 calc	$0.5H_2O = 0.25O_2(aq) + H^+ + e^-$	33.457	44	-20.775	27
152	kw	$H_2O = H^+ + OH^-$	13.362[4]	47	-14.000	47
		log K_r= -283.971-0.05069842T+13323/T-1.119669*$10^6/T^2$+102.24447Log_{10}T				
153	Sepiolite(d)	$Mg_2Si_3O_{7.5}OH \cdot 3H_2O+0.5H_2O+4H^+ = 2Mg^{2+}+3H_4SiO_4^\circ$	---[2]	---[2]	18.66	78
154	Diaspore	$AlOOH + 3H^+ = Al^{3+} + 2H_2O$	-24.681[5]	44	6.879[5]	44
155	Wairakite	$CaAl_2Si_4O_{12} \cdot 2H_2O + 10H_2O = Ca^{2+} + 2Al(OH)_4^- + 4H_4SiO_4^\circ$	26.140	80	-26.708	80
156	kFeH2PO4 +2	$Fe^{3+} + H_2PO_4^- = FeH_2PO_4^{2+}$	---[2]	---[2]	5.43	50
157	Allophane(a)	$[Al(OH)_3]_{(1-x)}[SiO_2]_x+(3-3x)H^+ = (1-x)Al^{3+}+xH_4SiO_4^\circ+(3-5x)H_2O$	---[2]	---[2]	6.06[10]	52
		log K_r= -5.7+1.68pH				
158	Allophane(P)	$[Al(OH)_3]_{(1-x)}[SiO_2]_x+(3-3x)H^+ = (1-x)Al^{3+}+xH_4SiO_4^\circ+(3-5x)H_2O$	---[2]	---[2]	5.24[10]	52
		log K_r= -5.4+1.52pH				
159	kFeHSO4 +2	$Fe^{3+} + HSO_4^- = FeHSO_4^{2+}$	---[2]	---[2]	2.48	37
160	kCaF +	$Ca^{2+} + F^- = CaF^+$	4.12	47	0.94	47
161	kBF(OH)3 -	$H_3BO_3^\circ + F^- = BF(OH)_3^-$	1.85	46	-0.4	46
162	kBF2(OH)2 -	$H_3BO_3^\circ + H^+ + 2F^- = BF_2(OH)_2^- + H_2O$	1.618[5]	46	7.63[5]	46

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
163	kBF3OH -	$H_3BO_3^o + 2H^+ + 3F^- = BF_3OH^- + 2H_2O$	-1.614[5]	46	13.67[5]	46
164	kBF4 -	$H_3BO_3^o + 3H^+ + 4F^- = BF_4^- + 3H_2O$	-1.846[5]	46	20.28[5]	46
165	kFeF +2	$Fe^{3+} + F^- = FeF^{2+}$	2.7	46	6.2	46
166	kFeF2 +	$Fe^{3+} + 2F^- = FeF_2^+$	4.8	46	10.8	46
167	kFeF3 aq	$Fe^{3+} + 3F^- = FeF_3^o$	5.4	46	14.0	46
168	kCaHSO4 +	$Ca^{2+} + HSO_4^- = CaHSO_4^+$	---[2]	---[2]	1.08	---[11]
169	kMn +3	$Mn^{2+} = Mn^{3+} + e^-$	25.8	47	-25.51	47
170	kMnCl +	$Mn^{2+} + Cl^- = MnCl^+$	---[2]	---[2]	0.61	47
171	kMnCl2 aq	$Mn^{2+} + 2Cl^- = MnCl_2^o$	---[2]	---[2]	0.25	47
172	kMnCl3 -	$Mn^{2+} + 3Cl^- = MnCl_3^-$	---[2]	---[2]	-0.31	47
173	kMnOH +	$Mn^{2+} + H_2O = MnOH^+ + H^+$	14.4	3	-10.59±0.04	3
174	kMn(OH)3 -	$Mn^{2+} + 3H_2O = Mn(OH)_3^- + 3H^+$	---[2]	---[2]	-34.8	3
175	kMnF +	$Mn^{2+} + F^- = MnF^+$	---[2]	---[2]	0.84	47
176	kMnSO4 aq	$Mn^{2+} + SO_4^{2-} = MnSO_4^o$	3.37	47	2.25	47
177	kMn(NO3)2 aq	$Mn^{2+} + 2NO_3^- = Mn(NO_3)_2^o$	-0.396	54	0.6	69
178	kMnHCO3 +	$Mn^{2+} + HCO_3^- = MnHCO_3^+$	---[2]	---[2]	1.95	47
179	kMnO4 -	$Mn^{2+} + 4H_2O = MnO_4^- + 8H^+ 5e^-$	176.62	54	-127.824	54
180	kMnO4 -2	$Mn^{2+} + 4H_2O = MnO_4^{2-} + 8H^+ + 4e^-$	150.02	54	-118.44	54
181	Fe(OH)2.7Cl.3	$Fe(OH)_{2.7}Cl_{0.3} + 2.7H^+ = Fe^{3+} + 2.7H_2O + 0.3\ Cl^-$	---[2]	---[2]	-3.04	6
182	MnSO4	$MnSO_4 = Mn^{2+} + SO_4^{2-}$	-15.48	54	2.669	54
183	Pyrolusite	$MnO_2 + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$	-65.11	47	41.38	47
184	Birnessite	$MnO_2 + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$	---[2]	---[2]	43.601	47
185	Nsutite	$MnO_2 + 4H^+ + 2e^- = Mn^{2+} + 2H_2O$	---[2]	---[2]	42.564	47
186	Bixbyite	$Mn_2O_3 + 6H^+ = 2Mn^{3+} + 3H_2O$	-15.245	54	-0.611	54
187	Hausmannite	$Mn_3O_4 + 8H^+ + 2e^- = 3Mn^{2+} + 4H_2O$	-100.64	47	61.03	47
188	Pyrochroite	$Mn(OH)_2 + 2H^+ = Mn^{2+} + 2H_2O$	---[2]	---[2]	15.2	47
189	Manganite	$MnOOH + 3H^+ + e^- = Mn^{2+} + 2H_2O$	---[2]	---[2]	25.34	47
190	Rhodochrosite (d)	$MnCO_{3(synthetic)} = Mn^{2+} + CO_3^{2-}$	---[2]	---[2]	-10.39	47
191	MnCl2, 4H2O	$MnCl_2 \cdot 4H_2O = Mn^{2+} + 2Cl^- + 4H_2O$	17.38	54	2.71	54

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
192	MnS Green	$MnS_{(green)} + H^+ = Mn^{2+} + HS^-$	-5.79	54	3.8	54
193	Mn3(PO4)2	$Mn_3(PO_4)_2 = 3Mn^{2+} + 2PO_4^{3-}$	2.12	54	-23.827	54
194	MnHPO4	$MnHPO_4 = Mn^{2+} + HPO_4^{2-}$	---[2]	---[2]	-12.947	54
195	α-Cryptomelane	$K_{0.8}Mn^{2+}_{0.6}Mn^{4+}_8O_{17}+34H^+ = 16Mn^{3+}+0.8K^++17H_2O-7.4Mn^{2+}$	---[2]	---[2]	---[2]	57,36[2]
196	Hollandite	$Ba_{0.82}Fe^{2+}_{0.57}Mn^{2+}_{0.59}Mn^{4+}_7O_{16} + 32H^+ =$ $14Mn^{3+} + 0.82Ba^{2+} + 0.57Fe^{2+} + 16H_2O$ - $6.41Mn^{2+}$	---[2]	---[2]	---[2]	12[2]
197	Psilomelane	$Ba_{0.78}Ca_{0.19}K_{0.03}Mn^{2+}Mn^{4+}_7O_{16}\cdot 2.5H_2O + 31.97H^+ =$ $0.78Ba^{2+} + 0.19Ca^{2+} + 0.03K^+ + 14Mn^{3+} + 18.485H_2O$ - $6Mn^{2+}$	---[2]	---[2]	---[2]	8[2]
198	Todorokite	$Ca_{0.393}Mg_{0.473}Mn^{2+}_{1.134}Mn^{4+}_5O_{12}\cdot 2H_2O + 24H^+ =$ $0.393Ca^{2+} + 0.473Mg^{2+} + 10Mn^{3+} + 14H_2O$ - $6Mn^{2+}$	---[2]	---[2]	---[2]	73[2]
199	Lithiophorite	$Li_2Al_8Mn^{2+}_2Mn^{4+}_{10}O_{35}\cdot 14H_2O + 70H^+ =$ $2Li^+ + 8Al^{3+} + 20Mn^{3+}$ $49H_2O$ - $8Mn^{2+}$	---[2]	---[2]	---[2]	76[2]
200	Rancieite	$Ca_{0.44}Mn^{2+}_{0.56}Mn^{4+}_4O_9\cdot 3H_2O + 18H^+ =$ $0.44Ca^{2+} + 8Mn^{3+} + 12H_2O$ - $3.44Mn^{2+}$	---[2]	---[2]	---[2]	60[2]
201	kSiF6 -2	$H_4SiO_4^o + 4H^+ + 6F^- = SiF_6^{2-} + 4H_2O$	-16.26	61	30.18	61
202	kHF aq	$H^+ + F^- = HF^o$ $\log K_r = -2.033+0.012645T+429.01/T$	3.18[4]	47	3.18±0.01	47
203	kHF2 -	$H^+ + 2F^- = HF_2^-$	4.55	47	3.76±0.06	47
204	Jarosite Na	$NaFe_3(SO_4)_2(OH)_6 + 6H^+ = Na^+ + 3Fe^{3+} + 2SO_4^{2-} + 6H_2O$	-36.18	4	-5.28±1.0	2
205	Jarosite K	$KFe_3(SO_4)_2(OH)_6 + 6H^+ = K^+ + 3Fe^{3+} + 2SO_4^{2-} + 6H_2O$	-31.28	4	-9.21±1.1	2
206	kCuCl2 -	$Cu^{2+} + 2Cl^- + e^- = CuCl_2^-$	1.23	22,44	8.22	69
207	kCuCl3 -2	$Cu^{2+} + 3Cl^- + e^- = CuCl_3^{2-}$	1.91	22,44	8.42	69
208	kCu +	$Cu^{2+} + e^- = Cu^+$	1.65	44	2.72	44
209	kCuCO3 aq	$Cu^{2+} + CO_3^{2-} = CuCO_3^o$	---[2]	---[2]	6.73±0.05	3
210	kCu(CO3)2 -2	$Cu^{2+} + 2CO_3^{2-} = Cu(CO_3)_2^{2-}$	---[2]	---[2]	9.83±0.04	3
211	kCuCl +	$Cu^{2+} + Cl^- = CuCl^+$	8.65	22	0.43	44
212	kCuCl2 aq	$Cu^{2+} + 2Cl^- = CuCl_2^o$	10.56	22	0.16	44
213	kCuCl3 -	$Cu^{2+} + 3Cl^- = CuCl_3^-$	13.69	22	-2.29	22
214	kCuCl4 -2	$Cu^{2+} + 4Cl^- = CuCl_4^{2-}$	17.78	22	-4.59	22

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
215	kCuF +	$Cu^{2+} + F^- = CuF^+$	1.62	44	1.26	44
216	kCuOH +	$Cu^{2+} + H_2O = CuOH^+ + H^+$	---[2]	---[2]	-8.0	3
217	kCu(OH)2 aq	$Cu^{2+} + 2H_2O = Cu(OH)_2^\circ + 2H^+$	---[2]	---[2]	-13.68	75
218	kCu(OH)3 -	$Cu^{2+} + 3H_2O = Cu(OH)_3^- + 3H^+$	---[2]	---[2]	-26.9	75
219	kCu(OH)4 -2	$Cu^{2+} + 4H_2O = Cu(OH)_4^{2-} + 4H^+$	---[2]	---[2]	-39.6	3
220	kCu2(OH)2 +2	$2Cu^{2+} + 2H_2O = Cu_2(OH)_2^{2+} + 2H^+$	17.539[4]	3	-10.359	3
		$\log K_r = 2.497\text{-}3833/T$				
221	kCuSO4 aq	$Cu2+ + SO_4^{2-} = CuSO_4^\circ$	1.22	45	2.31	3
222	kCu(HS)3 -	$Cu^{2+} + 3HS^- = Cu(HS)_3^-$	---[2]	---[2]	25.9	43
223	Cu Metal	$Cu = Cu^+ + e^-$	17.13	44	-8.76	44
224	Nantokite	$CuCl = Cu^+ + Cl^-$	9.98	44	-6.76	44
225	CuF	$CuF = Cu^+ + F^-$	-12.37	41	7.08	41
226	Cuprite	$Cu_2O + 2H^+ = 2Cu^+ + H_2O$	6.245	44	-1.55	44
227	Chalcocite	$Cu_2S + H^+ = 2Cu^+ + HS^-$	49.35	56	-34.619±0.16	56
228	Cu2SO4	$Cu_2SO_4 = 2Cu^+ + SO_4^{2-}$	-4.56	41	-1.95	19
229	Cuprous Ferrite	$CuFeO_2 + 4H^+ = Cu^+ + Fe^{3+} + 2H_2O$	-3.80	44	-8.92	44
230	Melanothallite	$CuCl_2 = Cu^{2+} + 2Cl^-$	-12.32	41	3.73	44
231	CuCO3	$CuCO_3 = Cu^{2+} + CO_3^{2-}$	---[2]	---[2]	-9.63	69
232	CuF2	$CuF_2 = Cu^{2+} + 2F^-$	-13.32	41	-0.62	41
233	CuF2, 2H2O	$CuF_2 \cdot 2H_2O = Cu^{2+} + 2F^- + 2H_2O$	-3.65	41	-4.55	41
234	Cu(OH)2	$Cu(OH)_2 + 2H^+ = Cu^{2+} + 2H_2O$	-15.25	41	8.64	3
235	Malachite	$Cu_2(OH)_2CO_3 + 3H^+ = 2Cu^{2+} + 2H_2O + HCO_3^-$	-19.76	44	5.15±0.08	3
236	Azurite	$Cu_3(OH)_2(CO_3)_2 + 4H^+ = 3Cu^{2+} + 2H_2O + 2HCO_3^-$	-30.87	44	3.75±0.09	3
237	Atacamite	$Cu_2(OH)_3Cl + 3H^+ = 2Cu^{2+} + 3H_2O + Cl^-$	-18.69	41	7.34	44
238	Cu2(OH)3NO3	$Cu_2(OH)_3NO_3 + 3H^+ = 2Cu^{2+} + 3H_2O + NO_3^-$	-17.35	41	9.24	44
239	Antlerite	$Cu_3(OH)_4SO_4 + 4H^+ = 3Cu^{2+} + 4H_2O + SO_4^{2-}$	---[2]	---[2]	8.29	44
240	Brochantite	$Cu_4(OH)_6SO_4 + 6H^+ = 4Cu^{2+} + 6H_2O + SO_4^{2-}$	---[2]	---[2]	15.34±0.16	69
241	Langite	$Cu_4(OH)_6SO_4 \cdot H_2O + 6H^+ = 4Cu^{2+} + 7H_2O + SO_4^{2-}$	-39.61	44	16.79	44
242	Tenorite	$CuO + 2H^+ = Cu^{2+} + H_2O$	-15.24	44	7.62	3

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
243	CuOCuSO4	$CuO \cdot CuSO_4 + 2H^+ = 2Cu^{2+} + H_2O + SO_4^{2-}$	-35.575	41	11.53	41
244	Cu3(PO4)2	$Cu_3(PO_4)_2 = 3Cu^{2+} + 2PO_4^{3-}$	---[2]	---[2]	-36.85	44
245	Cu3(PO4)2, 3H2O	$Cu_3(PO_4)_2 \cdot 3H_2O = 3Cu^{2+} + 2PO_4^{3-} + 3H_2O$	---[2]	---[2]	-35.12	41
246	Covellite	$CuS + H^+ = Cu^{2+} + HS^-$	24.01	56	-22.27±0.03	66
247	CuSO4	$CuSO_4 = Cu^{2+} + SO_4^{2-}$	-18.14	41	3.01	44
248	Chalcanthite	$CuSO_4 \cdot 5H_2O = Cu^{2+} + SO_4^{2-} + 5H_2O$	1.44	44	-2.64	44
249	Cupric Ferrite	$CuFe_2O_4 + 8H^+ = Cu^{2+} + 2Fe^{3+} + 4H_2O$	-38.69	44	5.88	44
250	Chalcopyrite	$CuFeS_2 + 2H^+ = Cu^{2+} + Fe^{2+} + 2HS^-$	35.48	41	-35.27	41
251	kZnCl +	$Zn^{2+} + Cl^- = ZnCl^+$	7.79	22	0.43	69
252	kZnCl2 aq	$Zn^{2+} + 2Cl^- = ZnCl_2^o$	8.5	22	0.45	--[12]
253	kZnCl3 -	$Zn^{2+} + 3Cl^- = ZnCl_3^-$	9.56	22	0.5	69
254	kZnCl4 -2	$Zn^{2+} + 4Cl^- = ZnCl_4^{2-}$	10.96	22	0.2	69
255	kZnF +	$Zn^{2+} + F^- = ZnF^+$	2.22	43	1.15	69
256	kZnOH +	$Zn^{2+} + H_2O = ZnOH^+ + H^+$	13.4	3	-8.96±0.05	3
257	kZn(OH)2 aq	$Zn^{2+} + 2H_2O = Zn(OH)_2^o + 2H^+$	---[2]	---[2]	-16.9	3
258	kZn(OH)3 -	$Zn^{2+} + 3H_2O = Zn(OH)_3^- + 3H^+$	---[2]	---[2]	-28.4±0.2	3
259	kZn(OH)4 -2	$Zn^{2+} + 4H_2O = Zn(OH)_4^{2-} + 4H^+$	---[2]	---[2]	-41.2±0.1	3
260	kZnOHCl aq	$Zn^{2+} + H_2O + Cl^- = ZnOHCl^o + H^+$	---[2]	---[2]	-7.48	44
261	kZn(HS)2 aq	$Zn^{2+} + 2HS^- = Zn(HS)_2^o$	---[2]	---[2]	14.94	43
262	kZn(HS)3 -	$Zn^{2+} + 3HS^- = Zn(HS)_3^-$	---[2]	---[2]	16.10	43
263	kZnSO4 aq	$Zn^{2+} + SO_4^{2-} = ZnSO_4^o$	1.36	14	2.37	45
264	kZn(SO4)2 -2	$Zn^{2+} + 2SO_4^{2-} = Zn(SO_4)_2^{2-}$	---[2]	---[2]	3.28	45
265	Zn Metal	$Zn = Zn^{2+} + 2e^-$	-36.78	44	25.757	44
266	Zn(BO2)2	$Zn(BO_2)_2 + 2H_2O + 2H^+ = Zn^{2+} + 2H_3BO_3^o$	---[2]	---[2]	8.29	44
267	ZnCl2	$ZnCl_2 = Zn^{2+} + 2Cl^-$	-17.48	44	7.03	44
268	Smithsonite	$ZnCO_3 = Zn^{2+} + CO_3^{2-}$	-4.36	44	-10.00	69
269	ZnCO3, H2O	$ZnCO_3 \cdot H_2O = Zn^{2+} + CO_3^{2-} + H_2O$	---[2]	---[2]	-10.26	44
270	ZnF2	$ZnF_2 = Zn^{2+} + 2F^-$	-13.08	44	-1.52	44
271	Zn(OH)2 (a)	$Zn(OH)_{2(amorph)} + 2H^+ = Zn^{2+} + 2H_2O$	---[2]	---[2]	12.45	3

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
272	Zn(OH)2 (c)	$Zn(OH)_{2(cryst)} + 2H^+ = Zn^{2+} + 2H_2O$	---[2]	---[2]	12.2	65
273	Zn(OH)2 (b)	$Zn(OH)_{2(\beta)} + 2H^+ = Zn^{2+} + 2H_2O$	---[2]	---[2]	11.75±0.02	3
274	Zn(OH)2 (g)	$Zn(OH)_{2(\gamma)} + 2H^+ = Zn^{2+} + 2H_2O$	---[2]	---[2]	11.71	3
275	Zn(OH)2 (e)	$Zn(OH)_{2(\epsilon)} + 2H^+ = Zn^{2+} + 2H_2O$	---[2]	---[2]	11.50±0.03	3
276	Zn2(OH)3Cl	$Zn_2(OH)_3Cl + 3H^+ = 2Zn^{2+} + 3H_2O + Cl^-$	---[2]	---[2]	15.2	44
277	Zn5(OH)8Cl2	$Zn_5(OH)_8Cl_2 + 8H^+ = 5Zn^{2+} + 8H_2O + 2Cl^-$	---[2]	---[2]	38.5	28
278	Zn2(OH)2SO4	$Zn_2(OH)_2SO_4 + 2H^+ = 2Zn^{2+} + 2H_2O + SO_4^{2-}$	---[2]	---[2]	7.5	44
279	Zn4(OH)6SO4	$Zn_4(OH)_6SO_4 + 6H^+ = 4Zn^{2+} + 6H_2O + SO_4^{2-}$	---[2]	---[2]	28.4	28
280	Zn(NO3)2, 6H2O	$Zn(NO_3)_2 \cdot 6H_2O = Zn^{2+} + 2NO_3^- + 6H_2O$	5.51	44	3.44	44
281	ZnO (a)	$ZnO_{(active)} + 2H^+ = Zn^{2+} + H_2O$	---[2]	---[2]	11.31	3
282	Zincite (c)	$ZnO_{(cryst)} + 2H^+ = Zn^{2+} + H_2O$	-21.86	44	11.14	3
283	Zn3O(SO4)2	$ZnO \cdot 2ZnSO_4 + 2H^+ = 3Zn^{2+} + 2SO_4^{2-} + H_2O$	-62.0	44	19.02	44
284	Zn3(PO4)2,4w	$Zn_3(PO_4)_2 \cdot 4H_2O = 3Zn^{2+} + 2PO_4^{3-} + 4H_2O$	---[2]	---[2]	-32.04	43
285	ZnS (a)	$ZnS_{(amorph)} + H^+ = Zn^{2+} + HS^-$	3.67	19	-9.052	19
286	Sphalerite (c)	$ZnS_{(sphaler)} + H^+ = Zn^{2+} + HS^-$	8.25	44	-11.618	44
287	Wurtzite	$ZnS_{(wurtz)} + H^+ = Zn^{2+} + HS^-$	5.06	44	-9.682	28
288	ZnSiO3	$ZnSiO_3 + 2H^+ + H_2O = Zn^{2+} + H_4SiO_4^\circ$	-18.27	44	2.93	19
289	Willemite	$Zn_2SiO_4 + 4H^+ = 2Zn^{2+} + H_4SiO_4^\circ$	-33.37	44	15.33	44
290	Zincosite	$ZnSO_4 = Zn^{2+} + SO_4^{2-}$	-19.20	44	3.01	44
291	ZnSO4, H2O	$ZnSO_4 \cdot H_2O = Zn^{2+} + SO_4^{2-} + H_2O$	-10.64	44	-0.57	44
292	Bianchite	$ZnSO_4 \cdot 6H_2O = Zn^{2+} + SO_4^{2-} + 6H_2O$	-0.16	44	-1.765	44
293	Goslarite	$ZnSO_4 \cdot 7H_2O = Zn^{2+} + SO_4^{2-} + 7H_2O$	3.3	44	-1.96	44
294	kCdCl +	$Cd^{2+} + Cl^- = CdCl^+$	0.59	44	1.98±0.03	69
295	kCdCl2 aq	$Cd^{2+} + 2Cl^- = CdCl_2^\circ$	1.24	44	2.6±0.1	69
296	kCdCl3 -	$Cd^{2+} + 3Cl^- = CdCl_3^-$	3.90	44	2.4±0.1	69
297	kCdF +	$Cd^{2+} + F^- = CdF^+$	---[2]	---[2]	1.1	28
298	kCdF2 aq	$Cd^{2+} + 2F^- = CdF_2^\circ$	---[2]	---[2]	1.5	28
299	kCd(CO3)2 -2	$Cd^{2+} + 2CO_3^{2-} = Cd(CO_3)_2^{2-}$	---[2]	---[2]	6.4	72
300	kCdOH +	$Cd^{2+} + H_2O = CdOH^+ + H^+$	13.1	3	-10.08±0.1	3

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
301	kCd(OH)2 aq	$Cd^{2+} + 2H_2O = Cd(OH)_2^o + 2H^+$	---[2]	---[2]	-20.35±0.2	3
302	kCd(OH)3 -	$Cd^{2+} + 3H_2O = Cd(OH)_3^- + 3H^+$	---[2]	---[2]	-33.3	3
303	kCd(OH)4 -2	$Cd^{2+} + 4H_2O = Cd(OH)_4^{2-} + 4H^+$	---[2]	---[2]	-47.35±0.1	3
304	kCd2OH +3	$2Cd^{2+} + H_2O = Cd_2OH^{3+} + H^+$	10.9	3	-9.39±0.05	3
305	kCdOHCl aq	$Cd^{2+} + H_2O + Cl^- = CdOHCl^o + H^+$	4.355	44	-7.404	44
306	kCdNO3 +	$Cd^{2+} + NO_3^- = CdNO_3^+$	-5.20	43	0.4	28
307	kCdSO4 aq	$Cd^{2+} + SO_4^{2-} = CdSO_4^o$	1.08	45	2.46	69
308	kCdHS +	$Cd^{2+} + HS^- = CdHS^+$	---[2]	---[2]	10.17	43
309	kCd(HS)2 aq	$Cd^{2+} + 2HS^- = Cd(HS)_2^o$	---[2]	---[2]	16.53	43
310	kCd(HS)3 -	$Cd^{2+} + 3HS^- = Cd(HS)_3^-$	---[2]	---[2]	18.71	43
311	kCd(HS)4 -2	$Cd^{2+} + 4HS^- = Cd(HS)_4^{2-}$	---[2]	---[2]	20.90	43
312	Cd Metal	$Cd = Cd^{2+} + 2e^-$	-18.0	44	13.49	44
313	Gamma Cd	$Cd_{(\gamma)} = Cd^{2+} + 2e^-$	-18.14	44	13.59	44
314	Cd(BO2)2	$Cd(BO_2)_2 + 2H_2O + 2H^+ = Cd^{2+} + 2H_3BO_3^o$	---[2]	---[2]	9.84	44
315	Otavite	$CdCO_3 = Cd^{2+} + CO_3^{2-}$	-0.019	72	-12.1±0.1	72
316	CdCl2	$CdCl_2 = Cd^{2+} + 2Cl^-$	-4.47	44	-0.68	44
317	CdCl2, H2O	$CdCl_2 \cdot H_2O = Cd^{2+} + 2Cl^- + H_2O$	-1.82	44	-1.71	44
318	CdCl2, 2.5H2O	$CdCl_2 \cdot 2.5H_2O = Cd^{2+} + 2Cl^- + 2.5H_2O$	1.71	44	-1.94	44
319	CdF2	$CdF_2 = Cd^{2+} + 2F^-$	-9.72	19	-2.98	19
320	Cd(OH)2 (a)	$Cd(OH)_{2(amorph)} + 2H^+ = Cd^{2+} + 2H_2O$	-20.77	44	13.73	44
321	Cd(OH)2 (c)	$Cd(OH)_{2(cryst)} + 2H^+ = Cd^{2+} + 2H_2O$	---[2]	---[2]	13.65±0.04	3
322	CdOHCl	$CdOHCl + H^+ = Cd^{2+} + H_2O + Cl^-$	-7.407	44	3.52	44
323	Cd3(OH)4SO4	$Cd_3(OH)_4SO_4 + 4H^+ = 3Cd^{2+} + 4H_2O + SO_4^{2-}$	---[2]	---[2]	22.56	44
324	Cd3(OH)2(SO4)2	$Cd_3(OH)_2(SO_4)_2 + 2H^+ = 3Cd^{2+} + 2H_2O + 2SO_4^{2-}$	---[2]	---[2]	6.71	44
325	Cd4(OH)6SO4	$Cd_4(OH)_6SO_4 + 6H^+ = 4Cd^{2+} + 6H_2O + SO_4^{2-}$	---[2]	---[2]	28.4	28
326	Monteponite	$CdO + 2H^+ = Cd^{2+} + H_2O$	-24.76	44	13.77	18
327	Cd3(PO4)2	$Cd_3(PO_4)_2 = 3Cd^{2+} + 2PO_4^{3-}$	---[2]	---[2]	-32.6	44
328	CdSiO3	$CdSiO_3 + H_2O + 2H^{2+} = Cd^{2+} + H_4SiO_4^o$	-16.63	44	9.06	44
329	CdSO4	$CdSO_4 = Cd^{2+} + SO_4^{2-}$	-14.74	44	-0.10	44

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
330	CdSO4, H2O	$CdSO_4 \cdot H_2O = Cd^{2+} + SO_4^{2-} + H_2O$	-7.52	44	-1.657	44
331	CdSO4, 2.7H2O	$CdSO_4 \cdot 2.67H_2O = Cd^{2+} + SO_4^{2-} + 2.67H_2O$	-4.30	44	-1.873	44
332	Greenockite	$CdS + H^+ = Cd^{2+} + HS^-$	16.36	44	-15.93	44
333	kFe(SO4)2 -	$Fe^{3+} + 2SO_4^{2-} = Fe(SO_4)_2^-$	4.60	47	5.38	47
334	kFe2(OH)2 +4	$2Fe^{3+} + 2H_2O = Fe_2(OH)_2^{4+} + 2H^+$	13.5	3	-2.95±0.05	3
335	kFe3(OH)4 +5	$3Fe^{3+} + 4H_2O = Fe_3(OH)_4^{5+} + 4H^+$	14.3	3	-6.3±0.1	3
336	kAl(OH)3 aq	$Al^{3+} + 3H_2O = Al(OH)_3^\circ + 3H^+$	39.89[4]	47	-16.9	47
		$\log K_r = 226.374 - 18247.8/T - 73.597 \log_{10} T$				
337	Jarosite H	$(H_3O)Fe_3(SO_4)_2(OH)_6 + 5H^+ = 3Fe^{3+} + 2SO_4^{2-} + 7H_2O$	-55.15	4	-5.39	4
338	Alum K	$KAl(SO_4)_2 \cdot 12H_2O = K^+ + Al^{3+} + 2SO_4^{2-} + 12H_2O$	7.22	4	-5.17	4
339	Melanterite	$FeSO_4 \cdot 7H_2O = Fe^{2+} + SO_4^{2-} + 7H_2O$	4.91[4]	47	-2.209	47
		$\log K_r = 1.447 - 0.004153T - 2.14949 * 10^5/T^2$				
340	Epsomite	$MgSO_4 \cdot 7H_2O = Mg^{2+} + SO_4^{2-} + 7H_2O$	2.82	45	-2.14	45
341	kPbCl +	$Pb^{2+} + Cl^- = PbCl^+$	4.38	14	1.60	44
342	kPbCl2 aq	$Pb^{2+} + 2Cl^- = PbCl_2^\circ$	1.08	22	1.80	44
343	kPbCl3 -	$Pb^{2+} + 3Cl^- = PbCl_3^-$	2.17	22	1.7	69
344	kPbCl4 -2	$Pb^{2+} + 4Cl^- = PbCl_4^{2-}$	3.53	22	1.38	22
345	kPb(CO3)2 -2	$Pb^{2+} + 2CO_3^{2-} = Pb(CO_3)_2^{2-}$	---[2]	---[2]	10.64	24
346	kPbF +	$Pb^{2+} + F^- = PbF^+$	---[2]	---[2]	1.25	44
347	kPbF2 aq	$Pb^{2+} + 2F^- = PbF_2^\circ$	---[2]	---[2]	2.56	44
348	kPbF3 -	$Pb^{2+} + 3F^- = PbF_3^-$	---[2]	---[2]	3.42	67
349	kPbF4 -2	$Pb^{2+} + 4F^- = PbF_4^{2-}$	---[2]	---[2]	3.1	67
350	kPbOH +	$Pb^{2+} + H_2O = PbOH^+ + H^+$	---[2]	---[2]	-7.71±0.1	3
351	kPb(OH)2 aq	$Pb^{2+} + 2H_2O = Pb(OH)_2^\circ + 2H^+$	---[2]	---[2]	-17.12±0.1	3
352	kPb(OH)3 -	$Pb^{2+} + 3H_2O = Pb(OH)_3^- + 3H^+$	---[2]	---[2]	-28.06±0.05	3
353	kPb2OH +3	$2Pb^{2+} + H_2O = Pb_2OH^{3+} + H^+$	---[2]	---[2]	-6.36±0.1	3
354	kPbNO3 +	$Pb^{2+} + NO_3^- = PbNO_3^+$	---[2]	---[2]	1.17±0.02	69
355	kPbSO4 aq	$Pb^{2+} + SO_4^{2-} = PbSO_4^\circ$	---[2]	---[2]	2.75±0.1	69
356	kPb(HS)2 aq	$Pb^{2+} + 2HS^- = Pb(HS)_2^\circ$	---[2]	---[2]	15.27	43

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
357	kPb(HS)3 -	$Pb^{2+} + 3HS^- = Pb(HS)_3^-$	---[2]	---[2]	16.57	43
358	kPb3(OH)4 +2	$3Pb^{2+} + 4H_2O = Pb_3(OH)_4^{2+} + 4H^+$	26.5	3	-23.88±0.2	3
359	kFeF +	$Fe^{2+} + F^- = FeF^+$	---[2]	---[2]	1.0	47
360	Pb Metal	$Pb = Pb^{2+} + 2e^-$	0.4	44	4.27	44
361	Pb(BO2)2	$Pb(BO_2)_2 + 2H_2O + 2H^+ = Pb^{2+} + 2H_3BO_3^o$	-5.80	43	7.61	43
362	Cotunnite	$PbCl_2 = Pb^{2+} + 2Cl^-$	5.60	44	-4.77	44
363	Matlockite	$PbClF = Pb^{2+} + Cl^- + F^-$	7.95	44	-9.43	44
364	Phosgenite	$PbCl_2 \cdot PbCO_3 = 2Pb^{2+} + 2Cl^- + CO_3^{2-}$	---[2]	---[2]	-19.81	44
365	Cerrusite	$PbCO_3 = Pb^{2+} + CO_3^{2-}$	4.86	44	-13.13	24
366	PbF2	$PbF_2 = Pb^{2+} + 2F^-$	-0.7	44	-7.44	69
367	Massicot	$PbO + 2H^+ = Pb^{2+} + H_2O$	-16.78	44	12.91	24
368	Litharge	$PbO + 2H^+ = Pb^{2+} + H_2O$	-16.38	44	12.72	3
369	PbO, 0.3H2O	$PbO \cdot 0.33H_2O + 2H^+ = Pb^{2+} + 1.33H_2O$	--	--	12.98	44
370	Pb2OCO3	$PbO \cdot PbCO_3 + 2H^+ = 2Pb^{2+} + CO_3^{2-} + H_2O$	-11.46	44	-0.5	44
371	Larnakite	$PbO \cdot PbSO_4 + 2H^+ = 2Pb^{2+} + SO_4^{2-} + H_2O$	-6.44	44	-0.28	44
372	Pb3O2SO4	$2PbO \cdot PbSO_4 + 4H^+ = 3Pb^{2+} + SO_4^{2-} + 2H_2O$	-20.75	44	10.4	44
373	Pb4O3SO4	$3PbO \cdot PbSO_4 + 6H^+ = 4Pb^{2+} + SO_4^{2-} + 3H_2O$	-35.07	44	22.1	44
374	PbHPO4	$PbHPO_4 = Pb^{2+} + HPO_4^{2-}$	7.04	51	-11.46	51
375	Pb3(PO4)2	$Pb_3(PO_4)_2 + 2H^+ = 3Pb^{2+} + 2HPO_4^{2-}$	-1.67	51	-19.67	51
376	Clpyromorphite	$Pb_5(PO_4)_3Cl = 5Pb^{2+} + 3PO_4^{3-} + Cl^-$	---[2]	---[2]	-84.43	51
377	Hxypyromorphite	$Pb_5(PO_4)_3OH + H^+ = 5Pb^{2+} + 3PO_4^{3-} + H_2O$	---[2]	---[2]	-62.79	51
378	Pb3O2CO3	$2PbO \cdot PbCO_3 + 4H^+ = 3Pb^{2+} + CO_3^{2-} + 2H_2O$	-26.43	19	11.02	19
379	Plumbogummite	$PbAl_3(PO_4)_2(OH)_5 \cdot H_2O + 5H^+ = Pb^{2+} + 3Al^{3+} + 2PO_4^{3-} + 6H_2O$	---[2]	---[2]	-32.79	51
380	Hinsdalite	$PbAl_3PO_4SO_4(OH)_6 + 6H^+ = Pb^{2+} + 3Al^{3+} + PO_4^{3-} + SO_4^{2-} + 6H_2O$	---[2]	---[2]	-2.5	51
381	Tsumebite	$Pb_2CuPO_4(OH)_3 \cdot 3H_2O + 3H^+ = 2Pb^{2+} + Cu^{2+} + PO_4^{3-} + 6H_2O$	---[2]	---[2]	-9.79	51
382	PbSiO3	$PbSiO_3 + H_2O + 2H^+ = Pb^{2+} + H_4SiO_4^o$	-9.26	44	7.32	44
383	Pb2SiO4	$Pb_2SiO_4 + 4H^+ = 2Pb^{2+} + H_4SiO_4^o$	-26.0	44	19.76	44
384	Anglesite	$PbSO_4 = Pb^{2+} + SO_4^{2-}$	2.15	44	-7.79±0.02	69
385	Galena	$PbS + H^+ = Pb^{2+} + HS^-$	19.4	44	-12.78	66

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
386	Plattnerite	$PbO_2 + 4H^+ + 2e^- = Pb^{2+} + 2H_2O$	-70.73	44	49.3	44
387	Pb2O3	$Pb_2O_3 + 6H^+ + 2e^- = 2Pb^{2+} + 3H_2O$	---[2]	---[2]	61.04	19
388	Minium	$Pb_3O_4 + 8H^+ + 2e^- = 3Pb^{2+} + 4H_2O$	-102.76	44	73.69	44
389	Pb(OH)2 (c)	$Pb(OH)_2 + 2H^+ = Pb^{2+} + 2H_2O$	-13.99	19	8.15	44
390	Laurionite	$PbOHCl + H^+ = Pb^{2+} + Cl^- + H_2O$	---[2]	---[2]	0.623	71
391	Pb2(OH)3Cl	$Pb_2(OH)_3Cl + 3H^+ = 2Pb^{2+} + 3H_2O + Cl^-$	---[2]	---[2]	8.793	71
392	Hydrocerrusite	$2PbCO_3 \cdot Pb(OH)_2 + 2H^+ = 3Pb^{2+} + 2CO_3^{2-} + 2H_2O$	---[2]	---[2]	-17.46	67
393	Pb2O(OH)2	$PbO \cdot Pb(OH)2 + 4H^+ = 2Pb^{2+} + 3H_2O$	---[2]	---[2]	26.2	67
394	Pb4(OH)6SO4	$Pb_4(OH)_6SO_4 + 6H^+ = 4Pb^{2+} + SO_4^{2-} + 6H_2O$	---[2]	---[2]	21.1	67
395	SiO2 (a)	$SiO_2 + 2H_2O = H_4SiO_4^o$ $\log K_r = -0.26-731/T$	3.34[4]	47	-2.71	47
396	FCO3Apatite	$Ca_{9.496}Na_{0.36}Mg_{0.144}(PO_4)_{4.8}(CO_3)_{1.2}F_{2.48} =$ $9.496Ca^{2+}+0.36Na^+ +0.144Mg^{2+}+4.8PO_4^{3-}+1.2CO_3^{2-}+2.48F^-$	39.39	13	-114.4	13
397	kAlHSO4 +2	$Al^{3+} + HSO_4^- = AlHSO_4^{2+}$	---[2]	---[2]	0.46	1
398	BaF2	$BaF_2 = Ba^{2+} + 2F^-$	1.0	44	-5.76	44
399	SrF2	$SrF_2 = Sr^{2+} + 2F^-$	1.25	44	-8.54	44
400	kNO3/NO2	$NO_3^- + 2H^+ + 2e^- = NO_2^- + H_2O$	-43.76	44	28.57	44
401	Dolomite (c)	$CaMg(CO_3)_2 = Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	-9.436	47	-17.09	47
402	Sulfur	$S + 2e^- = S^{2-}$	7.9	44	-15.026	44
403	kNiBr +	$Ni^{2+} + Br^- = NiBr^+$	---[2]	---[2]	0.5	67
404	kNiCl +	$Ni^{2+} + Cl^- = NiCl^+$	---[2]	---[2]	0.4	67
405	kNiF +	$Ni^{2+} F^- = NiF^+$	---[2]	---[2]	1.3	67
406	kNiOH +	$Ni^{2+} + H_2O = NiOH^+ + H^+$	12.42	44	-9.86±0.03	3
407	kNi(OH)2 aq	$Ni^{2+} + 2H_2O = Ni(OH)_2^o + 2H^+$	---[2]	---[2]	-19.0±1.0	3
408	kNi(OH)3 -	$Ni^{2+} + 3H_2O = Ni(OH)_3^- + 3H^+$	---[2]	---[2]	-30.0±0.5	3
409	kNiSO4 aq	$Ni^{2+} + SO_4^{2-} = NiSO_4^o$	1.52	14	2.29	44
410	NiCO3	$NiCO_3 = Ni^{2+} + CO_3^{2-}$	-9.94	43	-6.84	44
411	Ni(OH)2	$Ni(OH)_2 + 2H^+ = Ni^{2+} + 2H_2O$	30.45	44	10.8±0.1	3
412	Ni4(OH)6SO4	$Ni_4(OH)_6SO_4 + 6H^+ = 4Ni^{2+} + SO_4^{2-} + 6H_2O$	---[2]	---[2]	32.0	67

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
413	Bunsenite	$NiO + 2H^+ = Ni^{2+} + H_2O$	-23.92	44	12.45	44
414	Ni3(PO4)2	$Ni_3(PO_4)_2 = 3Ni^{2+} + 2PO_4^{3-}$	---[2]	---[2]	-31.3	44
415	Millerite	$NiS + H^+ = Ni^{2+} + HS^-$	2.5	44	-8.042	44
416	Retgersite	$NiSO_4 \cdot 6H_2O = Ni^{2+} + SO_4^{2-} + 6H_2O$	1.1	44	-2.04	44
417	Morenosite	$NiSO_4 \cdot 7H_2O = Ni^{2+} + SO_4^{2-} + 7H_2O$	2.94	44	-2.36	44
418	Ni2SiO4	$Ni_2SiO_4 + 4H^+ = 2Ni^{2+} + H_4SiO_4^\circ$	-33.36	43	14.54	43
419	Fe3(OH)8	$Fe_3(OH)_8 + 8H^+ = 2Fe^{3+} + Fe^{2+} + 8H_2O$	---[2]	---[2]	20.222	55
420	Dioptase	$CuSiO_3 \cdot H_2O + 2H^+ = Cu^{2+} + H_4SiO_4^\circ$	-8.96	43	6.50	43
421	kAgBr aq	$Ag^+ + Br^- = AgBr^\circ$	---[2]	---[2]	4.24	44
422	kAgBr2 -	$Ag^+ + 2Br^- = AgBr_2^-$	---[2]	---[2]	7.28	44
423	kAgCl aq	$Ag^+ Cl^- = AgCl^\circ$	-2.68	44	3.27	44
424	kAgCl2 -	$Ag^+ + 2Cl^- = AgCl_2^-$	-3.93	44	5.27	44
425	kAgCl3 -2	$Ag^+ + 3Cl^- = AgCl_3^{2-}$	---[2]	---[2]	5.29	22
426	kAgCl4 -3	$Ag^+ + 4Cl^- = AgCl_4^{3-}$	---[2]	---[2]	5.51	22
427	kAgF aq	$Ag^+ + F^- = AgF^\circ$	-2.83	44	0.36	44
428	kAgHS aq	$Ag^+ + HS^- = AgHS^\circ$	---[2]	---[2]	14.05	43
429	kAg(HS)2 -	$Ag^+ + 2HS^- = Ag(HS)_2^-$	---[2]	---[2]	18.45	43
430	kAgI aq	$Ag^+ + I^- = AgI^\circ$	---[2]	---[2]	6.6	44
431	kAgI2 -	$Ag^+ + 2I^- = AgI_2^-$	---[2]	---[2]	10.68	44
432	kAgOH aq	$Ag^+ + H_2O = AgOH^\circ + H^+$	---[2]	---[2]	-12.0±0.3	3
433	kAg(OH)2 -	$Ag^+ + 2H_2O = Ag(OH)_2^- + 2H^+$	---[2]	---[2]	-24.0±0.05	3
434	kAgSO4 -	$Ag^+ + SO_4^{2-} = AgSO_4^-$	1.49	44	1.29	44
435	kAgNO3 aq	$Ag^+ NO_3^- = AgNO_3^\circ$	---[2]	---[2]	-0.29	44
436	kAg(NO2)2 -	$Ag^+ + 2NO_2^- = Ag(NO_2)_2^-$	---[2]	---[2]	2.22	44
437	Ag Metal	$Ag = Ag^+ + e^-$	25.234	44	-13.51	44
438	Bromyrite	$AgBr = Ag^+ + Br^-$	20.17	44	-12.27	44
439	Cerargyrite	$AgCl = Ag^+ + Cl^-$	15.652	44	-9.75	44
440	Ag2CO3	$Ag_2CO_3 = 2Ag^+ + CO_3^{2-}$	9.53	44	-11.07	44
441	AgF, 4H2O	$AgF \cdot 4H_2O = Ag^+ + F^- + 4H_2O$	4.27	44	0.55	44

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
442	Iodyrite	$AgI = Ag^+ + I^-$	26.82	44	-16.07	44
443	Ag2O	$Ag_2O + 2H^+ = 2Ag^+ + H_2O$	-10.43	44	12.58±0.1	3
444	Ag3PO4	$Ag_3PO_4 = 3Ag^+ + PO_4^{3-}$	---[2]	---[2]	-17.55	69
445	Acanthite	$Ag_2S + H^+ = 2Ag^+ + HS^-$	53.3	44	-36.05	44
446	Ag2SO4	$Ag_2SO_4 = 2Ag^+ + SO_4^{2-}$	4.25	44	-4.92	44
447	kZnBr +	$Zn^{2+} + Br^- = ZnBr^+$	---[2]	---[2]	-0.58	44
448	kZnBr2 aq	$Zn^{2+} + 2Br^- = ZnBr_2^o$	---[2]	---[2]	-0.98	44
449	kZnI +	$Zn^{2+} + I^- = ZnI^+$	---[2]	---[2]	-2.91	44
450	kZnI2 aq	$Zn^{2+} + 2I^- = ZnI_2^o$	---[2]	---[2]	-1.69	44
451	kCdBr +	$Cd^{2+} + Br^- = CdBr^+$	-0.81	44	2.17	44
452	kCdBr2 aq	$Cd^{2+} + 2Br^- = CdBr_2^o$	---[2]	---[2]	2.9	44
453	kCdI +	$Cd^{2+} + I^- = CdI^+$	-2.37	44	2.15	44
454	kCdI2 aq	$Cd^{2+} + 2I^- = CdI_2^o$	---[2]	---[2]	3.59	44
455	kPbBr +	$Pb^{2+} + Br^- = PbBr^+$	2.88	44	1.77±0.1	69
456	kPbBr2 aq	$Pb^{2+} + 2Br^- = PbBr_2^o$	---[2]	---[2]	1.44	44
457	kPbI +	$Pb^{2+} + I^- = PbI^+$	---[2]	---[2]	1.94	44
458	kPbI2 aq	$Pb^{2+} + 2I^- = PbI_2^o$	---[2]	---[2]	3.2	69
459	CuBr	$CuBr = Cu^+ + Br^-$	13.08	44	-8.21	44
460	CuI	$CuI = Cu^+ + I^-$	20.14	44	-11.89	44
461	ZnBr2, 2H2O	$ZnBr_2 \cdot 2H_2O = Zn^{2+} + 2Br^- + 2H_2O$	-7.51	44	5.21	44
462	ZnI2	$ZnI_2 = Zn^{2+} + 2I^-$	-13.44	44	7.23	44
463	CdBr2, 4H2O	$CdBr_2 \cdot 4H_2O = Cd^{2+} + 2Br^- + 4H_2O$	7.23	44	-2.42	44
464	CdI2	$CdI_2 = Cd^{2+} + 2I^-$	4.08	44	-3.61	44
465	PbBr2	$PbBr_2 = Pb^{2+} + 2Br^-$	8.10	44	-5.18	44
466	PbBrF	$PbBrF = Pb^{2+} + Br^- + F^-$	---[2]	---[2]	-8.49	44
467	PbI2	$PbI_2 = Pb^{2+} + 2I^-$	15.16	44	-8.07	44
468	kPbCO3 aq	$Pb^{2+} + CO_3^{2-} = PbCO_3^o$	---[2]	---[2]	7.24	24
469	kPb(OH)4 -2	$Pb^{2+} + 4H_2O = Pb(OH)_4^{2-} + 4H^+$	---[2]	---[2]	-39.7	24
470	kPb(SO4)2 -2	$Pb^{2+} + 2SO_4^{2-} = Pb(SO_4)_2^{2-}$	---[2]	---[2]	3.47	24

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
471	Jurbanite	$AlOHSO_4 + H^+ = Al^{3+} + SO_4^{2-} + H_2O$	---[2]	---[2]	-3.23	58
472	Basaluminite	$Al_4(OH)_{10}SO_4 + 10H^+ = 4Al^{3+} + SO_4^{2-} + 10H_2O$	---[2]	---[2]	22.7	68
473	kAgBr3 -2	$Ag^+ + 3Br^- = AgBr_3^{2-}$	---[2]	---[2]	8.71	44
474	kAgI3 -2	$Ag^+ + 3I^- = AgI_3^{2-}$	-27.03	44	13.37	44
475	kAgI4 -3	$Ag^+ + 4I^- = AgI_4^{3-}$	---[2]	---[2]	14.08	44
476	kFe(HS)2 aq	$Fe^{2+} + 2HS^- = Fe(HS)_2^\circ$	---[2]	---[2]	8.95	43
477	kFe(HS)3 -	$Fe_{2+} + 3HS^- = Fe(HS)_3^-$	---[2]	---[2]	10.987	43
478	kH2AsO3 -	$H_3AsO_3^\circ = H^+ + H_2AsO_3^-$	6.56	44	-9.228	44
479	kHAsO3 -2	$H_3AsO_3^\circ = 2H^+ + HAsO_3^{2-}$	14.2	43	-21.33	43
480	KAsO3 -3	$H_3AsO_3^\circ = 3H^+ + AsO_3^{3-}$	20.25	43	-34.744	43
481	kH4AsO3 +	$H_3AsO_3^\circ + H^+ = H_4AsO_3^+$	---[2]	---[2]	-0.305	44
482	kH2AsO4 -	$H_3AsO_4^\circ = H^+ + H_2AsO_4^-$	-1.69	44	-2.243	44
483	kHAsO4 -2	$H_3AsO_4^\circ = 2H^+ + HAsO_4^{2-}$	-0.92	44	-9.001	44
484	kAsO4 -3	$H_3AsO_4^\circ = 3H^+ + AsO_4^{3-}$	3.43	44	-20.597	44
485	kCu(S4)2 -3	$Cu^{2+} + 2HS^- + 6S^\circ + e^- = Cu(S_4)_2^{3-} + 2H^+$	---[2]	---[2]	6.109	16
486	kCuS4S5 -3	$Cu^{2+} + 2HS^- + 7S^\circ + e^- = CuS_4S_5^{3-} + 2H^+$	---[2]	---[2]	5.382	16
487	kAs3/As5	$H_3AsO_3^\circ + H_2O = H_3AsO_4^\circ + 2H^+ + 2e^-$	30.015	44	-19.444	44
488	As2O5	$As_2O_5 + 3H_2O = 2H_3AsO_4^\circ$	-5.405	44	6.699	44
489	AlAsO4, 2H2O	$AlAsO_4 \cdot 2H_2O = Al^{3+} + AsO_4^{3-} + 2H_2O$	---[2]	---[2]	-15.837	43
490	Ca3(AsO4)2, 4w	$Ca_3(AsO_4)_2 \cdot 4H_2O = 3Ca^{2+} + 2AsO_4^{3-} + 4H_2O$	---[2]	---[2]	-18.905	43
491	Cu3(AsO4)2, 6w	$Cu_3(AsO_4)_2 \cdot 6H_2O = 3Cu^{2+} + 2AsO_4^{3-} + 6H_2O$	---[2]	---[2]	-35.123	43
492	Scorodite	$FeAsO_4 \cdot 2H_2O = Fe^{3+} + AsO_4^{3-} + 2H_2O$	---[2]	---[2]	-20.249	43
493	Mn3(AsO4), 8H2O	$Mn_3(AsO_4)_2 \cdot 8H_2O = 3Mn^{2+} + 2AsO_4^{3-} + 8H_2O$	---[2]	---[2]	-28.707	43
494	Ni3(AsO4)2, 8H2O	$Ni_3(AsO_4)_2 \cdot 8H_2O = 3Ni^{2+} + 2AsO_4^{3-} + 8H_2O$	---[2]	---[2]	-25.511	43
495	Pb3(AsO4)2	$Pb_3(AsO_4)_2 = 3Pb^{2+} + 2AsO_4^{3-}$	---[2]	---[2]	-35.403	43
496	Zn3(AsO4)2, 2.5w	$Zn_3(AsO_4)_2 \cdot 2.5H_2O = 3Zn^{2+} + 2AsO_4^{3-} + 2.5H_2O$	---[2]	---[2]	-27.546	44
497	Arsenolite	$As_4O_6 + 6H_2O = 4H_3AsO_3^\circ$	14.33	44	-2.801	44
498	Claudetite	$As_4O_6 + 6H_2O = 4H_3AsO_3^\circ$	13.29	44	-3.065	44
499	AsI3	$AsI_3 + 3H_2O = H_3AsO_3^\circ + 3I^- + 3H^+$	1.875	44	4.155	44

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
500	Orpiment	$As_2S_3 + 6H_2O = 2H_3AsO_3^o + 3HS^- + 3H^+$	82.89	44	-60.971	44
501	Realgar	$AsS + 3H_2O = H_3AsO_3^o + HS^- + 2H^+ + e^-$	30.545	43	-19.747	43
502	kS2 -2	$HS^- + S^o = S_2^{2-} + H^+$	11.4	44	-14.528	16
503	kS3 -2	$HS^- + 2S^o = S_3^{2-} + H^+$	10.4	44	-13.282	16
504	kS4 -2	$HS^- + 3S^o = S_4^{2-} + H^+$	9.7	44	-9.829	16
505	kS5 -2	$HS^- + 4S^o = S_5^{2-} + H^+$	9.3	44	-9.595	16
506	kS6 -2	$HS^- + 5S^o = S_6^{2-} + H^+$	---[2]	---[2]	-9.881	16
507	kAg(S4)2 -3	$Ag^+ + 2HS^- + 6S^o = Ag(S_4)_2^{3-} + 2H^+$	---[2]	---[2]	0.991	16
508	kAgS4S5 -3	$Ag^+ + 2HS^- + 7S^o = AgS_4S_5^{3-} + 2H^+$	---[2]	---[2]	0.680	16
509	kAg(HS)S4 -2	$Ag^+ + 2HS^- + 3S^o = Ag(HS)S_4^{2-} + H^+$	---[2]	---[2]	10.431	16
510	kCuHCO3 +	$Cu^{2+} + HCO_3^- = CuHCO_3^+$	---[2]	---[2]	2.7	81
511	kZnHCO3 +	$Zn^{2+} + HCO_3^- = ZnHCO_3^+$	---[2]	---[2]	2.1	81
512	kZnCO3 aq	$Zn^{2+} + CO_3^{2-} = ZnCO_3^o$	---[2]	---[2]	5.3	81
513	kZn(CO3)2 -2	$Zn^{2+} + 2CO_3^{2-} = Zn(CO_3)_2^{2-}$	---[2]	---[2]	9.63	37
514	kCdHCO3	$Cd^{2+} + HCO_3^- = CdHCO_3^+$	---[2]	---[2]	1.5	72
515	kCdCO3 aq	$Cd^{2+} + CO_3^{2-} = CdCO_3^o$	---[2]	---[2]	2.9±0.4	72
516	kCd(SO4)2 -2	$Cd^{2+} + 2SO_4^{2-} = Cd(SO_4)_2^{2-}$	---[2]	---[2]	3.5	81
517	kPbHCO3 +	$Pb^{2+} + HCO_3^- = PbHCO_3^+$	---[2]	---[2]	2.9	81
518	kNiCl2 aq	$Ni^{2+} + 2Cl^- = NiCl_2^o$	---[2]	---[2]	0.96	37
519	kNiHCO3 +	$Ni^{2+} + HCO_3^- = NiHCO_3^+$	---[2]	---[2]	2.14	37
520	kNiCO3 aq	$Ni^{2+} + CO_3^{2-} = NiCO_3^o$	---[2]	---[2]	6.87	37
521	kNi(CO3)2 -2	$Ni^{2+} + 2CO_3^{2-} = Ni(CO_3)_2^{2-}$	---[2]	---[2]	10.11	37
522	kNi(SO4)2 -2	$Ni^{2+} + 2SO_4^{2-} = Ni(SO_4)_2^{2-}$	---[2]	---[2]	1.02	37
523	kH Fulvate	$H^+ + L^{2-} = HL^-$	---[2]	---[2]	4.27	70[13]
524	kH Humate	$H^+ + L^{2-} = HL^-$	---[2]	---[2]	4.27	70[13]
525	kFe Fulvate	$Fe^{3+} + L^{2-} = FeL^+$	---[2]	---[2]	9.4	70[13]
526	kFe Humate	$Fe^{3+} + L^{2-} = FeL^+$	---[2]	---[2]	9.4	70[13]
527	kCu Fulvate	$Cu^{2+} + L^{2-} = CuL^o$	---[2]	---[2]	6.2	70[13]
528	kCu Humate	$Cu^{2+} + L^{2-} = CuL^o$	---[2]	---[2]	6.2	70[13]

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
529	kCd Fulvate	$Cd^{2+} + L^{2-} = CdL^o$	---[2]	---[2]	3.5	70[13]
530	kCd Humate	$Cd^{2+} + L^{2-} = CdL^o$	---[2]	---[2]	3.5	70[13]
531	kAg Fulvate	$Ag^+ + L^{2-} = AgL^-$	---[2]	---[2]	2.4	70[13]
532	kAg Humate	$Ag^+ + L^{2-} = AgL^-$	---[2]	---[2]	2.4	70[13]
533	Blaublei I	$Cu^{2+}_{0.9}Cu^{+}_{0.2}S + H^+ = 0.9Cu^{2+} + 0.2Cu^+ + HS^-$	---[2]	---[2]	-24.162±0.15	56
534	Blaublei II	$Cu^{2+}_{0.6}Cu^{+}_{0.8}S + H^+ = 0.6Cu^{2+} + 0.8Cu^+ + HS^-$	---[2]	---[2]	-27.279±0.15	56
535	Anilite	$Cu^{2+}_{0.25}Cu^{+}_{1.5}S + H^+ = 0.25Cu^{2+} + 1.5Cu^+ + HS^-$	43.535	56	-31.878±0.15	56
536	Djurleite	$Cu^{2+}_{0.066}Cu^{+}_{1.868}S + H^+ = 0.066Cu^{2+} + 1.868Cu^+ + HS^-$	47.881	56	-33.920±0.15	56
537	kH2F2 aq	$2H^+ + 2F^- = H_2F_2^-$	---[2]	---[2]	6.768	4
538	kpeS/H2S	$S_s + 2H^+ + 2e^- = H_2S^o$	-9.5	67	4.882	67
539	Portlandite	$Ca(OH)_2 + 2H^+ = Ca^{2+} + 2H_2O$	-31.0	47	22.8	47
540	kNaF aq	$Na^+ + F^- = NaF^o$	---[2]	---[2]	-0.24±0.05	47
541	Ba3(AsO4)2	$Ba_3(AsO_4)_2 = 3Ba^{2+} + 2AsO_4^{3-}$	9.5	44	-50.11	67
542	kFeCl +	$Fe^{2+} + Cl^- = FeCl^+$	---[2]	---[2]	0.14	47
543	kBaSO4 aq	$Ba^{2+} + SO_4^{2-} = BaSO_4^o$	---[2]	---[2]	2.7	69
544	kH2Se aq	$H_2Se^o = H^+ + HSe^-$	5.3	---[14]	-3.8	---[14]
545	kH2SeO3 aq	$SeO_3^{2-} + 2H^+ = H_2SeO_3^o$	---[2]	---[2]	11.25	---[14]
546	kHSeO3 -	$SeO_3^{2-} + H^+ = HSeO_3^-$	---[2]	---[2]	8.5	---[14]
547	kHSeO4 -	$SeO_4^{2-} + H^+ = HSeO_4^-$	4.91	---[14]	1.66	---[14]
548	kSe4/Se6	$SeO_3^{2-} + H_2O = SeO_4^{2-} + 2H^+ + 2e^-$	---[2]	---[2]	-30.256	---[14]
549	kSe4/Se-2	$SeO_3^{2-} + 7H^+ + 6e^- = HSe^- + 3H_2O$	---[2]	---[2]	42.514	---[14]
550	Se metal<Se=	$Se_s + H^+ + 2e^- = HSe^-$	---[2]	---[2]	-17.322	---[14]
551	Se metal<Se4	$Se_s + 3H_2O = SeO_3^{2-} + 6H^+ + 4e^-$	---[2]	---[2]	-59.836	---[14]
552	FeSe2	$FeSe_2 + 2H^+ + 2e^- = Fe^{2+} + 2HSe^-$	---[2]	---[2]	-18.58	---[14]
553	SeO2	$SeO_2 + H_2O = SeO_3^{2-} + 2H^+$	---[2]	---[2]	-8.38	---[14]
554	CaSeO3	$CaSeO_3 = Ca^{2+} + SeO_3^{2-}$	---[2]	---[2]	-5.6	---[14]
555	BaSeO3	$BaSeO_3 = Ba^{2+} + SeO_3^{2-}$	---[2]	---[2]	-6.39	---[14]
556	Fe2(SeO3)3	$Fe_2(SeO_3)_3 = 2Fe^{2+} + 3SeO_3^{2-}$	---[2]	---[2]	-35.43	---[14]
557	kAs3/As	$H_3AsO_3^o + 3H^+ + 3e^- = As_s + 3H_2O$	---[2]	---[2]	12.17	---[14]

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^\circ \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^\circ \pm 1\sigma$	Source
558	kFeHCO3 +	$Fe^{2+} + HCO_3^- = FeHCO_3^+$	---[2]	---[2]	2.0	47
559	kFeCO3 aq	$Fe^{2+} + CO_3^{2-} = FeCO_3^\circ$	---[2]	---[2]	4.38	47
560	kMnCO3 aq	$Mn^{2+} + CO_3^{2-} = MnCO_3^\circ$	---[2]	---[2]	4.90	47
561	kBaHCO3 +	$Ba^{2+} + HCO_3^- = BaHCO_3^+$	5.56[4]	47	0.982	47
		$\log K_r = -3.0938+0.013669T$				
562	kBaCO3 aq	$Ba^{2+} + CO_3^{2-} = BaCO_3^\circ$	3.55[4]	47	2.71	47
		$\log K_r = 0.113+0.008721T$				
563	kSrSO4 aq	$Sr^{2+} + SO_4^{2-} = SrSO_4^\circ$	2.08	47	2.29	47
564	Rhodochrosite (c)	$MnCO_{3(crystal)} = Mn^{2+} + CO_3^{2-}$	-1.43	47	-11.13	47
565	kU +4	$UO_2^{2+} + 4H^+ + 2e^- = U^{4+} + 2H_2O$	-34.43	33	9.04±0.04	21
566	kU +3	$U^{4+} + e^- = U^{3+}$	24.4±0.4	21	-8.796	33
567	kUOH +3	$U^{4+} + H_2O = UOH^{3+} + H^+$	11.21±2.16	21	-0.54±0.06	21
568	kU(OH)2 +2	$U^{4+} + 2H_2O = U(OH)_2^{2+} + 2H^+$	17.73	33	-2.27	33
569	kU(OH)3 +	$U^{4+} + 3H_2O = U(OH)_3^+ + 3H^+$	22.645	33	-4.935	33
570	kU(OH)4 aq	$U^{4+} + 4H_2O = U(OH)_4^\circ + 4H^+$	24.76	33	-8.498	33
571	Na4UO2(CO3)3	$Na_4UO_2(CO_3)_3 = 4Na^+ + UO_2^{2+} + 3CO_3^{2-}$	---[2]	---[2]	-16.29±0.16	21
572	kU6(OH)15 +9	$6U^{4+} + 15H_2O = U_6(OH)_{15}^{9+} + 15H^+$	---[2]	---[2]	-17.2	3
573	Uraninite (c)	$UO_2 + 4H^+ = U^{4+} + 2H_2O$	-18.61±0.96	21	-4.8±0.5	21
574	UO2 (a)	$UO_2 + 4H^+ = U^{4+} + 2H_2O$	---[2]	---[2]	0.1±0.7	21
575	U4O9 (c)	$U_4O_9 + 18H^+ + 2e^- = 4U^{4+} + 9H_2O$	-101.235	33	-3.384	33
576	U3O8 (c)	$U_3O_8 + 16H^+ + 4e^- = 3U^{4+} + 8H_2O$	-116.0±1.4	21	20.53±0.31	21
577	Coffinite	$USiO_4 + 4H^+ = U^{4+} + H_4SiO_4^\circ$	-14.3	21,63	-7.67	21
578	kUF +3	$U^{4+} + F^- = UF^{3+}$	-1.3±0.1	21	9.3±0.1	21
579	kUF2 +2	$U^{4+} + 2F^- = UF_2^{2+}$	-0.8±0.1	21	16.22±0.19	21
580	kUF3 +	$U^{4+} + 3F^- = UF_3^+$	0.1±1.0	21	21.6±1.0	21
581	kUF4 aq	$U^{4+} + 4F^- = UF_4^\circ$	-0.87±1.82	21	25.5±1.0	21
582	kUF5 -	$U^{4+} + 5F^- = UF_5^-$	4.85	33	27.01±0.31	21
583	kUF6 -2	$U^{4+} + 6F^- = UF_6^{2-}$	3.3	33	29.1±0.2	21
584	UF4 (c)	$UF_4 = U^{4+} + 4F^-$	-18.9	33	-18.606	33

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
585	UF4, 2.5H2O	$UF_4 \cdot 2.5H_2O = U^{4+} + 4F^- + 2.5H_2O$	-0.588	33	-27.57	33
586	kUCl +3	$U^{4+} + Cl^- = UCl^{3+}$	-4.54±2.15	21	1.72±0.13	21
587	kUSO4 +2	$U^{4+} + SO_4^{2-} = USO_4^{2+}$	1.9±0.7	21	6.58±0.19	21
588	kU(SO4)2 aq	$U^{4+} + 2SO_4^{2-} = U(SO_4)_2^o$	7.8±0.7	21	10.5±0.2	21
589	kU(CO3)4 -4	$U^{4+} + 4CO_3^{2-} = U(CO_3)_4^{4-}$	---[2]	---[2]	32.9±0.9	21
590	kU(CO3)5 -6	$U^{4+} + 5CO_3^{2-} = U(CO_3)_5^{6-}$	20.0	21	34.0±0.9	21
591	U(OH)2SO4	$U(OH)_2SO_4 + 2H^+ = U^{4+} + SO_4^{2-} + 2H_2O$	---[2]	---[2]	-3.2±0.5	21
592	UO2HPO4, 4H2O	$UO_2HPO_4 \cdot 4H_2O = UO_2^{2+} + HPO_4^{2-} + 4H_2O$	---[2]	---[2]	-11.85±0.09	21
593	U(HPO4)2, 4H2O	$U(HPO_4)_2 \cdot 4H_2O = U^{4+} + 2PO_4^{3-} + 2H^+ + 4H_2O$	3.84	33	-55.30±0.15	21
594	Ningyoite	$CaU(PO_4)_2 \cdot 2H_2O = U^{4+} + Ca^{2+} + 2PO_4^{3-} + 2H_2O$	-2.27	33	-53.906	33
595	kUO2 +	$UO_2^{2+} + e^- = UO_2^+$	-3.3	33	1.49±0.02	21
596	kUO2OH +	$UO_2^{2+} + H_2O = UO_2OH^+ + H^+$	11.015	33	-5.2±0.3	21
597	k(UO2)2(OH)2+2	$2UO_2^{2+} + 2H_2O = (UO_2)_2(OH)_2^{2+} + 2H^+$	10.23	33	-5.62±0.04	21
598	k(UO2)3(OH)5 +	$3UO_2^{2+} + 5H_2O = (UO_2)_3(OH)_5^+ + 5H^+$	25.075	33	-15.55±0.12	21
599	UO3 (γ)	$UO_3 + 2H^+ = UO_2^{2+} + H_2O$	-19.315	33	7.719	33
600	Gummite	$UO_3 + 2H^+ = UO_2^{2+} + H_2O$	-23.015	33	10.403	33
601	B-UO2(OH)2	$UO_2(OH)_2 + 2H^+ = UO_2^{2+} + 2H_2O$	-13.73	33	5.544	33
602	Schoepite	$UO_2(OH)_2 \cdot H_2O + 2H^+ = UO_2^{2+} + 3H_2O$	-12.045	33	5.404	33
603	kUO2CO3 aq	$UO_2^{2+} + CO_3^{2-} = UO_2CO_3^o$	1.20±0.48	21	9.63±0.05	21
604	kUO2(CO3)2 -2	$UO_2^{2+} + 2CO_3^{2-} = UO_2(CO_3)_2^{2-}$	4.42±0.96	21	17.0±0.1	21
605	kUO2(CO3)3 -4	$UO_2^{2+} + 3CO_3^{2-} = UO_2(CO_3)_3^{4-}$	-9.13±0.74	21	21.63±0.04	21
606	Rutherfordine	$UO_2CO_3 = UO_2^{2+} + CO_3^{2-}$	-1.44	33	-14.45±0.05	21
607	kUO2F +	$UO_2^{2+} + F^- = UO_2F^+$	0.41±0.02	21	5.09±0.13	21
608	kUO2F2 aq	$UO_2^{2+} + 2F^- = UO_2F_2^o$	0.50±0.05	21	8.62±0.04	21
609	kUO2F3 -	$UO_2^{2+} + 3F^- = UO_2F_3^-$	0.56±0.07	21	10.9±0.4	21
610	kUO2F4 -2	$UO_2^{2+} + 4F^- = UO_2F_4^{2-}$	0.07±0.11	21	11.7±0.7	21
611	kUO2Cl +	$UO_2^{2+} + Cl^- = UO_2Cl^+$	1.9±0.5	21	0.17±0.02	21
612	kUO2SO4 aq	$UO_2^{2+} + SO_4^{2-} = UO_2SO_4^o$	4.7±0.4	21	3.15±0.02	21
613	kUO2(SO4)2 -2	$UO_2^{2+} + 2SO_4^{2-} = UO_2(SO_4)_2^{2-}$	8.4±0.2	21	4.14±0.07	21

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
614	kUO2HPO4 aq	$UO_2^{2+} + PO_4^{3-} + H^+ = UO_2HPO_4^o$	-2.1	33	20.21±0.12	21
615	kUO2HPO4)2 -2	$UO_2^{2+} + 2PO_4^{3-} + 2H^+ = UO_2(HPO)_2^{2-}$	-11.8	33	43.441	33
616	kUO2H2PO4 +	$UO_2^{2+} + PO_4^{3-} + 2H^+ = UO_2H_2PO_4^+$	-3.70	33	22.87±0.06	21
617	kUO2H2PO4)2 aq	$UO_2^{2+} + 2PO_4^{3-} + 4H^+ = UO_2(H_2PO_4)_2^o$	-16.5	33	44.38±0.05	21
618	kUO2H2PO4)3 -	$UO_2^{2+} + 3PO_4^{3-} + 6H^+ = UO_2(H_2PO_4)_3^-$	-28.6	33	66.245	33
619	(UO2)3(PO4)2,4w	$(UO_2)_3(PO_4)_2 \cdot 4H_2O = 3UO_2^{2+} + 2PO_4^{3-} + 4H_2O$	41.5	33	-37.4±0.3	21
620	H-Autunite	$H_2(UO_2)_2(PO_4)_2 = 2H^+ + 2UO_2^{2+} + 2PO_4^{3-}$	-3.6	33	-47.931	33
621	Na-Autunite	$Na_2(UO_2)_2(PO_4)_2 = 2Na^+ + 2UO_2^{2+} + 2PO_4^{3-}$	-0.46	33	-47.409	33
622	K-Autunite	$K_2(UO_2)_2(PO_4)_2 = 2K^+ + 2UO_2^{2+} + 2PO_4^{3-}$	5.86	33	-48.244	33
623	Uramphite	$(NH_4)_2(UO_2)_2(PO_4)_2 = 2NH_4^+ + 2UO_2^{2+} + 2PO_4^{3-}$	9.70	33	-51.749	33
624	Saleeite	$Mg(UO_2)_2(PO_4)_2 = Mg^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-20.18	33	-43.646	33
625	Autunite	$Ca(UO_2)_2(PO_4)_2 = Ca^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-14.34	33	-43.927	33
626	Sr-Autunite	$Sr(UO_2)_2(PO_4)_2 = Sr^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-13.05	33	-44.457	33
627	Uranocircite	$Ba(UO_2)_2(PO_4)_2 = Ba^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-10.10	33	-44.631	33
628	Bassetite	$Fe(UO_2)_2(PO_4)_2 = Fe^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-19.9	33	-44.485	33
629	Torbernite	$Cu(UO_2)_2(PO_4)_2 = Cu^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-15.9	33	-45.279	33
630	Przhevalskite	$Pb(UO_2)_2(PO_4)_2 = Pb^{2+} + 2UO_2^{2+} + 2PO_4^{3-}$	-11.0	33	-44.365	33
631	Blank		---[9]	---[9]	---[9]	---[9]
632	Uranophane	$Ca(UO_2)_2(SiO_3OH)_2 + 6H^+ = Ca^{2+} + 2UO_2^{2+} + 2H_4SiO_4^o$	---[2]	---[2]	17.489	33
633	kUBr +3	$U^{4+} + Br^- = UBr^{3+}$	---[2]	---[2]	1.5±0.2	21
634	kUI +3	$U^{4+} + I^- = UI^{3+}$	---[2]	---[2]	1.3±0.3	21
635	kUNO3 +3	$U^{4+} + NO_3^- = UNO_3^{3+}$	---[2]	---[2]	1.47±0.13	21
636	kU(NO3)2 +2	$U^{4+} + 2NO_3^- = U(NO_3)_2^{2+}$	---[2]	---[2]	2.30±0.35	21
637	Blank		---[9]	---[9]	---[9]	---[9]
638	kUO2(OH)3 -	$UO_2^{2+} + 3H_2O = UO_2(OH)_3^- + 3H^+$	---[2]	---[2]	-19.2±0.4	21
639	kUO2(OH)4 -2	$UO_2^{2+} + 4H_2O = UO_2(OH)_4^{2-} + 4H^+$	---[2]	---[2]	-33.0±2.0	21
640	k(UO2)2OH +3	$2UO_2^{2+} + H_2O = (UO_2)_2OH^{3+} + H^+$	---[2]	---[2]	-2.7±1.0	21
641	k(UO2)3(OH)4+2	$3UO_2^{2+} + 4H_2O = (UO_2)_3(OH)_4^{2+} + 4H^+$	---[2]	---[2]	-11.9±0.3	21
642	k(UO2)3(OH)7 -	$3UO_2^{2+} + 7H_2O = (UO_2)_3(OH)_7^- + 7H^+$	---[2]	---[2]	-31.0±2.0	21

Table 2. Thermodynamic Data (continued)

I[1]	Species	Reaction	$\Delta H_r^o \pm 1\sigma$ (kcal/mol)	Source	Log $K_r^o \pm 1\sigma$	Source
643	k(UO2)4(OH)7 +	$4UO_2^{2+} + 7H_2O \rightleftharpoons (UO_2)_4(OH)_7^+ + 7H^+$	---[2]	---[2]	-21.9±1.0	21
644	kUO2Cl2 aq	$UO_2^{2+} + 2Cl^- \rightleftharpoons UO_2Cl_2^o$	3.6±1.4	21	-1.1±0.4	21
645	kUO2Br +	$UO_2^{2+} + Br^- \rightleftharpoons UO_2Br^+$	---[2]	---[2]	0.22±0.02	21
646	kUO2NO3 +	$UO_2^{2+} + NO_3^- \rightleftharpoons UO_2NO_3^+$	---[2]	---[2]	0.30±0.15	21
647	kUO2H3PO4 +2	$UO_2^{2+} + PO_4^{3-} + 3H^+ \rightleftharpoons UO_2H_3PO_4^{2+}$	---[2]	---[2]	22.87±0.06	21
648	k(UO2)3(CO3)6 -6	$3UO_2^{2+} + 6CO_3^{2-} \rightleftharpoons (UO_2)_3(CO_3)_6^{6-}$	---[2]	---[2]	54.0±1.0	21
649	kUO2PO4 -	$UO_2^{2+} + PO_4^{3-} \rightleftharpoons UO_2PO_4^-$	---[2]	---[2]	13.69±0.08	21
650	kUO2(CO3)3 -5	$UO_2^{2+} + 3CO_3^{2-} + e^- \rightleftharpoons UO_2(CO_3)_3^{5-}$	---[2]	---[2]	8.92±0.27	21
651	Blank		---[9]	---[9]	---[9]	---[9]
652	Blank		---[9]	---[9]	---[9]	---[9]
653	Blank		---[9]	---[9]	---[9]	---[9]

Footnotes to Table 2

[1]Reaction number.

[2]No thermodynamic data are presently available.

[3]Parenthetical letters after mineral names designate degree of crystallinity of phase: a=amorphous; b=beta; c=crystalline; d=disordered; e=eta; g=gamma; AB=Aberdeen; BF=Belle Fourche; Ca=calcium.

[4]Enthalpy derived from the temperature variation of log K using the vant Hoff relation.

[5]Changes in thermodynamic values reflect an alteration of the hydrolysis reaction from OH^- to H^+ and H_2O.

[6]Phlogopite solubility product constant was calculated from the average free energy of formation for phlogopite (-1389 kcal mol^{-1}, Bird and Anderson, 1973; Munoz and Ludington, 1974), the most recent evaluation of the free energy of potassium ion (Giordano and others, 1977), magnesium ion (Parker and others, 1971), aluminum ion and silicic acid (Hemingway and others, 1978). The enthalpy of phlogopite dissolution was calculated from the free energies previously cited and the entropies listed in Robie and others (1978).

[7]Changes in thermodynamic values reflect an alteration of the sulfide dissolution from S^{2-} to HS^-.

[8]Correction of error in sign in the original WATEQ.

[9]Not presently used.

[10]Calculated for 25°C and pH = 7.0.

[11]Assumes that divalent metal bisulfate ion pair stability constants are approximately equivalent (see Mattigod and Sposito, 1977). No reliable data exist.

[12]Estimated (Ball and others, 1980).

[13]Thermodynamic data are for oxalic acid.

[14]Tentative, based on preliminary review of the literature.

Data Sources for Table 2

1. Akitt and others (1969)
2. Alpers and others (1989)
3. Baes and Mesmer (1976)
4. Ball and others (1979)
5. Berner (1967)
6. Biedermann and Chow (1966)
7. Bird and Anderson (1973)
8. Bowser, C. J., written commun. (1975)
9. Bricker (1969)
10. Brown (1960)
11. Busenberg and others (1984)
12. Bystrom and Bystrom (1950)
13. Chien and Black (1976)
14. Christensen and others (1975)
15. Chughtai and others (1968)
16. Cloke (1963a, 1963b)
17. Cox and others (1989)
18. Dirkse (1986)
19. Garrels and Christ (1965)
20. Garrels and Thompson (1962)
21. Grenthe and others (1990)
22. Helgeson (1969)

23. Helgeson and others (1978)
24. Hem (1976)
25. Hemingway and Robie (1973)
26. Hess (1966)
27. Hoare (1985)
28. Hogfeldt and Sillen (Written commun., 1966)
29. Jones, B. F. (Oral commun., 1977)
30. Kittrick (1971a)
31. Kittrick (1971b)
32. Langmuir (1969)
33. Langmuir (1978)
34. Latimer (1952)
35. Linke and Seidell (1965)
36. Mathieson and Wadsley (1950)
37. Mattigod and Sposito (1977)
38. McCann (1968)
39. McGee and Hostetler (1975)
40. Mesmer and others (1972)
41. Mills (1974)
42. Munoz and Ludington (1974)
43. Naumov and others (1974)
44. NBS Technical Notes 270 (Wagman and others, 1968, 1969; Parker and others, 1971)
45. Nordstrom (1977)
46. Nordstrom and Jenne (1977)
47. Nordstrom and others (1990)
48. Nriagu (1971)
49 Nriagu (1972a)
50. Nriagu (1972b)
51. Nriagu (1974)
52. Paces (1973)
53. Plummer and Busenberg (1982)
54. Plummer and others (1976)
55. Ponnamperuma (1967)
56. Potter (1977)
57. Ramsdell (1942)
58. Rawajfih (1975)
59. Reesman and Keller (1968)
60. Richmond and others (1969)
61. Roberson and Barnes (1978)
62. Robie and Hemingway (1973)
63. Robie and others (1978)
64. Robie and Waldbaum (1968)
65. Schindler and others (1965)
66. Shea and Helz (1989)
67. Sillen and Martell (1964)
68. Singh (1969)
69. Smith and Martell (1976)
70. Smith and Martell (1977)
71. Staples, B. R. (Written commun., 1977)
72. Stipp (1991)

73. Straczek and others (1960)
74. Truesdell and Jones (1974)
75. Vuceta (1976)
76. Wadsley (1950)
77. Waterfield and others (1968)
78. Wollast and others (1968)
79. Yatsimirskii and Vasil'ev (1969)
80. Zen (1972)
81. Zirino and Yamamoto (1972)

Attachment A. Test Cases

Input Data Set for Test Problem Number 1:

```
****
DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data        1 A5
    0     0 000000       0       0  35.147       0       0       0       0
TEMP-.--- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--
   25.00     8.22    0.500     0.00     6.60        0
FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8--9
PPM     1.023361    3     1        0  0  0  0  0  0  3  2  0
EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.----SIGMPH-.----
       0     0.0      0.0       0.0         0.0         0.0
CA-----.----MG-----.----NA-----.----K------.----CL-----.----SO4----.----
       412.3      1291.8     10768.0       399.1     19353.0      2712.0
HCO3---.----FE TOT-.----H2S AQ-.----CO3----.----SIO2TOT.----NH4----.----
     141.682        .002         0.0         0.0        4.28         .29
B TOT--.----PO4----.----AL-----.----F------.----NO3----.----
        4.45         .06        .002        1.39         .29
$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++
CUN   48         .0004  80          .181  87         8.14  89          .02
CUN   94          .117  96          .062  97         67.3 109         .0002
CUN  130         .0007 145         .0049 160        .0001 182        .00005
CUN  202           .02 204         .0017 212       .00004 249          .004
```

Complete Aqueous Speciation, Mineral Saturation and Element Ratios Output

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```
DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data        1 A5
   0     0 000000       0       0  35.147       0
                    TEMP      =         25.000000
                    PH        =          8.220000
                    EH(0)     =           .500000
                    DOC       =           .000000
                    DOX       =          6.600000
                    CORALK    =          0
                    FLG       =        PPM
                    DENS      =          1.023361
                    PRNT      =          3
                    PUNCH     =          1
                    EHOPT(1)  =          0  Use measured Eh to calculate Fe species distribution
                    EHOPT(2)  =          0  Use measured Eh to calculate Mn species other than +2
                    EHOPT(3)  =          0  Use measured Eh to calculate Cu +1 species
                    EHOPT(4)  =          0  Use measured Eh to calculate As species distribution
                    EHOPT(5)  =          0  Use measured Eh to calculate Se species distribution
                    EHOPT(6)  =          0  Use measured Eh to calculate Ion Activity Products
                    EHOPT(7)  =          3  Use H2O/O2 classical Eh to calculate atmospheric pO2
                    EHOPT(8)  =          2  Use H2O2/O2 Sato Eh to calculate H2S from SO4
                    EHOPT(9)  =          0  Use measured Eh to calculate U species distribution
                    EMPOX     =          0
                    ITDS      =           .000000
                    COND      =           .000000
                    SIGMDO    =           .000000
                    SIGMEH    =           .000000
                    SIGMPH    =           .000000
```

Species	Index No	Input Concentration
Ca	0	412.30000000
Mg	1	1291.80000000
Na	2	10768.00000000
K	3	399.10000000
Cl	4	19353.00000000
SO4	5	2712.00000000
HCO3	6	141.68200000
Fe total	16	.00200000
H2S aq	13	.00000000
CO3	17	.00000000
SiO2 tot	34	4.28000000
NH4	38	.29000000
B tot	86	4.45000000
PO4	44	.06000000
Al	50	.00200000
F	61	1.39000000
NO3	84	.29000000
Cs	48	.00040000
Li	80	.18100000
Sr	87	8.14000000
Ba	89	.02000000
Rb	94	.11700000
I	96	.06200000
Br	97	67.30000000
Mn	109	.00020000
Cu	130	.00070000
Zn	145	.00490000
Cd	160	.00010000
Pb	182	.00005000
NO2	202	.02000000
Ni	204	.00170000
Ag	212	.00004000
As total	249	.00400000

ITER	S1-AnalCO3	S2-AnalSO4	S3-AnalF	S4-AnalPO4	S5-AnalCL	S6-AnalH2S	S7-AnalFULV	S8-AnalHUM
1	1.162973E-03	2.629247E-02	7.173270E-05	3.001007E-06	3.190657E-08	0.000000E+00	0.000000E+00	0.000000E+00
2	7.401058E-05	1.653941E-03	3.777427E-06	3.567761E-08	6.835840E-09	0.000000E+00	0.000000E+00	0.000000E+00
3	-1.195843E-07	-6.782150E-05	3.076308E-07	8.544126E-09	7.652298E-10	0.000000E+00	0.000000E+00	0.000000E+00
4	-5.505179E-07	-1.642316E-05	-6.398325E-09	3.197057E-10	-4.152254E-11	0.000000E+00	0.000000E+00	0.000000E+00

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data 1 A5 Date = 6/03/91 13:57

0 0 000000 0 0 35.147 0

DOX = 6.6000 DOC = .0 INPUT TDS = .0

Anal Cond = .0 Calc Cond = 46798.6 Activity H2S calc from SO4 and pe = 8.33E-63

Anal EPMCAT = 627.7348 Anal EPMAN = 627.6592 Percent difference in input cation/anion balance = .0120

Calc EPMCAT = 603.9316 Calc EPMAN = 603.8530 Percent difference in calc cation/anion balance = .0130

Total Ionic Strength (T.I.S.) from input data = .72279

Effective Ionic Strength (E.I.S.) from speciation = .67557

Input	Sigma	Fe3/Fe2	Sigma	NO3/NO2	Sigma	NO3/NH4	Sigma	SO4/S=	Sigma	S/S=	Sigma	Sato H2O2/O2	Sigma	H2O/O2	Sigma
								Eh							
.500	.000	.500	.000	.390	.000	.269	.000	9.900	.000	9.900	.000	.133	.000	.689	.000
								pe							
8.451	.000	8.451	.000	6.585	.000	4.551	.000	100.000	.000	100.000	.000	2.248	.000	11.643	.000

As5/As3	Sigma	As3/As	Sigma	Se6/Se4	Sigma	Se4/Se	Sigma	Se/Se=	Sigma	U6/U4	Sigma		Sigma		Sigma
								Eh							
.500	.000	-.830	.000	9.900	.000	9.900	.000	9.900	.000	9.900					
								pe							
8.451	.000	-14.037	.000	100.000	.000	100.000	.000	100.000	.000	100.000					

T	pH	TDS ppm	Effective Ionic Str	pO2 Atm	ppm O2 Atm	pCO2 Atm	ppm CO2 Atm	log pCO2	CO2 Tot	Ncrb Alk	aH2O
25.00	8.220	35164.5	.67557	2.06E-04	6.60E+00	4.67E-04	2.05E+01	-3.331	2.14E-03	6.05E-05	.9805

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
212	Ag	1	.000040	.000000	3.843E-10	4.017E-15	.00	3.001E-15	.7472	14.523
213	AgBr aq	0		.000000		2.912E-14	.00	3.402E-14	1.1683	13.468
214	AgBr2	-1		.000000		3.257E-14	.00	2.433E-14	.7472	13.614
244	AgBr3	-2		.000000		1.370E-15	.00	4.272E-16	.3118	15.369
215	AgCl aq	0		.000000		1.688E-12	.44	1.972E-12	1.1683	11.705
216	AgCl2	-1		.000016		9.308E-11	24.22	6.955E-11	.7472	10.158
217	AgCl3	-2		.000017		8.241E-11	21.44	2.569E-11	.3118	10.590
218	AgCl4	-3		.000050		2.071E-10	53.88	1.504E-11	.0726	10.823
219	AgF aq	0		.000000		1.626E-19	.00	1.900E-19	1.1683	18.721
222	AgI aq	0		.000000		3.870E-15	.00	4.521E-15	1.1683	14.345
223	AgI2	-1		.000000		2.752E-17	.00	2.057E-17	.7472	16.687
245	AgI3	-2		.000000		1.223E-20	.00	3.811E-21	.3118	20.419
246	AgI4	-3		.000000		1.018E-25	.00	7.396E-27	.0726	26.131
227	AgNO3 aq	0		.000000		4.772E-21	.00	5.576E-21	1.1683	20.254
228	Ag(NO2)2	-1		.000000		7.556E-26	.00	5.646E-26	.7472	25.248
224	AgOH aq	0		.000000		4.181E-19	.00	4.884E-19	1.1683	18.311
225	Ag(OH)2	-1		.000000		1.064E-22	.00	7.948E-23	.7472	22.100
226	AgSO4	-1		.000000		2.086E-16	.00	1.559E-16	.7472	15.807
50	Al	3	.002000	.000000	7.683E-08	5.190E-17	.00	3.769E-18	.0726	17.424
54	AlF	2		.000000		3.340E-15	.00	1.041E-15	.3118	14.982
55	AlF2	1		.000000		1.929E-14	.00	1.442E-14	.7472	13.841
56	AlF3 aq	0		.000000		4.292E-15	.00	5.014E-15	1.1683	14.300
57	AlF4	-1		.000000		7.379E-17	.00	5.514E-17	.7472	16.259
203	AlHSO4	2		.000000		5.442E-26	.00	1.697E-26	.3118	25.770
51	AlOH	2		.000000		1.956E-14	.00	6.097E-15	.3118	14.215
52	Al(OH)2	1		.000000		1.042E-11	.01	7.783E-12	.7472	11.109
181	Al(OH)3	0		.000012		1.598E-10	.21	1.867E-10	1.1683	9.729
53	Al(OH)4	-1		.007027		7.666E-08	99.78	5.728E-08	.7472	7.242
58	AlSO4	1		.000000		4.249E-17	.00	3.175E-17	.7472	16.498
59	Al(SO4)2	-1		.000000		3.576E-18	.00	2.672E-18	.7472	17.573
249	As total	0	.004000		5.533E-08					
253	AsO3	-3		.000000		2.561E-39	.00	1.860E-40	.0726	39.730
252	HAsO3	-2		.000000		9.326E-35	.00	2.907E-35	.3118	34.536
251	H2AsO3	-1		.000000		2.965E-31	.00	2.216E-31	.7472	30.654
250	H3AsO3aq	0		.000000		1.932E-30	.00	2.257E-30	1.1683	29.646
254	H4AsO3	1		.000000		9.017E-39	.00	6.738E-39	.7472	38.171
258	AsO4	-3		.000013		9.834E-11	.18	7.142E-12	.0726	11.146
257	HAsO4	-2		.007351		5.445E-08	98.41	1.698E-08	.3118	7.770
256	H2AsO4	-1		.000107		7.841E-10	1.42	5.859E-10	.7472	9.232
255	H3AsO4aq	0		.000000		5.288E-16	.00	6.178E-16	1.1683	15.209
86	B tot	0	4.450		4.266E-04					
35	H3BO3 aq	0		22.143		3.712E-04	87.00	4.336E-04	1.1683	3.363
36	H2BO3	-1		3.254		5.544E-05	13.00	4.143E-05	.7472	4.383
101	BF(OH)3	-1		.000498		6.383E-09	.00	4.769E-09	.7472	8.322
102	BF2(OH)2	-1		.000000		1.161E-13	.00	8.675E-14	.7472	13.062
103	BF3OH	-1		.000000		2.161E-20	.00	1.615E-20	.7472	19.792
104	BF4	-1		.000000		1.495E-26	.00	1.117E-26	.7472	25.952
89	Ba	2	.020	.015	1.509E-07	1.109E-07	73.47	3.457E-08	.3118	7.461
313	BaCO3 aq	0		.000023		1.197E-10	.08	1.398E-10	1.1683	9.854
312	BaHCO3	1		.000085		4.460E-10	.30	3.333E-10	.7472	9.477
90	BaOH	1		.000000		2.551E-13	.00	1.906E-13	.7472	12.720
201	BaSO4 aq	0		.008895		3.950E-08	26.17	4.615E-08	1.1683	7.336
97	Br	-1	67.300	67.299	8.730E-04	8.730E-04	100.00	6.523E-04	.7472	3.186
0	Ca	2	412.300	367.776	1.066E-02	9.511E-03	89.20	2.382E-03	.2504	2.623

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data 1 A5

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
30	CaCO3 aq	0		2.582		2.673E-05	.25	3.123E-05	1.1683	4.505
100	CaF	1		.044		7.670E-07	.00	5.731E-07	.7472	6.242
29	CaHCO3	1		3.987		4.088E-05	.38	3.055E-05	.7472	4.515
73	CaHPO4aq	0		.004773		3.636E-08	.00	4.248E-08	1.1683	7.372
75	CaH2PO4	1		.000034		2.574E-10	.00	1.924E-10	.7472	9.716
81	CaHSO4	1		.000008		5.981E-11	.00	4.469E-11	.7472	10.350
28	CaOH	1		.004741		8.608E-08	.00	6.432E-08	.7472	7.192
74	CaPO4	-1		.002908		2.232E-08	.00	1.668E-08	.7472	7.778
31	CaSO4 aq	0		142.306		1.083E-03	10.16	1.266E-03	1.1683	2.898
160	Cd	2	.000100	.000003	9.221E-10	2.731E-11	2.96	8.513E-12	.3118	11.070
233	CdBr	1		.000000		1.099E-12	.12	8.213E-13	.7472	12.085
234	CdBr2 aq	0		.000000		2.463E-15	.00	2.877E-15	1.1683	14.541
161	CdCl	1		.000055		3.838E-10	41.62	2.868E-10	.7472	9.542
162	CdCl2 aq	0		.000064		3.610E-10	39.15	4.217E-10	1.1683	9.375
163	CdCl3	-1		.000027		1.256E-10	13.62	9.387E-11	.7472	10.027
276	CdCO3	0		.000000		4.530E-14	.00	5.293E-14	1.1683	13.276
166	Cd(CO3)2	-2		.000000		4.199E-15	.00	1.309E-15	.3118	14.883
164	CdF	1		.000000		3.962E-15	.00	2.961E-15	.7472	14.529
165	CdF2 aq	0		.000000		1.759E-19	.00	2.054E-19	1.1683	18.687
275	CdHCO3	1		.000000		3.622E-13	.04	2.707E-13	.7472	12.568
235	CdI	1		.000000		6.089E-16	.00	4.550E-16	.7472	15.342
236	CdI2 aq	0		.000000		4.058E-21	.00	4.741E-21	1.1683	20.324
173	CdNO3	1		.000000		1.037E-16	.00	7.746E-17	.7472	16.111
167	CdOH	1		.000000		1.542E-13	.02	1.152E-13	.7472	12.938
168	Cd(OH)2	0		.000000		8.619E-16	.00	1.007E-15	1.1683	14.997
169	Cd(OH)3	-1		.000000		2.460E-20	.00	1.838E-20	.7472	19.736
170	Cd(OH)4	-2		.000000		8.553E-26	.00	2.666E-26	.3118	25.574
171	Cd2OH	3		.000000		6.616E-23	.00	4.805E-24	.0726	23.318
172	CdOHCl aq	0		.000003		1.650E-11	1.79	1.928E-11	1.1683	10.715
174	CdSO4 aq	0		.000001		5.597E-12	.61	6.539E-12	1.1683	11.184
277	Cd(SO4)2	-2		.000000		6.122E-13	.07	1.909E-13	.3118	12.719
4	Cl	-1	19353.000	19352.844	5.658E-01	5.658E-01	100.00	3.528E-01	.6235	.453
17	CO3	-2		2.176		3.759E-05	1.76	7.827E-06	.2082	5.106
6	HCO3	-1	141.682	87.626	2.407E-03	1.488E-03	69.57	1.005E-03	.6755	2.998
85	H2CO3 aq	0		.695		1.162E-05	.54	1.362E-05	1.1721	4.866
48	Cs	1	.000400	.000400	3.119E-09	3.119E-09	100.00	2.331E-09	.7472	8.632
127	Cu	1		.000000		5.464E-17	.00	4.083E-17	.7472	16.389
128	CuCl2	-1		.000000		2.150E-12	.02	1.607E-12	.7472	11.794
129	CuCl3	-2		.000000		2.881E-12	.03	8.983E-13	.3118	12.047
130	Cu	2	.000700	.000004	1.142E-08	7.056E-11	.62	2.200E-11	.3118	10.658
133	CuCl	1		.000003		2.795E-11	.24	2.089E-11	.7472	10.680
134	CuCl2 aq	0		.000000		3.387E-12	.03	3.957E-12	1.1683	11.403
135	CuCl3	-1		.000000		6.628E-15	.00	4.953E-15	.7472	14.305
136	CuCl4	-2		.000000		2.809E-17	.00	8.756E-18	.3118	17.058
131	CuCO3 aq	0		.000094		7.914E-10	6.93	9.246E-10	1.1683	9.034
132	Cu(CO3)2	-2		.000005		2.921E-11	.26	9.106E-12	.3118	11.041
137	CuF	1		.000000		1.480E-14	.00	1.106E-14	.7472	13.956
271	CuHCO3	1		.000002		1.483E-11	.13	1.109E-11	.7472	10.955
138	CuOH	1		.000004		4.790E-11	.42	3.580E-11	.7472	10.446
139	Cu(OH)2	0		.000981		1.042E-08	91.24	1.217E-08	1.1683	7.915
140	Cu(OH)3	-1		.000000		1.597E-13	.00	1.193E-13	.7472	12.923
141	Cu(OH)4	-2		.000000		1.243E-17	.00	3.875E-18	.3118	17.412
142	Cu2(OH)2	2		.000000		1.801E-15	.00	5.616E-16	.3118	15.251
143	CuSO4 aq	0		.000002		1.024E-11	.09	1.196E-11	1.1683	10.922
61	F	-1	1.390	.678	7.583E-05	3.697E-05	48.76	2.763E-05	.7472	4.559
125	HF aq	0		.000004		2.137E-10	.00	2.497E-10	1.1683	9.603
126	HF2	-1		.000000		3.541E-14	.00	2.646E-14	.7472	13.577
296	H2F2 aq	0		.000000		1.390E-19	.00	1.624E-19	1.1683	18.789
16	Fe total	2	.002000		3.712E-08					
7	Fe	2		.000000		3.322E-15	.00	1.036E-15	.3118	14.985
315	FeCl	1		.000000		6.748E-16	.00	5.043E-16	.7472	15.297
310	FeCO3 aq	0		.000000		1.664E-16	.00	1.944E-16	1.1683	15.711
308	FeF	1		.000000		3.829E-19	.00	2.861E-19	.7472	18.544
309	FeHCO3	1		.000000		1.393E-16	.00	1.041E-16	.7472	15.982
99	FeHPO4aq	0		.000000		1.148E-19	.00	1.341E-19	1.1683	18.873
64	FeH2PO4	1		.000000		2.193E-21	.00	1.638E-21	.7472	20.786
122	FeHSO4	1		.000000		2.600E-23	.00	1.943E-23	.7472	22.712
10	FeOH	1		.000000		7.131E-17	.00	5.329E-17	.7472	16.273
79	Fe(OH)2	0		.000000		6.317E-20	.00	7.380E-20	1.1683	19.132
11	Fe(OH)3	-1		.000000		5.972E-22	.00	4.462E-22	.7472	21.350
33	FeSO4 aq	0		.000000		4.198E-16	.00	4.905E-16	1.1683	15.309
8	Fe	3		.000000		3.850E-19	.00	2.796E-20	.0726	19.553
15	FeCl	2		.000000		9.556E-19	.00	2.979E-19	.3118	18.526
27	FeCl2	1		.000000		6.282E-19	.00	4.694E-19	.7472	18.328
32	FeCl3 aq	0		.000000		1.417E-20	.00	1.656E-20	1.1683	19.781
105	FeF	2		.000000		3.927E-18	.00	1.224E-18	.3118	17.912
106	FeF2	1		.000000		1.802E-18	.00	1.347E-18	.7472	17.871
107	FeF3 aq	0		.000000		5.046E-20	.00	5.895E-20	1.1683	19.229
12	FeHPO4	1		.000000		3.276E-22	.00	2.448E-22	.7472	21.611

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
98	FeH2PO4	2		.000000		7.621E-23	.00	2.376E-23	.3118	22.624
123	FeHSO4	2		.000000		4.227E-26	.00	1.318E-26	.3118	25.880
9	FeOH	2		.000000		9.424E-14	.00	2.938E-14	.3118	13.532
76	Fe(OH)2	1		.000184		2.119E-09	5.71	1.583E-09	.7472	8.800
77	Fe(OH)3	0		.002929		2.841E-08	76.53	3.319E-08	1.1683	7.479
78	Fe(OH)4	-1		.000788		6.592E-09	17.76	4.925E-09	.7472	8.308
179	Fe2(OH)2	4		.000000		2.460E-24	.00	2.324E-26	.0094	25.634
180	Fe3(OH)4	5		.000000		1.121E-29	.00	7.691E-33	.0007	32.114
14	FeSO4	1		.000000		1.093E-18	.00	8.167E-19	.7472	18.088
108	Fe(SO4)2	-1		.000000		6.365E-20	.00	4.756E-20	.7472	19.323
63	H	1		.000008		7.982E-09	.00	6.026E-09	.7549	8.220
96	I	-1	.062	.062	5.064E-07	5.064E-07	100.00	3.784E-07	.7472	6.422
3	K	1	399.100	392.963	1.058E-02	1.042E-02	98.46	6.495E-03	.6235	2.187
60	KHPO4	-1		.000072		5.512E-10	.00	4.119E-10	.7472	9.385
45	KSO4	-1		21.215		1.627E-04	1.54	1.216E-04	.7472	3.915
80	Li	1	.181	.179	2.704E-05	2.672E-05	98.85	1.997E-05	.7472	4.700
82	LiSO4	-1		.031		3.107E-07	1.15	2.322E-07	.7472	6.634
1	Mg	2	1291.800	1111.926	5.507E-02	4.740E-02	86.08	1.370E-02	.2891	1.863
20	MgCO3 aq	0		7.129		8.762E-05	.16	1.024E-04	1.1683	3.990
19	MgF	1		1.399		3.348E-05	.06	2.501E-05	.7472	4.602
21	MgHCO3	1		17.764		2.158E-04	.39	1.612E-04	.7472	3.793
72	MgHPO4aq	0		.033		2.828E-07	.00	3.304E-07	1.1683	6.481
40	MgH2PO4	1		.000221		1.886E-09	.00	1.410E-09	.7472	8.851
18	MgOH	1		.432		1.084E-05	.02	8.097E-06	.7472	5.092
39	MgPO4	-1		.020		1.732E-07	.00	1.295E-07	.7472	6.888
22	MgSO4 aq	0		850.591		7.324E-03	13.30	8.557E-03	1.1683	2.068
109	Mn	2	.000200	.000100	3.773E-09	1.888E-09	50.03	5.885E-10	.3118	9.230
110	Mn	3		.000000		7.080E-26	.00	5.142E-27	.0726	26.289
111	MnCl	1		.000099		1.132E-09	30.00	8.457E-10	.7472	9.073
112	MnCl2 aq	0		.000014		1.115E-10	2.95	1.302E-10	1.1683	9.885
113	MnCl3	-1		.000003		1.693E-11	.45	1.265E-11	.7472	10.898
311	MnCO3 aq	0		.000035		3.132E-10	8.30	3.659E-10	1.1683	9.437
116	MnF	1		.000000		1.505E-13	.00	1.125E-13	.7472	12.949
119	MnHCO3	1		.000008		7.057E-11	1.87	5.273E-11	.7472	10.278
118	Mn(NO3)2	0		.000000		2.631E-20	.00	3.074E-20	1.1683	19.512
121	MnO4	-2		.000000		2.331E-28	.00	7.266E-29	.3118	28.139
120	MnO4	-1		.000000		1.136E-29	.00	8.487E-30	.7472	29.071
114	MnOH	1		.000000		3.294E-12	.09	2.461E-12	.7472	11.609
115	Mn(OH)3	-1		.000000		5.378E-20	.00	4.019E-20	.7472	19.396
117	MnSO4 aq	0		.000035		2.386E-10	6.32	2.787E-10	1.1683	9.555
2	Na	1	10768.000	10628.569	4.855E-01	4.792E-01	98.71	3.387E-01	.7069	.470
41	NaCO3	-1		5.291		6.607E-05	.01	4.937E-05	.7472	4.307
297	NaF aq	0		.187		4.609E-06	.00	5.385E-06	1.1683	5.269
42	NaHCO3aq	0		13.287		1.639E-04	.03	1.915E-04	1.1683	3.718
49	NaHPO4	-1		.003300		2.875E-08	.00	2.148E-08	.7472	7.668
43	NaSO4	-1		695.034		6.051E-03	1.25	4.521E-03	.7472	2.345
37	NH3 aq	0		.015		9.213E-07	5.53	1.076E-06	1.1683	5.968
38	NH4	1	.290	.265	1.666E-05	1.522E-05	91.34	1.137E-05	.7472	4.944
91	NH4SO4	-1		.057		5.222E-07	3.13	3.902E-07	.7472	6.409
204	Ni	2	.001700	.000094	3.001E-08	1.654E-09	5.51	5.157E-10	.3118	9.288
205	NiBr	1		.000000		1.424E-12	.00	1.064E-12	.7472	11.973
206	NiCl	1		.000056		6.116E-10	2.04	4.570E-10	.7472	9.340
279	NiCl2	0		.000063		5.010E-10	1.67	5.853E-10	1.1683	9.233
281	NiCO3	0		.002934		2.561E-08	85.34	2.992E-08	1.1683	7.524
282	Ni(CO3)2	-2		.000225		1.305E-09	4.35	4.068E-10	.3118	9.391
207	NiF	1		.000000		3.804E-13	.00	2.843E-13	.7472	12.546
280	NiHCO3	1		.000011		9.579E-11	.32	7.158E-11	.7472	10.145
208	NiOH	1		.000001		1.550E-11	.05	1.158E-11	.7472	10.936
209	Ni(OH)2	0		.000000		1.169E-12	.00	1.366E-12	1.1683	11.865
210	Ni(OH)3	-1		.000000		2.974E-15	.00	2.222E-15	.7472	14.653
211	NiSO4 aq	0		.000034		2.292E-10	.76	2.678E-10	1.1683	9.572
283	Ni(SO4)2	-2		.000000		1.228E-13	.00	3.829E-14	.3118	13.417
202	NO2	-1	.020	.020	4.506E-07	4.506E-07	100.00	3.367E-07	.7472	6.473
84	NO3	-1	.290	.290	4.848E-06	4.848E-06	100.00	3.622E-06	.7472	5.441
26	OH	-1		.036		2.182E-06	.00	1.630E-06	.7472	5.788
182	Pb	2	.000050	.000000	2.501E-10	4.872E-12	1.95	1.519E-12	.3118	11.818
237	PbBr	1		.000000		7.808E-14	.03	5.834E-14	.7472	13.234
238	PbBr2 aq	0		.000000		1.524E-17	.00	1.780E-17	1.1683	16.750
183	PbCl	1		.000007		2.855E-11	11.41	2.133E-11	.7472	10.671
184	PbCl2 aq	0		.000003		1.021E-11	4.08	1.193E-11	1.1683	10.923
185	PbCl3	-1		.000001		4.472E-12	1.79	3.342E-12	.7472	11.476
186	PbCl4	-2		.000000		1.810E-12	.72	5.643E-13	.3118	12.249
241	PbCO3 aq	0		.000046		1.768E-10	70.70	2.066E-10	1.1683	9.685
187	Pb(CO3)2	-2		.000004		1.302E-11	5.21	4.060E-12	.3118	11.392
188	PbF	1		.000000		9.986E-16	.00	7.462E-16	.7472	15.127
189	PbF2 aq	0		.000000		3.603E-19	.00	4.209E-19	1.1683	18.376
190	PbF3	-1		.000000		1.127E-22	.00	8.423E-23	.7472	22.075
191	PbF4	-2		.000000		3.572E-27	.00	1.114E-27	.3118	26.953
278	PbHCO3	1		.000000		1.623E-12	.65	1.213E-12	.7472	11.916

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
239	PbI	1		.000000		6.699E-17	.00	5.006E-17	.7472	16.301
240	PbI2 aq	0		.000000		2.950E-22	.00	3.446E-22	1.1683	21.463
196	PbNO3	1		.000000		1.089E-16	.00	8.138E-17	.7472	16.089
192	PbOH	1		.000001		6.450E-12	2.58	4.819E-12	.7472	11.317
193	Pb(OH)2	0		.000000		2.612E-13	.10	3.051E-13	1.1683	12.516
194	Pb(OH)3	-1		.000000		7.629E-16	.00	5.701E-16	.7472	15.244
242	Pb(OH)4	-2		.000000		6.816E-19	.00	2.125E-19	.3118	18.673
195	Pb2OH	3		.000000		2.263E-21	.00	1.643E-22	.0726	21.784
200	Pb3(OH)4	2		.000000		1.045E-26	.00	3.258E-27	.3118	26.487
197	PbSO4 aq	0		.000000		1.947E-12	.78	2.275E-12	1.1683	11.643
243	Pb(SO4)2	-2		.000000		1.019E-13	.04	3.178E-14	.3118	13.498
44	PO4	-3	.060000	.000003	6.548E-07	3.351E-11	.00	2.434E-12	.0726	11.614
46	HPO4	-2		.009662		1.043E-07	15.93	3.253E-08	.3118	7.488
47	H2PO4	-1		.000395		4.225E-09	.65	3.157E-09	.7472	8.501
94	Rb	1	.117	.117	1.419E-06	1.419E-06	100.00	1.060E-06	.7472	5.975
34	SiO2 tot	0	4.280		7.383E-05					
23	H4SiO4aq	0		6.594		7.111E-05	96.31	8.308E-05	1.1683	4.081
24	H3SiO4	-1		.250		2.722E-06	3.69	2.034E-06	.7472	5.692
25	H2SiO4	-2		.000007		7.369E-11	.00	2.297E-11	.3118	10.639
124	SiF6	-2		.000000		2.556E-34	.00	7.969E-35	.3118	34.099
5	SO4	-2	2712.000	1355.923	2.926E-02	1.463E-02	50.00	2.663E-03	.1821	2.575
62	HSO4	-1		.000196		2.089E-09	.00	1.561E-09	.7472	8.807
87	Sr	2	8.140	7.286	9.629E-05	8.618E-05	89.51	2.114E-05	.2453	4.675
95	SrCO3 aq	0		.033		2.300E-07	.24	1.056E-07	.4594	6.976
68	SrHCO3	1		.069		4.814E-07	.50	3.252E-07	.6755	6.488
88	SrOH	1		.000027		2.659E-10	.00	1.764E-10	.6634	9.753
314	SrSO4 aq	0		1.665		9.396E-06	9.76	1.098E-05	1.1683	4.959
145	Zn	2	.004900	.001554	7.769E-08	2.464E-08	31.71	7.681E-09	.3118	8.115
229	ZnBr	1		.000000		1.764E-12	.00	1.318E-12	.7472	11.880
230	ZnBr2 aq	0		.000000		2.929E-16	.00	3.422E-16	1.1683	15.466
146	ZnCl	1		.000949		9.760E-09	12.56	7.293E-09	.7472	8.137
147	ZnCl2 aq	0		.000303		2.306E-09	2.97	2.694E-09	1.1683	8.570
148	ZnCl3	-1		.000236		1.427E-09	1.84	1.066E-09	.7472	8.972
149	ZnCl4	-2		.000121		6.047E-10	.78	1.885E-10	.3118	9.725
273	ZnCO3	0		.001242		1.027E-08	13.22	1.199E-08	1.1683	7.921
274	Zn(CO3)2	-2		.001151		6.434E-09	8.28	2.006E-09	.3118	8.698
150	ZnF	1		.000000		4.011E-12	.00	2.997E-12	.7472	11.523
272	ZnHCO3	1		.000159		1.301E-09	1.67	9.722E-10	.7472	9.012
231	ZnI	1		.000000		4.785E-18	.00	3.575E-18	.7472	17.447
232	ZnI2 aq	0		.000000		1.922E-23	.00	2.245E-23	1.1683	22.649
151	ZnOH	1		.000146		1.834E-09	2.36	1.370E-09	.7472	8.863
152	Zn(OH)2	0		.000210		2.192E-09	2.82	2.560E-09	1.1683	8.592
153	Zn(OH)3	-1		.000000		1.763E-12	.00	1.318E-12	.7472	11.880
154	Zn(OH)4	-2		.000000		1.090E-16	.00	3.398E-17	.3118	16.469
155	ZnOHCl aq	0		.001421		1.250E-08	16.09	1.460E-08	1.1683	7.836
158	ZnSO4 aq	0		.000639		4.105E-09	5.28	4.796E-09	1.1683	8.319
159	Zn(SO4)2	-2		.000083		3.328E-10	.43	1.038E-10	.3118	9.984

Weight ratios from analytical ppm - Mole ratios from analytical molality

Ca/Cl	2.1304E-02	Ca/Cl	1.8845E-02
Ca/SO4	1.5203E-01	Ca/SO4	3.6437E-01
Mg/Cl	6.6749E-02	Mg/Cl	9.7337E-02
Mg/SO4	4.7633E-01	Mg/SO4	1.8821E+00
Na/Cl	5.5640E-01	Na/Cl	8.5803E-01
Na/SO4	3.9705E+00	Na/SO4	1.6591E+01
K /Cl	2.0622E-02	K /Cl	1.8698E-02
K /SO4	1.4716E-01	K /SO4	3.6153E-01
Al/Cl	1.0334E-07	Al/Cl	1.3579E-07
Al/SO4	7.3746E-07	Al/SO4	2.6256E-06
Fe/Cl	1.0334E-07	Fe/Cl	6.5605E-08
Fe/SO4	7.3746E-07	Fe/SO4	1.2685E-06
Mn/Cl	1.0334E-08	Mn/Cl	6.6690E-09
Mn/SO4	7.3746E-08	Mn/SO4	1.2895E-07
Sr/Cl	4.2061E-04	Sr/Cl	1.7019E-04
Sr/SO4	3.0015E-03	Sr/SO4	3.2906E-03
Ba/Cl	1.0334E-06	Ba/Cl	2.6677E-07
Ba/SO4	7.3746E-06	Ba/SO4	5.1581E-06
Li/Cl	9.3526E-06	Li/Cl	4.7784E-05
Li/SO4	6.6740E-05	Li/SO4	9.2394E-04
Cs/Cl	2.0669E-08	Cs/Cl	5.5134E-09
Cs/SO4	1.4749E-07	Cs/SO4	1.0661E-07
Rb/Cl	6.0456E-06	Rb/Cl	2.5077E-06
Rb/SO4	4.3142E-05	Rb/SO4	4.8488E-05
Cu/Cl	3.6170E-08	Cu/Cl	2.0180E-08
Cu/SO4	2.5811E-07	Cu/SO4	3.9018E-07
Zn/Cl	2.5319E-07	Zn/Cl	1.3732E-07
Zn/SO4	1.8068E-06	Zn/SO4	2.6551E-06
Cd/Cl	5.1672E-09	Cd/Cl	1.6298E-09
Cd/SO4	3.6873E-08	Cd/SO4	3.1513E-08
Pb/Cl	2.5836E-09	Pb/Cl	4.4209E-10
Pb/SO4	1.8437E-08	Pb/SO4	8.5479E-09
Ni/Cl	8.7842E-08	Ni/Cl	5.3045E-08
Ni/SO4	6.2684E-07	Ni/SO4	1.0256E-06
As/Cl	2.0669E-07	As/Cl	9.7804E-08
As/SO4	1.4749E-06	As/SO4	1.8911E-06
B /Cl	2.2994E-04	B /Cl	7.5405E-04
B /SO4	1.6409E-03	B /SO4	1.4580E-02
F /Cl	7.1823E-05	F /Cl	1.3403E-04
F /SO4	5.1254E-04	F /SO4	2.5915E-03
Br/Cl	3.4775E-03	Br/Cl	1.5429E-03
Br/SO4	2.4816E-02	Br/SO4	2.9834E-02
I /Cl	3.2036E-06	I /Cl	8.9499E-07
I /SO4	2.2861E-05	I /SO4	1.7305E-05
Ca/HCO3=	2.9100E+00	Ca/HCO3=	4.4302E+00
Mg/HCO3=	9.1176E+00	Mg/HCO3=	2.2883E+01
Na/HCO3=	7.6001E+01	Na/HCO3=	2.0171E+02
K /HCO3=	2.8169E+00	K /HCO3=	4.3956E+00
F /HCO3=	9.8107E-03	F /HCO3=	3.1509E-02
Sr/HCO3=	5.7453E-02	Sr/HCO3=	4.0009E-02
Ca/Mg	3.1917E-01	Ca/Mg	1.9360E-01
Na/K	2.6981E+01	Na/K	4.5890E+01
Zn/Cd	4.9000E+01	Zn/Cd	8.4253E+01
Na/Ca	2.6117E+01	Na/Ca	4.5532E+01
Sr/Ca	1.9743E-02	Sr/Ca	9.0310E-03
B/F	3.2014E+00	B/F	5.6260E+00
B/As	1.1125E+03	B/As	7.7098E+03
Mn/Fe	1.0000E-01	Mn/Fe	1.0165E-01
Cu/Fe	3.5000E-01	Cu/Fe	3.0760E-01
Zn/Fe	2.4500E+00	Zn/Fe	2.0931E+00
Cd/Fe	5.0000E-02	Cd/Fe	2.4843E-02
Pb/Fe	2.5000E-02	Pb/Fe	6.7386E-03
Ni/Fe	8.5000E-01	Ni/Fe	8.0855E-01
Ag/Fe	2.0000E-02	Ag/Fe	1.0355E-02
As/Fe	2.0000E+00	As/Fe	1.4908E+00

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
195	a-Cryptomeln		-74.732			
39	Adularia	-1.030	-21.603		-20.573	
437	Ag metal	-9.464	-22.974		-13.510	
440	Ag2CO3	-23:082	-34.152		-11.070	
443	Ag2O	-25.194	-12.614		12.580	.100
446	Ag2SO4	-26.700	-31.620		-4.920	
444	Ag3PO4	-37.632	-55.182		-17.550	
441	AgF, 4H2O	-19.666	-19.116		.550	
489	AlAsO4, 2H2O	-12.750	-28.587		-15.837	
40	Albite	-1.883	-19.885		-18.002	
157	Allophane(a)	-2.348	5.762		8.110	
158	Allophane(P)	-1.333	5.762		7.094	
140	Al(OH)3 (a)	-3.589	7.211		10.800	
338	Alum k	-19.693	-24.863		-5.170	
50	Alunite	-8.939	-10.339		-1.400	
42	Analcime	-3.130	-15.831		-12.701	
384	Anglesite	-6.603	-14.393		-7.790	.020
17	Anhydrite	-.837	-5.198		-4.361	
113	Annite	19.105	-66.540		-85.645	
41	Anorthite	-5.486	-25.200		-19.714	
239	Antlerite	-9.992	-1.702		8.290	
21	Aragonite	.607	-7.730		-8.336	.020
497	Arsenolite	-115.734	-118.535		-2.801	
150	Artinite	-3.555	6.045		9.600	
488	As2O5	-37.092	-30.393		6.699	
499	AsI3	-77.702	-73.547		4.155	
237	Atacamite	-4.473	2.867		7.340	
236	Azurite	-8.855	-5.105		3.750	.090
541	Ba3(AsO4)2	5.434	-44.676		-50.110	
398	BaF2	-10.819	-16.579		-5.760	
144	Barite	-.066	-10.036		-9.970	
472	Basaluminite	-12.855	9.845		22.700	
48	Beidellite	-3.026	-48.298		-45.272	
292	Bianchite	-8.975	-10.740		-1.765	
184	Birnessite	-3.065	40.536		43.601	
186	Bixbyite	-2.672	-3.283		-.611	
52	Boehmite	-1.365	7.219		8.584	
240	Brochantite	-11.276	4.064		15.340	.160
438	Bromyrite	-5.438	-17.708		-12.270	
19	Brucite	-2.280	14.560		16.840	
413	Bunsenite	-5.306	7.144		12.450	
490	Ca3AsO4)2,4w	-11.291	-30.196		-18.905	
12	Calcite	.750	-7.730		-8.480	.020
312	Cd metal	-41.463	-27.973		13.490	
314	Cd(BO2)2	-11.179	-1.339		9.840	
320	Cd(OH)2 (a)	-8.377	5.353		13.730	
321	Cd(OH)2 (c)	-8.297	5.353		13.650	.040
323	Cd3(OH)4SO4	-25.498	-2.938		22.560	
327	Cd3(PO4)2	-23.837	-56.437		-32.600	
324	Cd3OH)2SO4)2	-28.646	-21.936		6.710	
325	Cd4(OH)6SO4	-25.985	2.415		28.400	
463	CdBr2, 4H2O	-15.055	-17.475		-2.420	
317	CdCl2, 1H2O	-10.273	-11.983		-1.710	
316	CdCl2	-11.295	-11.975		-.680	
318	CdCl2,2.5H2O	-10.056	-11.996		-1.940	
319	CdF2	-17.207	-20.187		-2.980	
464	CdI2	-20.304	-23.914		-3.610	
322	CdOHCl	-6.831	-3.311		3.520	
328	CdSiO3	-7.762	1.298		9.060	
330	CdSO4, 1H2O	-11.996	-13.653		-1.657	
329	CdSO4	-13.544	-13.644		-.100	
331	CdSO4,2.7H2O	-11.794	-13.667		-1.873	
143	Celestite	-.618	-7.249		-6.631	
439	Cerargyrite	-5.225	-14.975		-9.750	
365	Cerrusite	-3.795	-16.925		-13.130	
248	Chalcanthite	-10.635	-13.275		-2.640	
97	Chalcedony	-.512	-4.063		-3.551	
49	Chlorite 14A	6.684	75.064		68.380	6.000
125	Chlorite 7A	3.312	75.064		71.752	6.000
20	Chrysotile	3.361	35.561		32.200	
498	Claudetite	-115.470	-118.535		-3.065	
29	Clinoenstite	-.837	10.505		11.342	
56	Clinoptilolt		-27.803			
376	Clpyromorph	-9.956	-94.386		-84.430	
362	Cotunnite	-7.953	-12.723		-4.770	
99	Cristobalite	-.476	-4.063		-3.587	
223	Cu metal	-16.080	-24.840		-8.760	
234	Cu(OH)2	-2.875	5.765		8.640	
238	Cu2(OH)3NO3	-11.362	-2.122		9.240	

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
228	Cu2SO4	-33.403	-35.353		-1.950	
244	Cu3(PO4)2	-18.350	-55.200		-36.850	
245	Cu3(PO4)2,3w	-20.106	-55.226		-35.120	
491	Cu3AsO4)2,6w	-19:193	-54.316		-35.123	
459	CuBr	-11.365	-19.575		-8.210	
231	CuCO3	-6.134	-15.764		-9.630	
225	CuF	-28.028	-20.948		7.080	
232	CuF2	-19.155	-19.775		-.620	
233	CuF2, 2H2O	-15.242	-19.792		-4.550	
460	CuI	-10.921	-22.811		-11.890	
243	CuOCuSO4	-35.428	-23.898		11.530	
248	CupricFerrit	10.081	15.961		5.880	
226	Cuprite	-14.797	-16.347		-1.550	
229	CuprousFerit	5.840	-3.080		-8.920	
247	CuSO4	-16.242	-13.232		3.010	
154	Diaspore	.340	7.219		6.879	
28	Diopside	.356	20.250		19.894	
420	Dioptase	-4.798	1.702		6.500	
11	Dolomite (d)	1.841	-14.699		-16.540	
401	Dolomite (c)	2.391	-14.699		-17.090	
340	Epsomite	-2.357	-4.497		-2.140	
55	Erionite		-21.943			
396	FCO3 Apatite	15.874	-98.526		-114.400	
419	Fe3(OH)8	-8.622	11.600		20.222	
181	FeOH)2.7Cl.3	5.522	2.482		-3.040	
112	Ferrihydrite	.190	5.081		4.891	
96	Fluorapatite	2.123	-15.477		-17.600	
62	Fluorite	-1.141	-11.740		-10.600	
27	Forsterite	-3.233	25.073		28.306	
313	Gamma Cd	-41.563	-27.973		13.590	
51	Gibbsite (c)	-.899	7.211		8.110	.200
110	Goethite	6.090	5.090		-1.000	.800
293	Goslarite	-8.789	-10.749		-1.960	
111	Greenalite	-24.614	-3.804		20.810	
18	Gypsum	-.634	-5.215		-4.581	
64	Halite	-2.505	-.923		1.582	
47	Halloysite	-6.195	6.303		12.498	
187	Hausmannite	-6.092	54.938		61.030	
108	Hematite	14.196	10.188		-4.008	
380	Hinsdalite	-26.509	-29.009		-2.500	
196	Hollandite		-60.634			
117	Huntite	1.330	-28.638		-29.968	
377	Hxypyromorph	-22.932	-85.722		-62.790	
392	Hydcerrusite	-11.785	-29.245		-17.460	
38	Hydrmagnesit	-4.591	-13.353		-8.762	
95	Hydroxyapati	.714	-2.707		-3.421	
45	Illite	-2.218	-42.485		-40.267	
442	Iodyrite	-4.875	-20.945		-16.070	
205	Jarosite K	-7.518	-16.728		-9.210	1.100
337	Jarosite H	-17.379	-22.769		-5.390	
204	Jarosite Na	-9.731	-15.011		-5.280	1.000
133	Jarosite(ss)	-10.083	-18.083		-8.000	
471	Jurbanite	-8.557	-11.787		-3.230	
46	Kaolinite	-1.132	6.303		7.435	
43	Kmica	2.797	15.500		12.703	1.300
241	Langite	-12.735	4.055		16.790	
371	Larnakite	-9.500	-9.780		-.280	
128	Laumontite	-2.401	-33.361		-30.960	
390	Laurionite	-4.683	-4.060		.623	
147	Leonhardite	3.043	-66.713		-69.756	
368	Litharge	-8.107	4.613		12.720	
199	Lithiophorit		-25.742			
98	Magadiite	-8.154	-22.454		-14.300	
109	Maghemite	3.802	10.188		6.386	
10	Magnesite	1.059	-6.970		-8.029	
107	Magnetite	7.897	11.634		3.737	
235	Malachite	-4.820	.330		5.150	.080
189	Manganite	-1.476	23.864		25.340	
367	Massicot	-8.297	4.613		12.910	
363	Matlockite	-7.400	-16.830		-9.430	
230	Melanothalit	-15.293	-11.563		3.730	
339	Melanterite	-15.410	-17.619		-2.209	
388	Minium	-26.517	47.173		73.690	
66	Mirabilite	-2.486	-3.600		-1.114	
134	Mn2(SO4)3	-54.590	-60.301		-5.711	
193	Mn3(PO4)2	-27.091	-50.918		-23.827	
493	Mn3AsO4)2,8w	-21.344	-50.051		-28.707	
191	MnCl2, 4H2O	-12.879	-10.169		2.710	
194	MnHPO4	-3.771	-16.718		-12.947	

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
182	MnSO4	-14.474	-11.805		2.669	
326	Monteponite	-8.408	5.362		13.770	
115	Montmoril BF	2.099	-32.814		-34.913	
116	Montmoril AB	1.910	-27.778		-29.688	
63	Montmoril Ca	-3.598	-48.625		-45.027	
57	Mordenite		-25.767			
417	Morenosite	-9.562	-11.922		-2.360	
58	Nahcolite	-2.920	-3.468		-.548	
224	Nantokite	-10.082	-16.842		-6.760	
60	Natron	-4.821	-6.132		-1.311	
149	Nesquehonite	-1.374	-6.995		-5.621	
411	Ni(OH)2	-3.665	7.135		10.800	.100
418	Ni2SiO4	-4.316	10.224		14.540	
414	Ni3(PO4)2	-19.790	-51.090		-31.300	
494	Ni3AsO4)2,8w	-24.712	-50.223		-25.511	
412	Ni4(OH)6SO4	-22.456	9.544		32.000	
410	NiCO3	-7.554	-14.394		-6.840	
185	Nsutite	-2.028	40.536		42.564	
315	Otavite	-4.076	-16.176		-12.100	.100
360	Pb metal	-32.991	-28.721		4.270	
361	Pb(BO2)2	-9.697	-2.087		7.610	
389	Pb(OH)2 (c)	-3.546	4.604		8.150	
391	Pb2(OH)3Cl	-8.248	.545		8.793	
393	Pb2O(OH)2	-16.983	9.217		26.200	
387	Pb2O3	-18.480	42.560		61.040	
370	Pb2OCO3	-11.812	-12.312		-.500	
383	Pb2SiO4	-14.597	5.163		19.760	
495	Pb3(AsO4)2	-22.345	-57.748		-35.403	
375	Pb3(PO4)2	-14.321	-33.991		-19.670	
378	Pb3O2CO3	-18.719	-7.699		11.020	
372	Pb3O2SO4	-15.567	-5.167		10.400	
394	Pb4(OH)6SO4	-21.680	-.580		21.100	
373	Pb4O3SO4	-22.654	-.554		22.100	
465	PbBr2	-13.010	-18.190		-5.180	
466	PbBrF	-11.073	-19.563		-8.490	
366	PbF2	-13.496	-20.936		-7.440	
374	PbHPO4	-7.846	-19.306		-11.460	
467	PbI2	-16.593	-24.663		-8.070	
369	PbO, 0.3H2O	-8.370	4.610		12.980	
382	PbSiO3	-6.770	.550		7.320	
54	Phillipsite	-.879	-20.753		-19.874	
44	Phlogopite	-21.206	22.094		43.300	3.000
364	Phosgenite	-9.838	-29.648		-19.810	
386	Plattnerite	-11.353	37.947		49.300	
379	Plumbgummite	-13.478	-46.268		-32.790	
539	Portlandite	-9.000	13.800		22.800	
141	Prehnite	-3.768	-15.463		-11.695	
197	Psilomelane		-56.410			
188	Pyrocroite	-8.007	7.193		15.200	
183	Pyrolusite	-.844	40.536		41.380	
53	Pyrophyllite	1.170	-47.144		-48.314	
101	Quartz	-.083	-4.063		-3.980	
200	Rancieite		-31.855			
416	Retgersite	-9.873	-11.913		-2.040	
190	Rhodochrs(d)	-3.947	-14.337		-10.390	
564	Rhodochrs(c)	-3.207	-14.337		-11.130	
492	Scorodite	-10.468	-30.717		-20.249	
153	Sepiolite(d)	-1.744	16.916		18.660	
36	Sepiolite(c)	1.156	16.916		15.760	
9	Siderite (d)	-9.641	-20.091		-10.450	
94	Siderite (c)	-9.201	-20.091		-10.890	
100	Silica gel	-1.045	-4.063		-3.018	
395	SiO2 (a)	-1.352	-4.063		-2.712	
268	Smithsonite	-3.221	-13.221		-10.000	
399	SrF2	-5.252	-13.792		-8.540	
146	Strengite	-4.784	-31.184		-26.400	
142	Strontianite	-.511	-9.781		-9.271	
37	Talc	6.044	27.443		21.399	2.000
242	Tenorite	-1.846	5.774		7.620	
65	Thenardite	-3.336	-3.515		-.179	
61	Thermonatrit	-6.180	-6.055		.125	
198	Todorokite		-31.956			
31	Tremolite	11.368	67.942		56.574	
59	Trona	-8.737	-9.532		-.795	
381	Tsumebite	-11.510	-21.300		-9.790	
106	Vivianite	-32.250	-68.250		-36.000	
155	Wairakite	-6.636	-33.344		-26.708	
289	Willemite	-2.760	12.570		15.330	
145	Witherite	-4.006	-12.568		-8.562	

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
282	Zincite (c)	-2.823	8.317		11.140	
290	Zincosite	-13.699	-10.689		3.010	
265	Zn metal	-50.774	-25.017		25.757	
266	Zn(BO2)2	-6.673	1.617		8.290	
275	Zn(OH)2 (e)	-3.192	8.308		11.500	.030
272	Zn(OH)2 (c)	-3.892	8.308		12.200	
274	Zn(OH)2 (g)	-3.402	8.308		11.710	
273	Zn(OH)2 (b)	-3.442	8.308		11.750	.020
271	Zn(OH)2 (a)	-4.142	8.308		12.450	
278	Zn2(OH)2SO4	-9.881	-2.381		7.500	
276	Zn2(OH)3Cl	-7.247	7.953		15.200	
284	Zn3(PO4)2,4w	-15.565	-47.605		-32.040	
496	Zn3AsO422.5w	-19.111	-46.657		-27.546	
283	Zn3O(SO4)2	-32.081	-13.061		19.020	
279	Zn4(OH)6SO4	-14.164	14.236		28.400	
277	Zn5(OH)8Cl	-14.286	24.214		38.500	
461	ZnBr2, 2H2O	-19.713	-14.503		5.210	
267	ZnCl2	-16.050	-9.020		7.030	
269	ZnCO3, 1H2O	-2.970	-13.230		-10.260	
270	ZnF2	-15.712	-17.232		-1.520	
462	ZnI2	-28.189	-20.959		7.230	
280	ZnNO3)2,6H2O	-22.488	-19.048		3.440	
281	ZnO (a)	-2.993	8.317		11.310	
288	ZnSiO3	1.323	4.253		2.930	
291	ZnSO4, 1H2O	-10.128	-10.698		-.570	

Minimum Output for Test Problem #1

```
DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data        1 A5
   0     0 000000       0       0  35.147       0
                    TEMP      =         25.000000
                    PH        =          8.220000
                    EH(0)     =           .500000
                    DOC       =           .000000
                    DOX       =          6.600000
                    CORALK    =          0
                    FLG       =        PPM
                    DENS      =          1.023361
                    PRNT      =          0
                    PUNCH     =          1
                    EHOPT(1)  =          0  Use measured Eh to calculate Fe species distribution
                    EHOPT(2)  =          0  Use measured Eh to calculate Mn species other than +2
                    EHOPT(3)  =          0  Use measured Eh to calculate Cu +1 species
                    EHOPT(4)  =          0  Use measured Eh to calculate As species distribution
                    EHOPT(5)  =          0  Use measured Eh to calculate Se species distribution
                    EHOPT(6)  =          0  Use measured Eh to calculate Ion Activity Products
                    EHOPT(7)  =          3  Use H2O/O2 classical Eh to calculate atmospheric pO2
                    EHOPT(8)  =          2  Use H2O2/O2 Sato Eh to calculate H2S from SO4
                    EHOPT(9)  =          0  Use measured Eh to calculate U species distribution
                    EMPOX     =          0
                    ITDS      =           .000000
                    COND      =           .000000
                    SIGMDO    =           .000000
                    SIGMEH    =           .000000
                    SIGMPH    =           .000000
```

Species	Index No	Input Concentration
Ca	0	412.30000000
Mg	1	1291.80000000
Na	2	10768.00000000
K	3	399.10000000
Cl	4	19353.00000000
SO4	5	2712.00000000
HCO3	6	141.68200000
Fe total	16	.00200000
H2S aq	13	.00000000
CO3	17	.00000000
SiO2 tot	34	4.28000000
NH4	38	.29000000
B tot	86	4.45000000
PO4	44	.06000000
Al	50	.00200000
F	61	1.39000000
NO3	84	.29000000
Cs	48	.00040000
Li	80	.18100000
Sr	87	8.14000000
Ba	89	.02000000
Rb	94	.11700000
I	96	.06200000
Br	97	67.30000000
Mn	109	.00020000
Cu	130	.00070000
Zn	145	.00490000
Cd	160	.00010000
Pb	182	.00005000
NO2	202	.02000000
Ni	204	.00170000
Ag	212	.00004000
As total	249	.00400000

ITER	S1-AnalCO3	S2-AnalSO4	S3-AnalF	S4-AnalPO4	S5-AnalCL	S6-AnalH2S	S7-AnalFULV	S8-AnalHUM
1	1.162973E-03	2.629247E-02	7.173270E-05	3.001007E-06	3.190657E-08	0.000000E+00	0.000000E+00	0.000000E+00
2	7.401058E-05	1.653941E-03	3.777427E-06	3.567761E-08	6.835840E-09	0.000000E+00	0.000000E+00	0.000000E+00
3	-1.195843E-07	-6.782150E-05	3.076308E-07	8.544126E-09	7.652298E-10	0.000000E+00	0.000000E+00	0.000000E+00
4	-5.505179E-07	-1.642316E-05	-6.398325E-09	3.197057E-10	-4.152254E-11	0.000000E+00	0.000000E+00	0.000000E+00

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data 1 A5 Date = 6/03/91 13:57

0 0 000000 0 0 35.147 0

DOX = 6.6000 DOC = .0 INPUT TDS = .0

Anal Cond = .0 Calc Cond = 46798.6 Activity H2S calc from SO4 and pe = 8.33E-63

Anal EPMCAT = 627.7348 Anal EPMAN = 627.6592 Percent difference in input cation/anion balance = .0120

Calc EPMCAT = 603.9316 Calc EPMAN = 603.8530 Percent difference in calc cation/anion balance = .0130

Total Ionic Strength (T.I.S.) from input data = .72279

Effective Ionic Strength (E.I.S.) from speciation = .67557

Input	Sigma	Fe3/Fe2	Sigma	NO3/NO2	Sigma	NO3/NH4	Sigma	SO4/S=	Sigma	S/S=	Sigma	Sato H2O2/O2	Sigma	H2O/O2	Sigma
							Eh								
.500	.000	.500	.000	.390	.000	.269	.000	9.900	.000	9.900	.000	.133	.000	.689	.000
							pe								
8.451	.000	8.451	.000	6.585	.000	4.551	.000	100.000	.000	100.000	.000	2.248	.000	11.643	.000

As5/As3	Sigma	As3/As	Sigma	Se6/Se4	Sigma	Se4/Se	Sigma	Se/Se=	Sigma	U6/U4	Sigma		Sigma		Sigma
							Eh								
.500	.000	-.830	.000	9.900	.000	9.900	.000	9.900	.000	9.900					
							pe								
8.451	.000	-14.037	.000	100.000	.000	100.000	.000	100.000	.000	100.000					

T	pH	TDS ppm	Effective Ionic Str	pO2 Atm	ppm O2 Atm	pCO2 Atm	ppm CO2 Atm	log pCO2	CO2 Tot		Ncrb Alk	aH2O
25.00	8.220	35164.5	.67557	2.06E-04	6.60E+00	4.67E-04	2.05E+01	-3.331	2.14E-03		6.05E-05	.9805

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
212	Ag	1	.000040	.000000	3.843E-10	4.017E-15	.00	3.001E-15	.7472	14.523
216	AgCl2	-1		.000016		9.308E-11	24.22	6.955E-11	.7472	10.158
217	AgCl3	-2		.000017		8.241E-11	21.44	2.569E-11	.3118	10.590
218	AgCl4	-3		.000050		2.071E-10	53.88	1.504E-11	.0726	10.823
50	Al	3	.002000	.000000	7.683E-08	5.190E-17	.00	3.769E-18	.0726	17.424
53	Al(OH)4	-1		.007027		7.666E-08	99.78	5.728E-08	.7472	7.242
249	As total	0	.004000		5.533E-08					
257	HAsO4	-2		.007351		5.445E-08	98.41	1.698E-08	.3118	7.770
256	H2AsO4	-1		.000107		7.841E-10	1.42	5.859E-10	.7472	9.232
86	B tot	0	4.450		4.266E-04					
35	H3BO3 aq	0		22.143		3.712E-04	87.00	4.336E-04	1.1683	3.363
36	H2BO3	-1		3.254		5.544E-05	13.00	4.143E-05	.7472	4.383
89	Ba	2	.020	.015	1.509E-07	1.109E-07	73.47	3.457E-08	.3118	7.461
201	BaSO4 aq	0		.008895		3.950E-08	26.17	4.615E-08	1.1683	7.336
97	Br	-1	67.300	67.299	8.730E-04	8.730E-04	100.00	6.523E-04	.7472	3.186
0	Ca	2	412.300	367.776	1.066E-02	9.511E-03	89.20	2.382E-03	.2504	2.623
31	CaSO4 aq	0		142.306		1.083E-03	10.16	1.266E-03	1.1683	2.898
160	Cd	2	.000100	.000003	9.221E-10	2.731E-11	2.96	8.513E-12	.3118	11.070
161	CdCl	1		.000055		3.838E-10	41.62	2.868E-10	.7472	9.542
162	CdCl2 aq	0		.000064		3.610E-10	39.15	4.217E-10	1.1683	9.375
163	CdCl3	-1		.000027		1.256E-10	13.62	9.387E-11	.7472	10.027
172	CdOHCl aq	0		.000003		1.650E-11	1.79	1.928E-11	1.1683	10.715
4	Cl	-1	19353.000	19352.844	5.658E-01	5.658E-01	100.00	3.528E-01	.6235	.453
17	CO3	-2		2.176		3.759E-05	1.76	7.827E-06	.2082	5.106
6	HCO3	-1	141.682	87.626	2.407E-03	1.488E-03	69.57	1.005E-03	.6755	2.998
48	Cs	1	.000400	.000400	3.119E-09	3.119E-09	100.00	2.331E-09	.7472	8.632
130	Cu	2	.000700	.000004	1.142E-08	7.056E-11	.62	2.200E-11	.3118	10.658
131	CuCO3 aq	0		.000094		7.914E-10	6.93	9.246E-10	1.1683	9.034
139	Cu(OH)2	0		.000981		1.042E-08	91.24	1.217E-08	1.1683	7.915
61	F	-1	1.390	.678	7.583E-05	3.697E-05	48.76	2.763E-05	.7472	4.559
16	Fe total	2	.002000		3.712E-08					
76	Fe(OH)2	1		.000184		2.119E-09	5.71	1.583E-09	.7472	8.800
77	Fe(OH)3	0		.002929		2.841E-08	76.53	3.319E-08	1.1683	7.479
78	Fe(OH)4	-1		.000788		6.592E-09	17.76	4.925E-09	.7472	8.308
63	H	1		.000008		7.982E-09	.00	6.026E-09	.7549	8.220
96	I	-1	.062	.062	5.064E-07	5.064E-07	100.00	3.784E-07	.7472	6.422
3	K	1	399.100	392.963	1.058E-02	1.042E-02	98.46	6.495E-03	.6235	2.187
45	KSO4	-1		21.215		1.627E-04	1.54	1.216E-04	.7472	3.915
80	Li	1	.181	.179	2.704E-05	2.672E-05	98.85	1.997E-05	.7472	4.700
82	LiSO4	-1		.031		3.107E-07	1.15	2.322E-07	.7472	6.634
1	Mg	2	1291.800	1111.926	5.507E-02	4.740E-02	86.08	1.370E-02	.2891	1.863
22	MgSO4 aq	0		850.591		7.324E-03	13.30	8.557E-03	1.1683	2.068
109	Mn	2	.000200	.000100	3.773E-09	1.888E-09	50.03	5.885E-10	.3118	9.230
111	MnCl	1		.000099		1.132E-09	30.00	8.457E-10	.7472	9.073
112	MnCl2 aq	0		.000014		1.115E-10	2.95	1.302E-10	1.1683	9.885
311	MnCO3 aq	0		.000035		3.132E-10	8.30	3.659E-10	1.1683	9.437
119	MnHCO3	1		.000008		7.057E-11	1.87	5.273E-11	.7472	10.278
117	MnSO4 aq	0		.000035		2.386E-10	6.32	2.787E-10	1.1683	9.555
2	Na	1	10768.000	10628.569	4.855E-01	4.792E-01	98.71	3.387E-01	.7069	.470
43	NaSO4	-1		695.034		6.051E-03	1.25	4.521E-03	.7472	2.345
37	NH3 aq	0		.015		9.213E-07	5.53	1.076E-06	1.1683	5.968
38	NH4	1	.290	.265	1.666E-05	1.522E-05	91.34	1.137E-05	.7472	4.944
91	NH4SO4	-1		.057		5.222E-07	3.13	3.902E-07	.7472	6.409
204	Ni	2	.001700	.000094	3.001E-08	1.654E-09	5.51	5.157E-10	.3118	9.288

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data 1 A5

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
206	NiCl	1		.000056		6.116E-10	2.04	4.570E-10	.7472	9.340
279	NiCl2	0		.000063		5.010E-10	1.67	5.853E-10	1.1683	9.233
281	NiCO3	0		.002934		2.561E-08	85.34	2.992E-08	1.1683	7.524
282	Ni(CO3)2	-2		.000225		1.305E-09	4.35	4.068E-10	.3118	9.391
202	NO2	-1	.020	.020	4.506E-07	4.506E-07	100.00	3.367E-07	.7472	6.473
84	NO3	-1	.290	.290	4.848E-06	4.848E-06	100.00	3.622E-06	.7472	5.441
26	OH	-1		.036		2.182E-06	.00	1.630E-06	.7472	5.788
182	Pb	2	.000050	.000000	2.501E-10	4.872E-12	1.95	1.519E-12	.3118	11.818
183	PbCl	1		.000007		2.855E-11	11.41	2.133E-11	.7472	10.671
184	PbCl2 aq	0		.000003		1.021E-11	4.08	1.193E-11	1.1683	10.923
185	PbCl3	-1		.000001		4.472E-12	1.79	3.342E-12	.7472	11.476
241	PbCO3 aq	0		.000046		1.768E-10	70.70	2.066E-10	1.1683	9.685
187	Pb(CO3)2	-2		.000004		1.302E-11	5.21	4.060E-12	.3118	11.392
192	PbOH	1		.000001		6.450E-12	2.58	4.819E-12	.7472	11.317
44	PO4	-3	.060000	.000003	6.548E-07	3.351E-11	.00	2.434E-12	.0726	11.614
46	HPO4	-2		.009662		1.043E-07	15.93	3.253E-08	.3118	7.488
94	Rb	1	.117	.117	1.419E-06	1.419E-06	100.00	1.060E-06	.7472	5.975
34	SiO2 tot	0	4.280		7.383E-05					
23	H4SiO4aq	0		6.594		7.111E-05	96.31	8.308E-05	1.1683	4.081
24	H3SiO4	-1		.250		2.722E-06	3.69	2.034E-06	.7472	5.692
5	SO4	-2	2712.000	1355.923	2.926E-02	1.463E-02	50.00	2.663E-03	.1821	2.575
87	Sr	2	8.140	7.286	9.629E-05	8.618E-05	89.51	2.114E-05	.2453	4.675
314	SrSO4 aq	0		1.665		9.396E-06	9.76	1.098E-05	1.1683	4.959
145	Zn	2	.004900	.001554	7.769E-08	2.464E-08	31.71	7.681E-09	.3118	8.115
146	ZnCl	1		.000949		9.760E-09	12.56	7.293E-09	.7472	8.137
147	ZnCl2 aq	0		.000303		2.306E-09	2.97	2.694E-09	1.1683	8.570
148	ZnCl3	-1		.000236		1.427E-09	1.84	1.066E-09	.7472	8.972
273	ZnCO3	0		.001242		1.027E-08	13.22	1.199E-08	1.1683	7.921
274	Zn(CO3)2	-2		.001151		6.434E-09	8.28	2.006E-09	.3118	8.698
272	ZnHCO3	1		.000159		1.301E-09	1.67	9.722E-10	.7472	9.012
151	ZnOH	1		.000146		1.834E-09	2.36	1.370E-09	.7472	8.863
152	Zn(OH)2	0		.000210		2.192E-09	2.82	2.560E-09	1.1683	8.592
155	ZnOHCl aq	0		.001421		1.250E-08	16.09	1.460E-08	1.1683	7.836
158	ZnSO4 aq	0		.000639		4.105E-09	5.28	4.796E-09	1.1683	8.319

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
39	Adularia	-1.030	-21.603		-20.573	
437	Ag metal	-9.464	-22.974		-13.510	
40	Albite	-1.883	-19.885		-18.002	
140	Al(OH)3 (a)	-3.589	7.211		10.800	
50	Alunite	-8.939	-10.339		-1.400	
42	Analcime	-3.130	-15.831		-12.701	
384	Anglesite	-6.603	-14.393		-7.790	.020
17	Anhydrite	-.837	-5.198		-4.361	
239	Antlerite	-9.992	-1.702		8.290	
21	Aragonite	.607	-7.730		-8.336	.020
497	Arsenolite	-115.734	-118.535		-2.801	
237	Atacamite	-4.473	2.867		7.340	
236	Azurite	-8.855	-5.105		3.750	.090
144	Barite	-.066	-10.036		-9.970	
472	Basaluminite	-12.855	9.845		22.700	
240	Brochantite	-11.276	4.064		15.340	.160
19	Brucite	-2.280	14.560		16.840	
413	Bunsenite	-5.306	7.144		12.450	
12	Calcite	.750	-7.730		-8.480	.020
143	Celestite	-.618	-7.249		-6.631	
439	Cerargyrite	-5.225	-14.975		-9.750	
365	Cerrusite	-3.795	-16.925		-13.130	
97	Chalcedony	-.512	-4.063		-3.551	
20	Chrysotile	3.361	35.561		32.200	
99	Cristobalite	-.476	-4.063		-3.587	
226	Cuprite	-14.797	-16.347		-1.550	
154	Diaspore	.340	7.219		6.879	
11	Dolomite (d)	1.841	-14.699		-16.540	
401	Dolomite (c)	2.391	-14.699		-17.090	
340	Epsomite	-2.357	-4.497		-2.140	
396	FCO3 Apatite	15.874	-98.526		-114.400	
112	Ferrihydrite	.190	5.081		4.891	
96	Fluorapatite	2.123	-15.477		-17.600	
62	Fluorite	-1.141	-11.740		-10.600	
51	Gibbsite (c)	-.899	7.211		8.110	.200
110	Goethite	6.090	5.090		-1.000	.800
18	Gypsum	-.634	-5.215		-4.581	
64	Halite	-2.505	-.923		1.582	
47	Halloysite	-6.195	6.303		12.498	
392	Hydcerrusite	-11.785	-29.245		-17.460	
205	Jarosite K	-7.518	-16.728		-9.210	1.100
46	Kaolinite	-1.132	6.303		7.435	
128	Laumontite	-2.401	-33.361		-30.960	
10	Magnesite	1.059	-6.970		-8.029	
235	Malachite	-4.820	.330		5.150	.080
189	Manganite	-1.476	23.864		25.340	
315	Otavite	-4.076	-16.176		-12.100	.100
141	Prehnite	-3.768	-15.463		-11.695	
183	Pyrolusite	-.844	40.536		41.380	
101	Quartz	-.083	-4.063		-3.980	
190	Rhodochrs(d)	-3.947	-14.337		-10.390	
492	Scorodite	-10.468	-30.717		-20.249	
153	Sepiolite(d)	-1.744	16.916		18.660	
36	Sepiolite(c)	1.156	16.916		15.760	
9	Siderite (d)	-9.641	-20.091		-10.450	
395	SiO2 (a)	-1.352	-4.063		-2.712	
268	Smithsonite	-3.221	-13.221		-10.000	
146	Strengite	-4.784	-31.184		-26.400	
142	Strontianite	-.511	-9.781		-9.271	
242	Tenorite	-1.846	5.774		7.620	
106	Vivianite	-32.250	-68.250		-36.000	
145	Witherite	-4.006	-12.568		-8.562	
282	Zincite (c)	-2.823	8.317		11.140	
281	ZnO (a)	-2.993	8.317		11.310	

Input Data Set for Test Problem Number 2:

```
****
DK Nordstrom Test Data - Test Case #2 - Surface Water                    2 B5
  162     0 000000       0     2.5      .13       0       0       0       0
TEMP-.-- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--
    9.50     8.01    0.440     2.50    10.94        0
FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8--9
MG/L    1.0          0     1        0  0  0  0  0  0  3  5  0
EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.----SIGMPH-.----
       0     0.0    162.0        0.0         0.0         0.0
CA-----.----MG-----.----NA-----.----K------.----CL-----.----SO4----.----
        12.2         7.5        12.0         1.4         9.9         7.7
HCO3---.----FE TOT-.----H2S AQ-.----CO3----.----SIO2TOT.----NH4----.----
        75.2       .0157        .002        -1.0       18.23        .144
B TOT--.----PO4----.----AL-----.----F------.----NO3----.----
         .05         .21        .005          .1        .898
$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++
CUN    7          .015  96         .0018  97          .006 109         .0044
CUN  130         .0005 145        .00049 160         .0001 182        .00003
CUN  202          .019 204         .0018 212        .00004 249         .002
```

Minimum Output for Test Problem #2

```
DK Nordstrom Test Data - Test Case #2 - Surface Water                    2 B5
 162     0 000000       0     2.5     .13       0
                    TEMP      =          9.500000
                    PH        =          8.010000
                    EH(0)     =           .440000
                    DOC       =          2.500000
                    DOX       =         10.940000
                    CORALK    =          0
                    FLG       =         MG/L
                    DENS      =          1.000000
                    PRNT      =          0
                    PUNCH     =          1
                    EHOPT(1)  =          0  Use measured Eh to calculate Fe species distribution
                    EHOPT(2)  =          0  Use measured Eh to calculate Mn species other than +2
                    EHOPT(3)  =          0  Use measured Eh to calculate Cu +1 species
                    EHOPT(4)  =          0  Use measured Eh to calculate As species distribution
                    EHOPT(5)  =          0  Use measured Eh to calculate Se species distribution
                    EHOPT(6)  =          0  Use measured Eh to calculate Ion Activity Products
                    EHOPT(7)  =          3  Use H2O/O2 classical Eh to calculate atmospheric pO2
                    EHOPT(8)  =          5  Use S=/SO4 Eh to calculate H2S from SO4
                    EHOPT(9)  =          0  Use measured Eh to calculate U species distribution
                    EMPOX     =          0
                    ITDS      =           .000000
                    COND      =        162.000000
                    SIGMDO    =           .000000
                    SIGMEH    =           .000000
                    SIGMPH    =           .000000

    Species     Index No      Input Concentration
    ----------------------------------------------
    Ca          :     0   :        12.20000000
    Mg          :     1   :         7.50000000
    Na          :     2   :        12.00000000
    K           :     3   :         1.40000000
    Cl          :     4   :         9.90000000
    SO4         :     5   :         7.70000000
    HCO3        :     6   :        75.20000000
    Fe total    :    16   :           .01570000
    H2S aq      :    13   :           .00200000
    CO3         :    17   :        -1.00000000
    SiO2 tot    :    34   :        18.23000000
    NH4         :    38   :           .14400000
    B tot       :    86   :           .05000000
    PO4         :    44   :           .21000000
    Al          :    50   :           .00500000
    F           :    61   :           .10000000
    NO3         :    84   :           .89800000
    Fe          :     7   :           .01500000
    I           :    96   :           .00180000
    Br          :    97   :           .00600000
    Mn          :   109   :           .00440000
    Cu          :   130   :           .00050000
    Zn          :   145   :           .00049000
    Cd          :   160   :           .00010000
    Pb          :   182   :           .00003000
    NO2         :   202   :           .01900000
    Ni          :   204   :           .00180000
    Ag          :   212   :           .00004000
    As total    :   249   :           .00200000
```

ITER	S1-AnalCO3	S2-AnalSO4	S3-AnalF	S4-AnalPO4	S5-AnalCL	S6-AnalH2S	S7-AnalFULV	S8-AnalHUM
1	1.578326E-05	5.310843E-06	7.243660E-08	4.340160E-07	1.279901E-10	3.106834E-08	0.000000E+00	0.000000E+00
2	-2.991425E-07	2.233015E-08	1.842873E-10	1.775415E-09	1.353077E-12	6.421184E-09	0.000000E+00	0.000000E+00
3	-4.792144E-09	-3.622872E-10	-2.447801E-12	-2.940534E-11	1.682508E-13	1.391181E-09	0.000000E+00	0.000000E+00
4	-6.084537E-10	-4.855595E-12	-3.988941E-14	-4.097580E-13	3.229457E-14	2.934523E-10	0.000000E+00	0.000000E+00
5	-1.305742E-10	2.757330E-14	-2.363291E-16	-2.986992E-15	6.883379E-15	6.136173E-11	0.000000E+00	0.000000E+00
6	-2.715144E-11	1.429437E-13	9.132548E-16	1.070408E-14	1.439877E-15	1.280474E-11	0.000000E+00	0.000000E+00

DK Nordstrom Test Data - Test Case #2 - Surface Water 2 B5 Date = 6/03/91 13:58

162 0 000000 0 2.5 .13 0

DOX = 10.9400 DOC = 2.5 INPUT TDS = .0

Anal Cond = 162.0 Calc Cond = 176.3 Activity H2S calc from SO4 and pe = 3.97E-09

Anal EPMCAT = 1.7932 Anal EPMAN = 1.6994 Percent difference in input cation/anion balance = 5.3688

Calc EPMCAT = 1.7714 Calc EPMAN = 1.6742 Percent difference in calc cation/anion balance = 5.6431

Total Ionic Strength (T.I.S.) from input data = .00245

Effective Ionic Strength (E.I.S.) from speciation = .00240

Input	Sigma	Fe3/Fe2	Sigma	NO3/NO2	Sigma	NO3/NH4	Sigma	SO4/S=	Sigma	S/S=	Sigma	Sato H2O2/O2	Sigma	H2O/O2	Sigma
							Eh								
.440	.000	.095	.000	.445	.000	.328	.000	-.229	.000	-.066	.000	.141	.000	.743	.000
							pe								
7.845	.000	1.688	.000	7.927	.000	5.845	.000	-4.080	.000	-1.177	.000	2.508	.000	13.248	.000

As5/As3	Sigma	As3/As	Sigma	Se6/Se4	Sigma	Se4/Se	Sigma	Se/Se=	Sigma	U6/U4	Sigma		Sigma		Sigma
							Eh								
.440	.000	-.714	.000	9.900	.000	9.900	.000	9.900	.000	9.900					
							pe								
7.845	.000	-12.737	.000	100.000	.000	100.000	.000	100.000	.000	100.000					

T	pH	TDS ppm	Effective Ionic Str	pO2 Atm	ppm O2 Atm	pCO2 Atm	ppm CO2 Atm	log pCO2	CO2 Tot		Ncrb Alk	aH2O
9.50	8.010	145.6	.00240	2.64E-04	8.44E+00	6.05E-04	2.66E+01	-3.218	1.25E-03		4.96E-06	.9999

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
212	Ag	1	.000040	.000000	3.709E-10	1.282E-16	.00	1.216E-16	.9487	15.915
220	AgHS aq	0		.000052		3.702E-10	99.82	3.704E-10	1.0006	9.431
50	Al	3	.005000	.000000	1.853E-07	6.048E-15	.00	3.765E-15	.6224	14.424
53	Al(OH)4	-1		.017		1.840E-07	99.30	1.746E-07	.9487	6.758
249	As total	0	.002000		2.670E-08					
257	HAsO4	-2		.003552		2.539E-08	95.10	2.057E-08	.8100	7.687
256	H2AsO4	-1		.000184		1.303E-09	4.88	1.236E-09	.9487	8.908
86	B tot	0	.050		4.626E-06					
35	H3BO3 aq	0		.274		4.428E-06	95.74	4.431E-06	1.0006	5.354
36	H2BO3	-1		.012		1.971E-07	4.26	1.870E-07	.9487	6.728
97	Br	-1	.006000	.006000	7.510E-08	7.510E-08	100.00	7.125E-08	.9487	7.147
0	Ca	2	12.200	11.935	3.044E-04	2.978E-04	97.83	2.421E-04	.8130	3.616
160	Cd	2	.000100	.000000	8.898E-10	2.443E-12	.27	1.979E-12	.8100	11.704
175	CdHS	1		.000122		8.376E-10	94.13	7.946E-10	.9487	9.100
176	Cd(HS)2	0		.000009		4.940E-11	5.55	4.943E-11	1.0006	10.306
4	Cl	-1	9.900	9.900	2.793E-04	2.793E-04	100.00	2.648E-04	.9483	3.577
6	HCO3	-1	75.200	73.698	1.233E-03	1.208E-03	96.34	1.147E-03	.9496	2.940
85	H2CO3 aq	0		2.042		3.292E-05	2.63	3.294E-05	1.0006	4.482
130	Cu	2	.000500	.000000	7.869E-09	5.065E-12	.06	4.102E-12	.8100	11.387
131	CuCO3 aq	0		.000010		8.286E-11	1.05	8.291E-11	1.0006	10.081
139	Cu(OH)2	0		.000087		8.969E-10	11.40	8.974E-10	1.0006	9.047
144	Cu(HS)3	-1		.001119		6.875E-09	87.36	6.522E-09	.9487	8.186
61	F	-1	.100	.099	5.264E-06	5.193E-06	98.64	4.926E-06	.9487	5.307
7	Fe	2	.015	.013	2.686E-07	2.257E-07	80.26	1.828E-07	.8100	6.738
310	FeCO3 aq	0		.001910		1.649E-08	5.87	1.650E-08	1.0006	7.782
309	FeHCO3	1		.002583		2.210E-08	7.86	2.097E-08	.9487	7.678
8	Fe	3	.000700	.000000	1.254E-08	5.584E-19	.00	3.475E-19	.6224	18.459
77	Fe(OH)3	0		.001103		1.032E-08	3.67	1.033E-08	1.0006	7.986
63	H	1		.000010		1.026E-08	.00	9.772E-09	.9521	8.010
96	I	-1	.001800	.001800	1.419E-08	1.419E-08	100.00	1.346E-08	.9487	7.871
3	K	1	1.400	1.400	3.581E-05	3.580E-05	99.97	3.395E-05	.9483	4.469
1	Mg	2	7.500	7.339	3.085E-04	3.019E-04	97.85	2.459E-04	.8144	3.609
21	MgHCO3	1		.284		3.335E-06	1.08	3.163E-06	.9487	5.500
109	Mn	2	.004400	.003290	8.010E-08	5.990E-08	74.78	4.852E-08	.8100	7.314
311	MnCO3 aq	0		.001666		1.450E-08	18.10	1.450E-08	1.0006	7.839
119	MnHCO3	1		.000606		5.229E-09	6.53	4.961E-09	.9487	8.304
2	Na	1	12.000	11.989	5.220E-04	5.216E-04	99.91	4.950E-04	.9490	3.305
37	NH3 aq	0		.002323		1.364E-07	1.71	1.365E-07	1.0006	6.865
38	NH4	1	.144	.141	7.984E-06	7.841E-06	98.21	7.439E-06	.9487	5.128
204	Ni	2	.001800	.000075	3.066E-08	1.282E-09	4.18	1.039E-09	.8100	8.984
281	NiCO3	0		.003437		2.896E-08	94.43	2.897E-08	1.0006	7.538
202	NO2	-1	.019	.019	4.131E-07	4.131E-07	100.00	3.919E-07	.9487	6.407
84	NO3	-1	.898	.898	1.448E-05	1.448E-05	100.00	1.374E-05	.9487	4.862
26	OH	-1		.005136		3.020E-07	.00	2.865E-07	.9487	6.543
182	Pb	2	.000030	.000000	1.448E-10	2.486E-12	1.72	2.014E-12	.8100	11.696
241	PbCO3 aq	0		.000035		1.316E-10	90.89	1.317E-10	1.0006	9.880
187	Pb(CO3)2	-2		.000000		1.537E-12	1.06	1.245E-12	.8100	11.905
278	PbHCO3	1		.000000		1.934E-12	1.34	1.835E-12	.9487	11.736
198	Pb(HS)2	0		.000000		2.762E-12	1.91	2.764E-12	1.0006	11.558
192	PbOH	1		.000000		4.235E-12	2.92	4.018E-12	.9487	11.396
44	PO4	-3	.210000	.000007	2.212E-06	6.973E-11	.00	4.340E-11	.6224	10.363
46	HPO4	-2		.155		1.610E-06	72.81	1.304E-06	.8100	5.885
47	H2PO4	-1		.023		2.372E-07	10.72	2.250E-07	.9487	6.648
66	HS	-1		.000946		2.862E-08	48.75	2.715E-08	.9487	7.566

DK Nordstrom Test Data - Test Case #2 - Surface Water 2 B5

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	.Act Coeff	-Log Act
13	H2S aq	0	.002000	.000135	5.869E-08	3.965E-09	6.76	3.967E-09	1.0006	8.402
34	SiO2 tot	0	18.230		3.034E-04					
23	H4SiO4aq	0		28.908		3.008E-04	99.13	3.010E-04	1.0006	3.521
5	SO4	-2	7.700	7.220	8.017E-05	7.517E-05	93.76	6.104E-05	.8121	4.214
145	Zn	2	.000490	.000199	7.497E-09	3.051E-09	40.70	2.471E-09	.8100	8.607
273	ZnCO3	0		.000232		1.855E-09	24.74	1.856E-09	1.0006	8.732
274	Zn(CO3)2	-2		.000034		1.843E-10	2.46	1.493E-10	.8100	9.826
272	ZnHCO3	1		.000048		3.762E-10	5.02	3.569E-10	.9487	9.447
156	Zn(HS)2	0		.000209		1.586E-09	21.15	1.587E-09	1.0006	8.800
151	ZnOH	1		.000007		8.456E-11	1.13	8.022E-11	.9487	10.096
152	Zn(OH)2	0		.000032		3.256E-10	4.34	3.257E-10	1.0006	9.487

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
445	Acanthite	6.806	-31.386		-38.192	
39	Adularia	.020	-21.791		-21.812	
437	Ag metal	-9.236	-23.760		-14.524	
40	Albite	-1.585	-20.628		-19.043	
140	Al(OH)3 (a)	-2.259	9.606		11.865	
50	Alunite	-8.731	-8.111		.620	
42	Analcime	-3.673	-17.106		-13.433	
384	Anglesite	-8.034	-15.910		-7.876	.020
17	Anhydrite	-3.494	-7.830		-4.336	
239	Antlerite	-14.625	-6.335		8.290	
21	Aragonite	-.787	-9.040		-8.253	.020
497	Arsenolite	-102.021	-105.398		-3.377	
237	Atacamite	-10.412	-2.321		8.091	
236	Azurite	-12.992	-8.002		4.991	.090
472	Basaluminite	-4.512	18.188		22.700	
240	Brochantite	-17.042	-1.702		15.340	.160
19	Brucite	-5.519	12.411		17.929	
413	Bunsenite	-6.375	7.036		13.411	
12	Calcite	-.632	-9.040		-8.409	.020
439	Cerargyrite	-9.113	-19.492		-10.379	
365	Cerrusite	-3.795	-17.120		-13.325	
97	Chalcedony	.220	-3.521		-3.741	
227	Chalcocite	3.890	-32.713		-36.603	.160
250	Chalcopyrite	19.459	-17.238		-36.696	
20	Chrysotile	-4.033	30.189		34.222	
246	Covellite	12.292	-10.943		-23.235	.300
99	Cristobalite	.287	-3.521		-3.808	
226	Cuprite	-15.336	-17.137		-1.801	
154	Diaspore	1.735	9.606		7.871	
11	Dolomite (d)	-1.980	-18.074		-16.094	
401	Dolomite (c)	-1.363	-18.074		-16.711	
340	Epsomite	-5.570	-7.824		-2.253	
396	FCO3 Apatite	10.524	-105.459		-115.983	
112	Ferrihydrite	.680	5.571		4.891	
96	Fluorapatite	-.218	-17.011		-16.793	
62	Fluorite	-3.427	-14.231		-10.804	
385	Galena	2.307	-11.252		-13.560	
51	Gibbsite (c)	.579	9.606		9.026	.200
110	Goethite	6.571	5.571		-1.000	.800
332	Greenockite	5.328	-11.260		-16.588	
118	Greigite	3.154	-41.881		-45.035	
18	Gypsum	-3.238	-7.830		-4.592	
64	Halite	-8.428	-6.882		1.545	
47	Halloysite	-1.934	12.168		14.103	
392	Hydcerrusite	-12.457	-29.917		-17.460	
205	Jarosite K	-12.262	-20.215		-7.953	1.100
46	Kaolinite	3.315	12.168		8.854	
128	Laumontite	1.335	-31.218		-32.552	
10	Magnesite	-1.253	-9.034		-7.781	
235	Malachite	-7.629	-1.684		5.944	.080
189	Manganite	-.779	24.561		25.340	
415	Millerite	-.397	-8.540		-8.142	
500	Orpiment	-35.125	-99.428		-64.303	
315	Otavite	-5.029	-17.128		-12.099	.100
141	Prehnite	-3.179	-15.292		-12.113	
114	Pyrite	28.773	9.840		-18.933	
183	Pyrolusite	-3.581	40.416		43.997	
101	Quartz	.700	-3.521		-4.221	
501	Realgar	-36.806	-57.781		-20.975	
190	Rhodochrs(d)	-2.349	-12.739		-10.390	
492	Scorodite	-9.658	-29.907		-20.249	
153	Sepiolite(d)	-4.403	14.257		18.660	
36	Sepiolite(c)	-1.933	14.257		16.190	
9	Siderite (d)	-1.712	-12.162		-10.450	
395	SiO2 (a)	-.675	-3.521		-2.846	
268	Smithsonite	-4.207	-14.032		-9.825	
286	Sphalerit(c)	3.786	-8.163		-11.950	
146	Strengite	-2.503	-28.822		-26.318	
242	Tenorite	-3.600	4.633		8.233	
106	Vivianite	-4.939	-40.939		-36.000	
287	Wurtzite	1.722	-8.163		-9.885	
282	Zincite (c)	-4.606	7.413		12.019	
281	ZnO (a)	-3.897	7.413		11.310	
285	ZnS (a)	1.036	-8.163		-9.200	

Input Data Set for Test Problem Number 3:

```
****
N Dubrovsky Se Test Data - Test Case #3 - Airport Well (24') 870423          3 C5
11500  7030 870423       0     2.2       0       0       0    .004        0
TEMP-.-- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--
   21.00     7.85    0.391     2.20     0.20        0
FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8--9
MG/L    1.0         0     1        0  0  0  0  0  0  3  2  0
EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.-----SIGMPH-.----
       0  7030.0  11500.0        0.0         0.0         0.0
CA-----.----MG-----.----NA-----.----K------.----CL-----.----SO4----.----
       130.0       130.0      2200.0         4.6      2600.0      1600.0
HCO3---.----FE TOT-.----H2S AQ-.----CO3----.----SIO2TOT.----NH4----.----
       643.7         .02         0.0         0.0        24.0         0.0
B TOT--.----PO4----.----AL-----.----F------.----NO3----.----
         4.6         0.0         0.0          .4        5.75
$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++
CUN   80          .34  87          2.7  96          .08  97          8.2
CUN  109          .37 130         .002 145          .02 204         .002
CUN  212         .001 249         .001 298          .46 300         .018
CUN  301         .442
```

Minimum Output for Test Problem #3

```
 N Dubrovsky Se Test Data - Test Case #3 - Airport Well (24') 870423        3 C5
11500  7030 870423       0     2.2       0       0       0    .004       0
                    TEMP      =          21.000000
                    PH        =           7.850000
                    EH(0)     =            .391000
                    DOC       =           2.200000
                    DOX       =            .200000
                    CORALK    =           0
                    FLG       =         MG/L
                    DENS      =           1.000000
                    PRNT      =           0
                    PUNCH     =           1
                    EHOPT(1)  =           0  Use measured Eh to calculate Fe species distribution
                    EHOPT(2)  =           0  Use measured Eh to calculate Mn species other than +2
                    EHOPT(3)  =           0  Use measured Eh to calculate Cu +1 species
                    EHOPT(4)  =           0  Use measured Eh to calculate As species distribution
                    EHOPT(5)  =           0  Use measured Eh to calculate Se species distribution
                    EHOPT(6)  =           0  Use measured Eh to calculate Ion Activity Products
                    EHOPT(7)  =           3  Use H2O/O2 classical Eh to calculate atmospheric pO2
                    EHOPT(8)  =           2  Use H2O2/O2 Sato Eh to calculate H2S from SO4
                    EHOPT(9)  =           0  Use measured Eh to calculate U species distribution
                    EMPOX     =           0
                    ITDS      =        7030.000000
                    COND      =       11500.000000
                    SIGMDO    =            .000000
                    SIGMEH    =            .000000
                    SIGMPH    =            .000000

     Species     Index No       Input Concentration
     ----------------------------------------------
     Ca          :     0   :       130.00000000
     Mg          :     1   :       130.00000000
     Na          :     2   :      2200.00000000
     K           :     3   :         4.60000000
     Cl          :     4   :      2600.00000000
     SO4         :     5   :      1600.00000000
     HCO3        :     6   :       643.70000000
     Fe total    :    16   :          .02000000
     H2S aq      :    13   :          .00000000
     CO3         :    17   :          .00000000
     SiO2 tot    :    34   :        24.00000000
     NH4         :    38   :          .00000000
     B tot       :    86   :         4.60000000
     PO4         :    44   :          .00000000
     Al          :    50   :          .00000000
     F           :    61   :          .40000000
     NO3         :    84   :         5.75000000
     Li          :    80   :          .34000000
     Sr          :    87   :         2.70000000
     I           :    96   :          .08000000
     Br          :    97   :         8.20000000
     Mn          :   109   :          .37000000
     Cu          :   130   :          .00200000
     Zn          :   145   :          .02000000
     Ni          :   204   :          .00200000
     Ag          :   212   :          .00100000
     As total    :   249   :          .00100000
     Se4 tot     :   300   :          .01800000
     Se6 tot     :   301   :          .44200000


ITER  S1-AnalCO3     S2-AnalSO4     S3-AnalF       S4-AnalPO4     S5-AnalCL      S6-AnalH2S     S7-AnalFULV    S8-AnalHUM
  1  8.031056E-04   4.978863E-03   2.560259E-06   0.000000E+00   3.188538E-07   0.000000E+00   0.000000E+00   0.000000E+00
  2  4.401277E-05   3.162427E-04   1.548773E-07   0.000000E+00   1.930752E-08   0.000000E+00   0.000000E+00   0.000000E+00
  3  1.555897E-06   5.181723E-06   8.392706E-09   0.000000E+00   3.323267E-09   0.000000E+00   0.000000E+00   0.000000E+00
```

N Dubrovsky Se Test Data - Test Case #3 - Airport Well (24') 870423 3 C5 Date = 6/03/91 13:59

11500 7030 870423 0 2.2 0 0 0 .004 0

DOX = .2000 DOC = 2.2 INPUT TDS = 7030.0

Anal Cond = 11500.0 Calc Cond = 10721.8 Activity H2S calc from SO4 and pe = 3.68E-58

Anal EPMCAT = 113.9574 Anal EPMAN = 118.2855 Percent difference in input cation/anion balance = -3.7273

Calc EPMCAT = 107.0777 Calc EPMAN = 111.4200 Percent difference in calc cation/anion balance = -3.9747

Total Ionic Strength (T.I.S.) from input data = .14159

Effective Ionic Strength (E.I.S.) from speciation = .12823

Input	Sigma	Fe3/Fe2	Sigma	NO3/NO2	Sigma	NO3/NH4	Sigma	SO4/S=	Sigma	S/S=	Sigma	Sato H2O2/O2	Sigma	H2O/O2	Sigma
							Eh								
.391	.000	.391	.000	9.900	.000	9.900	.000	9.900	.000	9.900	.000	.130	.000	.698	.000
							pe								
6.699	.000	6.699	.000	100.000	.000	100.000	.000	100.000	.000	100.000	.000	2.235	.000	11.963	.000

As5/As3	Sigma	As3/As	Sigma	Se6/Se4	Sigma	Se4/Se	Sigma	Se/Se=	Sigma	U6/U4	Sigma		Sigma		Sigma
							Eh								
.391	.000	-.707	.000	.479	.000	-1.671	.000	9.900	.000	9.900					
							pe								
6.699	.000	-12.109	.000	8.215	.000	-28.627	.000	100.000	.000	100.000					

T	pH	TDS ppm	Effective Ionic Str	pO2 Atm	ppm O2 Atm	pCO2 Atm	ppm CO2 Atm	log pCO2	CO2 Tot		Ncrb Alk	aH2O
21.00	7.850	7355.2	.12823	5.86E-06	1.88E-01	6.81E-03	3.00E+02	-2.167	1.07E-02		2.61E-05	.9966

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
212	Ag	1	.001000	.000001	9.339E-09	1.163E-11	.12	8.945E-12	.7692	11.048
215	AgCl aq	0		.000135		9.495E-10	10.17	9.780E-10	1.0300	9.010
216	AgCl2	-1		.001282		7.223E-09	77.34	5.556E-09	.7692	8.255
217	AgCl3	-2		.000178		8.383E-10	8.98	2.935E-10	.3502	9.532
218	AgCl4	-3		.000071		2.852E-10	3.05	2.690E-11	.0943	10.570
249	As total	0	.001000		1.345E-08					
257	HAsO4	-2		.001799		1.295E-08	96.33	4.535E-09	.3502	8.343
256	H2AsO4	-1		.000068		4.855E-10	3.61	3.735E-10	.7692	9.428
86	B tot	0	4.600		4.286E-04					
35	H3BO3 aq	0		25.042		4.080E-04	95.19	4.202E-04	1.0300	3.376
36	H2BO3	-1		1.245		2.063E-05	4.81	1.587E-05	.7692	4.800
97	Br	-1	8.200	8.200	1.034E-04	1.034E-04	100.00	7.953E-05	.7692	4.099
0	Ca	2	130.000	95.894	3.268E-03	2.410E-03	73.77	8.842E-04	.3668	3.053
29	CaHCO3	1		10.358		1.032E-04	3.16	7.940E-05	.7692	4.100
31	CaSO4 aq	0		97.693		7.229E-04	22.12	7.446E-04	1.0300	3.128
4	Cl	-1	2600.000	2599.884	7.388E-02	7.388E-02	100.00	5.521E-02	.7473	1.258
6	HCO3	-1	643.700	588.304	1.063E-02	9.713E-03	90.89	7.524E-03	.7746	2.124
85	H2CO3 aq	0		15.042		2.443E-04	2.29	2.522E-04	1.0322	3.598
130	Cu	2	.002000	.000024	3.171E-08	3.764E-10	1.19	1.318E-10	.3502	9.880
131	CuCO3 aq	0		.001934		1.577E-08	49.75	1.625E-08	1.0300	7.789
132	Cu(CO3)2	-2		.000244		1.340E-09	4.23	4.691E-10	.3502	9.329
271	CuHCO3	1		.000080		6.461E-10	2.04	4.970E-10	.7692	9.304
139	Cu(OH)2	0		.001289		1.331E-08	41.97	1.371E-08	1.0300	7.863
61	F	-1	.400	.354	2.121E-05	1.878E-05	88.55	1.445E-05	.7692	4.840
16	Fe total	2	.020		3.608E-07					
76	Fe(OH)2	1		.004528		5.077E-08	14.07	3.905E-08	.7692	7.408
77	Fe(OH)3	0		.031		2.888E-07	80.05	2.974E-07	1.0300	6.527
78	Fe(OH)4	-1		.002599		2.114E-08	5.86	1.626E-08	.7692	7.789
63	H	1		.000017		1.730E-08	.00	1.413E-08	.8164	7.850
96	I	-1	.080	.080	6.351E-07	6.351E-07	100.00	4.885E-07	.7692	6.311
3	K	1	4.600	4.475	1.185E-04	1.153E-04	97.29	8.616E-05	.7473	4.065
45	KSO4	-1		.431		3.215E-06	2.71	2.473E-06	.7692	5.607
80	Li	1	.340	.334	4.936E-05	4.843E-05	98.12	3.726E-05	.7692	4.429
82	LiSO4	-1		.095		9.268E-07	1.88	7.129E-07	.7692	6.147
1	Mg	2	130.000	93.018	5.387E-03	3.855E-03	71.56	1.483E-03	.3848	2.829
21	MgHCO3	1		14.148		1.670E-04	3.10	1.285E-04	.7692	3.891
22	MgSO4 aq	0		159.279		1.333E-03	24.75	1.373E-03	1.0300	2.862
109	Mn	2	.370	.163	6.785E-06	2.982E-06	43.96	1.044E-06	.3502	5.981
111	MnCl	1		.027		3.053E-07	4.50	2.349E-07	.7692	6.629
311	MnCO3 aq	0		.211		1.848E-06	27.24	1.904E-06	1.0300	5.720
119	MnHCO3	1		.105		9.104E-07	13.42	7.003E-07	.7692	6.155
117	MnSO4 aq	0		.110		7.315E-07	10.78	7.535E-07	1.0300	6.123
2	Na	1	2200.000	2146.361	9.640E-02	9.406E-02	97.57	7.240E-02	.7697	1.140
43	NaSO4	-1		238.141		2.015E-03	2.09	1.550E-03	.7692	2.810
204	Ni	2	.002000	.000030	3.432E-08	5.167E-10	1.51	1.809E-10	.3502	9.742
281	NiCO3	0		.003522		2.989E-08	87.09	3.078E-08	1.0300	7.512
282	Ni(CO3)2	-2		.000622		3.505E-09	10.21	1.227E-09	.3502	8.911
84	NO3	-1	5.750	5.750	9.342E-05	9.342E-05	100.00	7.186E-05	.7692	4.143
26	OH	-1		.011		6.746E-07	.00	5.189E-07	.7692	6.285
300	Se4 tot	0	.018		2.297E-07					
301	Se6 tot	0	.442		5.639E-06					
304	HSeO3	-1		.020		1.539E-07	2.62	1.184E-07	.7692	6.927
305	SeO3	-2		.009541		7.571E-08	1.29	2.651E-08	.3502	7.577
307	SeO4	-2		.800		5.639E-06	96.09	1.975E-06	.3502	5.705
34	SiO2 tot	0	24.000		4.024E-04					
23	H4SiO4aq	0		37.931		3.976E-04	98.80	4.095E-04	1.0300	3.388
24	H3SiO4	-1		.455		4.819E-06	1.20	3.707E-06	.7692	5.431
5	SO4	-2	1600.000	1210.630	1.678E-02	1.270E-02	75.67	4.384E-03	.3453	2.358
87	Sr	2	2.700	2.006	3.104E-05	2.307E-05	74.31	8.520E-06	.3693	5.070
68	SrHCO3	1		.163		1.104E-06	3.56	8.554E-07	.7746	6.068
314	SrSO4 aq	0		1.229		6.741E-06	21.71	6.943E-06	1.0300	5.158
145	Zn	2	.020000	.003474	3.082E-07	5.353E-08	17.37	1.875E-08	.3502	7.727
273	ZnCO3	0		.010		8.335E-08	27.04	8.584E-08	1.0300	7.066
274	Zn(CO3)2	-2		.022		1.202E-07	39.01	4.210E-08	.3502	7.376
272	ZnHCO3	1		.002895		2.308E-08	7.49	1.776E-08	.7692	7.751
158	ZnSO4 aq	0		.002905		1.813E-08	5.88	1.867E-08	1.0300	7.729

Input Data Set for Test Problem Number 4:

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****
USBM-1 Table  Potter et al.  Report 79-1144                                    4 D5
    0     0 000000       0       0       0       0       0       0       0
TEMP-.-- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--
   24.50     6.90    -0.131     0.00     0.00        0
FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8--9
MG/L    1.0          0     1        0  0  0  0  0  0  0  0  0
EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.----SIGMPH-.----
       0     0.0      0.0        0.0         0.0         0.0
CA-----.----MG-----.----NA-----.----K------.---CL-----.----SO4----.----
        48.6         5.4       153.0        11.9        94.0        65.0
HCO3---.----FE TOT-.----H2S AQ-.----CO3----.---SIO2TOT.----NH4----.----
       328.0         .12         0.0         0.0        38.0          .1
B TOT--.----PO4----.----AL-----.----F------.----NO3----.----
         1.1         .05        .003         .55         0.0
$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++
CUN  316      0.01
```

Minimum Output for Test Problem #4

N Dubrovsky Se Test Data - Test Case #3 - Airport Well (24') 870423 3 C5

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
437	Ag metal	-3.986	-17.747		-13.762	
17	Anhydrite	-1.065	-5.412		-4.347	
239	Antlerite	-8.894	-.604		8.290	
21	Aragonite	.619	-7.693		-8.312	.020
497	Arsenolite	-96.854	-99.798		-2.944	
237	Atacamite	-4.999	2.527		7.526	
236	Azurite	-6.548	-2.490		4.058	.090
240	Brochantite	-10.127	5.213		15.340	.160
19	Brucite	-4.242	12.868		17.110	
413	Bunsenite	-6.732	5.956		12.688	
12	Calcite	.766	-7.693		-8.458	.020
143	Celestite	-.804	-7.428		-6.623	
439	Cerargyrite	-2.400	-12.306		-9.906	
97	Chalcedony	.214	-3.385		-3.598	
20	Chrysotile	-.866	31.837		32.702	
99	Cristobalite	.257	-3.385		-3.642	
226	Cuprite	-10.440	-12.052		-1.612	
11	Dolomite (d)	1.269	-15.161		-16.429	
401	Dolomite (c)	1.835	-15.161		-16.996	
340	Epsomite	-3.029	-5.197		-2.168	
556	Fe2(SeO3)3	-21.830	-57.260		-35.430	
112	Ferrihydrite	1.390	6.281		4.891	
62	Fluorite	-2.087	-12.734		-10.647	
110	Goethite	7.282	6.282		-1.000	.800
18	Gypsum	-.834	-5.415		-4.581	
64	Halite	-3.971	-2.398		1.573	
205	Jarosite K	-4.587	-13.485		-8.898	1.100
10	Magnesite	.500	-7.468		-7.968	
235	Malachite	-3.684	1.663		5.347	.080
189	Manganite	-1.075	24.265		25.340	
183	Pyrolusite	-3.215	38.814		42.029	
101	Quartz	.655	-3.385		-4.040	
190	Rhodochrs(d)	-.230	-10.620		-10.390	
492	Scorodite	-9.152	-29.401		-20.249	
553	SeO2	-14.895	-23.275		-8.380	
153	Sepiolite(d)	-3.080	15.580		18.660	
36	Sepiolite(c)	-.287	15.580		15.867	
9	Siderite (d)	-5.036	-15.486		-10.450	
395	SiO2 (a)	-.640	-3.385		-2.745	
268	Smithsonite	-2.410	-12.366		-9.957	
142	Strontianite	-.440	-9.709		-9.269	
242	Tenorite	-1.953	5.818		7.772	
282	Zincite (c)	-3.386	7.971		11.358	
281	ZnO (a)	-3.339	7.971		11.310	

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USBM-1 Table  Potter et al. - Test Case #4 -  Report 79-1144                4 D5
   0     0 000000       0       0       0       0       0       0       0
                    TEMP      =        24.500000
                    PH        =         6.900000
                    EH(0)     =         -.131000
                    DOC       =          .000000
                    DOX       =          .000000
                    CORALK    =         0
                    FLG       =        MG/L
                    DENS      =         1.000000
                    PRNT      =         0
                    PUNCH     =         1
                    EHOPT(1)  =         0  Use measured Eh to calculate Fe species distribution
                    EHOPT(2)  =         0  Use measured Eh to calculate Mn species other than +2
                    EHOPT(3)  =         0  Use measured Eh to calculate Cu +1 species
                    EHOPT(4)  =         0  Use measured Eh to calculate As species distribution
                    EHOPT(5)  =         0  Use measured Eh to calculate Se species distribution
                    EHOPT(6)  =         0  Use measured Eh to calculate Ion Activity Products
                    EHOPT(7)  =         0  Use measured Eh to calculate atmospheric pO2
                    EHOPT(8)  =         0  Use measured Eh to calculate H2S from SO4
                    EHOPT(9)  =         0  Use measured Eh to calculate U species distribution
                    EMPOX     =         0
                    ITDS      =          .000000
                    COND      =          .000000
                    SIGMDO    =          .000000
                    SIGMEH    =          .000000
                    SIGMPH    =          .000000

    Species     Index No      Input Concentration
    ----------------------------------------------
    Ca          :     0   :       48.60000000
    Mg          :     1   :        5.40000000
    Na          :     2   :      153.00000000
    K           :     3   :       11.90000000
    Cl          :     4   :       94.00000000
    SO4         :     5   :       65.00000000
    HCO3        :     6   :      328.00000000
    Fe total    :    16   :         .12000000
    H2S aq      :    13   :         .00000000
    CO3         :    17   :         .00000000
    SiO2 tot    :    34   :       38.00000000
    NH4         :    38   :         .10000000
    B tot       :    86   :        1.10000000
    PO4         :    44   :         .05000000
    Al          :    50   :         .00300000
    F           :    61   :         .55000000
    NO3         :    84   :         .00000000
    U total     :   316   :         .01000000


ITER  S1-AnalCO3     S2-AnalSO4     S3-AnalF      S4-AnalPO4     S5-AnalCL      S8-AnalH2S     S7-AnalFULV    S8-AnalHUM
  1  8.096104E-05  9.141527E-05  5.307843E-07  9.322684E-08  3.542700E-09  0.000000E+00  0.000000E+00  0.000000E+00
  2  8.628703E-07  1.461683E-06  5.730421E-09  4.610094E-10  4.664940E-11  0.000000E+00  0.000000E+00  0.000000E+00
  3 -6.714829E-09 -2.311989E-08 -3.946429E-11 -3.094758E-11  1.873367E-13  0.000000E+00  0.000000E+00  0.000000E+00
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USBM-1 Table Potter et al. - Test Case #4 - Report 79-1144 4 D5 Date = 6/03/91 13:59

0 0 000000 0 0 0 0 0 0 0

DOX = .0000 DOC = .0 INPUT TDS = .0

Anal Cond = .0 Calc Cond = 963.5 Activity H2S calc from SO4 and pe = 1.15E-14

Anal EPMCAT = 0.8465 Anal EPMAN = 0.4179 Percent difference in input cation/anion balance = 4.4499

Calc EPMCAT = 0.6171 Calc EPMAN = 0.1876 Percent difference in calc cation/anion balance = 4.5675

Total Ionic Strength (T.I.S.) from input data = .01175

Effective Ionic Strength (E.I.S.) from speciation = .01131

Input	Sigma	Fe3/Fe2	Sigma	NO3/NO2	Sigma	NO3/NH4	Sigma	SO4/S=	Sigma	S/S=	Sigma	Sato H2O2/O2	Sigma	H2O/O2	Sigma
							Eh								
-.131	.000	-.131	.000	0.900	.000	0.900	.000	0.900	.000	0.900	.000	0.900	.000	0.900	.000
							pe								
-2.218	.000	-2.218	.000	100.000	.000	100.000	.000	100.000	.000	100.000	.000	100.000	.000	100.000	.000

As5/As3	Sigma	As3/As	Sigma	Se6/Se4	Sigma	Se4/Se	Sigma	Se/Se=	Sigma	U6/U4	Sigma		Sigma		Sigma
							Eh								
0.900	.000	0.900	.000	0.900	.000	0.900	.000	0.900	.000	-.131					
							pe								
100.000	.000	100.000	.000	100.000	.000	100.000	.000	100.000	.000	-2.218					

T	pH	TDS ppm	Effective Ionic Str	pO2 Atm	ppm O2 Atm	pCO2 Atm	ppm CO2 Atm	log pCO2	CO2 Tot		Mcrb Alk	aH2O
24.50	6.900	745.8	.01131	2.75E-65	8.80E-61	9.93E-02	1.73E+03	-1.406	6.73E-03		1.69E-06	.9997

I	Species		Anal ppm	Calc ppm	Anal Molal	Calc Molal	% of Total	Activity	Act Coeff	-Log Act
50	Al	3	.003000	.000000	1.113E-07	2.941E-12	.00	1.106E-12	.3761	11.956
55	AlF2	1		.000260		4.000E-09	3.59	3.588E-09	.8970	8.445
56	AlF3 aq	0		.000096		1.149E-09	1.03	1.152E-09	1.0026	8.939
52	Al(OH)2	1		.000342		5.618E-09	5.05	5.039E-09	.8970	8.298
181	Al(OH)3	0		.000442		5.672E-09	5.10	5.686E-09	1.0026	8.245
53	Al(OH)4	-1		.008947		9.425E-08	84.70	8.455E-08	.8970	7.073
86	B tot	0	1.100		1.018E-04					
35	H3BO3 aq	0		6.259		1.013E-04	99.50	1.016E-04	1.0026	3.993
0	Ca	2	48.600	44.300	1.213E-03	1.106E-03	91.16	7.268E-04	.6570	3.139
29	CaHCO3	1		4.938		4.888E-05	4.03	4.385E-05	.8970	4.358
31	CaSO4 aq	0		7.619		5.601E-05	4.62	5.616E-05	1.0026	4.251
4	Cl	-1	94.000	93.989	2.653E-03	2.653E-03	100.00	2.375E-03	.8952	2.624
6	HCO3	-1	328.000	322.723	5.380E-03	5.294E-03	78.70	4.767E-03	.9005	2.322
85	H2CO3 aq	0		83.892		1.354E-03	20.13	1.357E-03	1.0028	2.867
61	F	-1	.550	.540	2.897E-05	2.844E-05	98.17	2.551E-05	.8970	4.593
16	Fe total	2	.120		2.150E-06					
7	Fe	2		.085		1.517E-06	70.53	9.820E-07	.6475	6.008
310	FeCO3 aq	0		.004782		4.131E-08	1.92	4.141E-08	1.0026	7.383
309	FeHCO3	1		.061		5.218E-07	24.27	4.681E-07	.8970	6.330
33	FeSO4 aq	0		.010		6.714E-08	3.12	6.732E-08	1.0026	7.172
63	H	1		.000139		1.384E-07	.00	1.259E-07	.9095	6.900
3	K	1	11.900	11.867	3.046E-04	3.037E-04	99.73	2.719E-04	.8952	3.566
1	Mg	2	5.400	4.896	2.223E-04	2.015E-04	90.67	1.334E-04	.6617	3.875
21	MgHCO3	1		.705		8.274E-06	3.72	7.422E-06	.8970	5.129
22	MgSO4 aq	0		1.440		1.198E-05	5.39	1.201E-05	1.0026	4.921
2	Na	1	153.000	152.314	6.660E-03	6.631E-03	99.56	5.956E-03	.6982	2.225
38	NH4	1	.100	.099	5.548E-06	5.499E-06	99.12	4.933E-06	.8970	5.307
26	OH	-1		.001451		8.538E-08	.00	7.659E-08	.8970	7.116
44	PO4	-3	.050000	.000000	5.269E-07	1.107E-12	.00	4.164E-13	.3761	12.381
46	HPO4	-2		.017		1.814E-07	34.42	1.174E-07	.6475	6.930
47	H2PO4	-1		.026		2.662E-07	50.53	2.388E-07	.8970	6.622
34	SiO2 tot	0	38.000		6.329E-04					
23	H4SiO4aq	0		60.702		6.321E-04	99.87	6.337E-04	1.0026	3.198
5	SO4	-2	65.000	57.140	6.772E-04	5.953E-04	87.92	3.891E-04	.6535	3.410
316	U total	0	.010		4.204E-08					
323	U(OH)4	0		.001494		4.884E-09	11.62	4.897E-09	1.0026	8.310
344	UO2CO3)2	-2		.009212		2.364E-08	56.23	1.531E-08	.6475	7.815
345	UO2CO3)3	-4		.003051		6.785E-09	16.14	1.193E-09	.1758	8.923
354	UO2HPO42	-2		.002803		6.072E-09	14.44	3.932E-09	.6475	8.405

USBM-1 Table Potter et al. - Test Case #4 - Report 79-1144 4 D5

	Phase	Log IAP/KT	Log IAP	Sigma(A)	Log KT	Sigma(T)
39	Adularia	.379	-20.232		-20.611	
40	Albite	-.857	-18.891		-18.034	
140	Al(OH)3 (a)	-2.089	8.743		10.833	
50	Alunite	-3.517	-4.855		-1.338	
42	Analcime	-2.970	-15.693		-12.723	
17	Anhydrite	-2.190	-6.549		-4.359	
21	Aragonite	-.561	-8.894		-8.333	.020
625	Autunite	-10.590	-54.499		-43.909	
622	K-Autunite	-10.240	-58.492		-48.251	
472	Basaluminite	-4.936	17.764		22.700	
19	Brucite	-6.949	9.925		16.873	
12	Calcite	-.416	-8.894		-8.477	.020
97	Chalcedony	.359	-3.198		-3.557	
20	Chrysotile	-8.883	23.379		32.262	
577	Coffinite	4.677	-2.979		-7.656	
99	Cristobalite	.396	-3.198		-3.594	
154	Diaspore	1.834	8.744		6.909	
11	Dolomite (d)	-1.997	-18.523		-16.526	
401	Dolomite (c)	-1.445	-18.523		-17.078	
340	Epsomite	-5.142	-7.286		-2.143	
396	FCO3 Apatite	5.562	-108.887		-114.449	
112	Ferrihydrite	-5.449	-.558		4.891	
96	Fluorapatite	-2.801	-20.377		-17.575	
62	Fluorite	-1.720	-12.325		-10.605	
51	Gibbsite (c)	.605	8.743		8.138	.200
110	Goethite	.442	-.558		-1.000	.800
600	Gummite	-9.931	.500		10.431	
18	Gypsum	-1.968	-6.549		-4.581	
64	Halite	-6.430	-4.849		1.581	
47	Halloysite	-1.456	11.091		12.547	
205	Jarosite K	-23.588	-32.760		-9.171	1.100
46	Kaolinite	3.613	11.091		7.478	
128	Laumontite	.933	-30.076		-31.009	
10	Magnesite	-1.609	-9.630		-8.021	
594	Ningyoite	-1.378	-55.281		-53.903	
141	Prehnite	-4.508	-16.216		-11.708	
101	Quartz	.790	-3.198		-3.988	
606	Rutherfordin	-4.606	-19.055		-14.448	.050
602	Schoepite	-4.919	.500		5.419	
153	Sepiolite(d)	-8.404	10.256		18.660	
36	Sepiolite(c)	-5.517	10.256		15.773	
9	Siderite (d)	-1.313	-11.763		-10.450	
395	SiO2 (a)	-.482	-3.198		-2.716	
146	Strengite	-7.241	-33.639		-26.398	
574	UO2 (a)	.119	.219		.100	.700
601	B-UO2(OH)2	-5.061	.500		5.561	
599	UO3 (c)	-7.243	.500		7.743	
576	U3O8 (c)	-1.289	19.384		20.673	.310
573	Uraninite(c)	4.996	.219		-4.777	.500
632	Uranophane	-12.223	5.266		17.489	
106	Vivianite	-6.786	-42.786		-36.000	

Attachment B. Listing of WATEQ4F Data Base

I	Page2	dH	LogKto		Error
0	kFe2/Fe3	9.680	-13.020		
1	kFeOH +2	10.400	-2.190		.020
2	kFeOH +	13.200	-9.500		.100
3	kFe(OH)3 -	30.300	-31.000		1.500
4	kFeSO4 +	3.910	4.040		
5	kFeCl +2	5.600	1.480		
6	kFeCl2 +		2.130		
7	kFeCl3 aq		1.130		
8	kFeSO4 aq	3.230	2.250		
9	Siderite ppt		-10.450		
10	Magnesite	-6.169	-8.029		
11	Dolomite (d)	-11.090	-16.540		
12	Calcite	-2.297	-8.480	*	.020
13	kH3SiO4 -	6.120	-9.830	*	
14	kH2SiO4 -2	17.600	-23.000	*	
15	kHPO4 -2	-3.530	12.346		
16	kH2PO4 -	-4.520	19.553		
17	Anhydrite	-1.710	-4.360	*	
18	Gypsum	-.109	-4.580	*	
19	Brucite	-27.100	16.840		
20	Chrysotile	-46.800	32.200	*	
21	Aragonite	-2.589	-8.336	*	.020
22	kMgF +	3.200	1.820		
23	kCaSO4 aq	1.650	2.300		
24	kMgOH +	15.952	-11.440		.050
25	kH3BO3 aq	3.224	-9.240	*	
26	kNH3 aq	12.480	-9.252	*	
27	Forsterite	-48.578	28.306		
28	Diopside	-32.348	19.894		
29	Clinoenstite	-20.049	11.342		
30	kNaHPO4 -		.290		
31	Tremolite	-96.853	56.574		
32	kKHPO4 -		.290		
33	kMgHPO4 aq	3.300	2.870		
34	kCaHPO4 aq	3.300	2.739		
35	kH2CO3 aq	-2.247	6.351	*	.010
36	Sepiolite(c)	-10.700	15.760		
37	Talc	-46.352	21.399		2.000
38	Hydrmagnesit	-52.244	-8.762		
39	Adularia	30.820	-20.573		
40	Albite	25.896	-18.002		
41	Anorthite	11.580	-19.714		
42	Analcime	18.206	-12.701		
43	Kmica	-59.376	12.703		1.300
44	Phlogopite	-42.300	43.300		3.000
45	Illite	54.684	-40.267		
46	Kaolinite	-35.300	7.435		
47	Halloysite	-39.920	12.498		
48	Beidellite	60.355	-45.272		
49	Chlorite 14A	-151.494	68.380		6.000
50	Alunite	-50.250	-1.400		
51	Gibbsite (c)	-22.800	8.110		.200
52	Boehmite	-28.181	8.584		
53	Pyrophyllite		-48.314		
54	Phillipsite		-19.874		
55	Erionite				
56	Clinoptilolt				
57	Mordenite				
58	Nahcolite	3.720	-.548		
59	Trona	-18.000	-.795		
60	Natron	15.745	-1.311		
61	Thermonatrit	-2.802	.125		
62	Fluorite	4.690	-10.600	*	

I	Page1	Z	DHa	GFW
0	Ca	2	5.0	40.0800
1	Mg	2	5.5	24.3120
2	Na	1	4.0	22.9898
3	K	1	3.5	39.1020
4	Cl	-1	3.5	35.4530
5	SO4	-2	5.0	96.0616
6	HCO3	-1	5.4	61.0173
7	Fe	2	6.0	55.8470
8	Fe	3	9.0	55.8470
9	FeOH	2	5.0	72.8544
10	FeOH	1	5.0	72.8544
11	Fe(OH)3	-1	5.0	106.8691
12	FeHPO4	1	5.4	151.8264
13	H2S aq	0	.0	34.0799
14	FeSO4	1	5.0	151.9086
15	FeCl	2	5.0	91.3000
16	Fe total	2	.0	55.8470
17	CO3	-2	5.4	60.0094
18	MgOH	1	6.5	41.3194
19	MgF	1	4.5	43.3104
20	MgCO3 aq	0	.0	84.3214
21	MgHCO3	1	4.0	85.3293
22	MgSO4 aq	0	.0	120.3736
23	H4SiO4aq	0	.0	96.1155
24	H3SiO4	-1	4.0	95.1075
25	H2SiO4	-2	5.4	94.0995
26	OH	-1	3.5	17.0074
27	FeCl2	1	5.0	126.7530
28	CaOH	1	6.0	57.0874
29	CaHCO3	1	6.0	101.0973
30	CaCO3 aq	0	.0	100.0894
31	CaSO4 aq	0	.0	136.1416
32	FeCl3 aq	0	.0	162.2060
33	FeSO4 aq	0	.0	151.9086
34	SiO2 tot	0	.0	60.0848
35	H3BO3 aq	0	.0	61.8331
36	H2BO3	-1	2.5	60.8251
37	NH3 aq	0	.0	17.0306
38	NH4	1	2.5	18.0386
39	MgPO4	-1	5.4	119.2834
40	MgH2PO4	1	5.4	121.2993
41	NaCO3	-1	5.4	82.9992
42	NaHCO3aq	0	.0	84.0071
43	NaSO4	-1	5.4	119.0514
44	PO4	-3	5.0	94.9714
45	KSO4	-1	5.4	135.1636
46	HPO4	-2	5.0	95.9794
47	H2PO4	-1	5.4	96.9873
48	Cs	1	.0	132.9050
49	NaHPO4	-1	5.4	118.9692
50	Al	3	9.0	26.9815
51	AlOH	2	5.4	43.9889
52	Al(OH)2	1	5.4	60.9962
53	Al(OH)4	-1	4.5	95.0110
54	AlF	2	5.4	45.9799
55	AlF2	1	5.4	64.9783
56	AlF3 aq	0	.0	83.9767
57	AlF4	-1	4.5	102.9751
58	AlSO4	1	4.5	123.0431
59	Al(SO4)2	-1	4.5	219.1047
60	KHPO4	-1	5.4	135.0814
61	F	-1	3.5	18.9984
62	HSO4	-1	4.5	97.0696

I	Page2	dH	LogKto		Error
63	Montmoril Ca	58.373	-45.027		
64	Halite	.918	1.582		
65	Thenardite	-.572	-.179		
66	Mirabilite	18.987	-1.114		
67	Mackinawite		-4.648		
68	kHCO3 -	-3.561	10.329	*	.010
69	kNaCO3 -	8.910	1.270		
70	kNaHCO3 aq		-.250		
71	kNaSO4 -	1.120	.700		.050
72	kKSO4 -	2.250	.850	*	.050
73	kMgCO3 aq	2.713	2.980	*	.030
74	kMgHCO3 +	.790	1.070	*	.030
75	kMgSO4 aq	4.550	2.370		.020
76	kCaOH +		-12.780		
77	kCaHCO3 +	2.690	1.106	*	.050
78	kCaCO3 aq	3.545	3.224	*	.080
79	kSrHCO3 +	6.050	1.180	*	
80	kAlOH +2	11.490	-5.000	*	.020
81	kAl(OH)2 +	26.900	-10.100	*	.200
82	kAl(OH)4 -	42.300	-22.700	*	.300
83	kAlF +2	1.060	7.000		
84	kAlF2 +	1.980	12.700		
85	kAlF3 aq	2.160	16.800		
86	kAlF4 -	2.200	19.400		
87	kAlSO4 +	2.290	3.500		
88	kAl(SO4)2 -	3.110	5.000		
89	kHSO4 -	3.850	1.988	*	
90	kSO4/H2S	-65.440	40.644		
91	kH2S aq	5.300	-6.994	*	
92	kHS -	12.100	-12.918		
93	koxy	34.157	-20.780		
94	Siderite (c)	-2.480	-10.890		
95	Hydroxyapati	-36.155	-3.421		
96	Fluorapatite	-20.070	-17.600		
97	Chalcedony	4.720	-3.550	*	
98	Magadiite		-14.300		
99	Cristobalite	5.500	-3.587		
100	Silica gel	4.440	-3.018		
101	Quartz	5.990	-3.980	*	
102	kFe(OH)2 +	17.100	-5.670		.100
103	kFe(OH)3 aq	24.800	-12.560		
104	kFe(OH)4 -	31.900	-21.600		.200
105	kFe(OH)2 aq	28.565	-20.570		1.000
106	Vivianite		-36.000		
107	Magnetite	-50.460	3.737		
108	Hematite	-30.845	-4.008		
109	Maghemite		6.386		
110	Goethite		-1.000		.800
111	Greenalite		20.810		
112	Ferrihydrite		4.891		
113	Annite	62.480	-85.645		
114	Pyrite	11.300	-18.479		
115	Montmoril BF		-34.913		
116	Montmoril AB		-29.688		
117	Huntite	-25.760	-29.968		
118	Greigite		-45.035		
119	FeS ppt		-3.915		
120	kFeH2PO4 +		2.700		
121	kCaPO4 -	3.100	6.459		
122	kCaH2PO4 +	3.400	1.408		
123	kMgPO4 -	3.100	6.589		
124	kMgH2PO4 +	3.400	1.513		
125	Chlorite 7A	-155.261	71.752		6.000

I	Page1	Z	DHa	GFW
63	H	1	9.0	1.0080
64	FeH2PO4	1	5.4	152.8343
65	H2S calc	0	.0	34.0799
66	HS	-1	3.5	33.0720
67	S	-2	5.0	32.0640
68	SrHCO3	1	5.4	148.6373
69	pO2	0	.0	31.9988
70	Blank	0	.0	.0000
71	AH2O	0	.0	18.0153
72	MgHPO4aq	0	.0	120.2914
73	CaHPO4aq	0	.0	136.0594
74	CaPO4	-1	5.4	135.0514
75	CaH2PO4	1	5.4	137.0673
76	Fe(OH)2	1	5.4	89.8617
77	Fe(OH)3	0	.0	106.8691
78	Fe(OH)4	-1	5.4	123.8765
79	Fe(OH)2	0	.0	89.8617
80	Li	1	6.0	6.9390
81	CaHSO4	1	.0	137.1496
82	LiSO4	-1	5.0	103.0006
83	NH4calc	1	2.5	18.0386
84	NO3	-1	3.0	62.0049
85	H2CO3 aq	0	.0	62.0253
86	B tot	0	.0	10.8110
87	Sr	2	5.2	87.6200
88	SrOH	1	5.0	104.6274
89	Ba	2	5.0	137.3400
90	BaOH	1	5.0	154.3474
91	NH4SO4	-1	5.0	114.1002
92	Blank	0	.0	.0000
93	Blank	0	.0	.0000
94	Rb	1	.0	85.4700
95	SrCO3 aq	0	.0	147.6294
96	I	-1	.0	126.9044
97	Br	-1	4.0	79.9040
98	FeH2PO4	2	5.4	152.8343
99	FeHPO4aq	0	.0	151.8264
100	CaF	1	5.0	59.0784
101	BF(OH)3	-1	2.5	80.8315
102	BF2(OH)2	-1	2.5	82.8225
103	BF3OH	-1	2.5	84.8136
104	BF4	-1	2.5	86.8046
105	FeF	2	5.0	74.8454
106	FeF2	1	5.0	93.8438
107	FeF3 aq	0	.0	112.8422
108	Fe(SO4)2	-1	.0	247.9702
109	Mn	2	6.0	54.9380
110	Mn	3	9.0	54.9380
111	MnCl	1	5.0	90.3910
112	MnCl2 aq	0	.0	125.8440
113	MnCl3	-1	5.0	161.2970
114	MnOH	1	5.0	71.9454
115	Mn(OH)3	-1	5.0	105.9601
116	MnF	1	5.0	73.9364
117	MnSO4 aq	0	.0	150.9996
118	Mn(NO3)2	0	.0	178.9478
119	MnHCO3	1	5.0	115.9553
120	MnO4	-1	3.0	118.9356
121	MnO4	-2	5.0	118.9356
122	FeHSO4	1	.0	152.9166
123	FeHSO4	2	.0	152.9166
124	SiF6	-2	5.0	142.0764
125	HF aq	0	.0	20.0064

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126	kLiSO4 -		.640		
127	kNH4/NO3	187.055	-119.077		
128	Laumontite	39.610	-30.960		
129	kSrOH +		-13.290		
130	kBaOH +		-13.470		
131	kNH4SO4 -		1.110		
132	Blank				
133	Jarosite(ss)		-8.000		
134	Mn2(SO4)3	-39.060	-5.711		
135	kSrCO3 aq	5.220	2.810	*	
136	kO2 Sato		-11.385		
137	kH2CO3 aq	-4.776	-1.468	*	
138	kFeHPO4 aq		3.600		
139	kFeHPO4 +	5.760	5.430		
140	Al(OH)3 (a)	-26.500	10.800		
141	Prehnite	10.390	-11.695		
142	Strontianite	-.400	-9.271	*	
143	Celestite	-1.037	-6.630	*	
144	Barite	6.350	-9.970	*	
145	Witherite	.703	-8.562	*	
146	Strengite	-2.030	-26.400		
147	Leonhardite	90.070	-69.756		
148	kFeHSO4 +		1.080		
149	Nesquehonite	-5.789	-5.621		
150	Artinite	-28.742	9.600		
151	kO2 calc	33.457	-20.780		
152	kw	13.362	-14.000	*	
153	Sepiolite(a)		18.660		
154	Diaspore	-24.681	6.879		
155	Wairakite	26.140	-26.708		
156	kFeH2PO4 +2		5.430		
157	Allophane(a)		6.060	*	
158	Allophane(f)		5.240	*	
159	kFeHSO4 +2		2.480		
160	kCaF +	4.120	.940		
161	kBF(OH)3 -	1.850	-.400		
162	kBF2(OH)2 -	1.618	7.630		
163	kBF3OH -	-1.614	13.670		
164	kBF4 -	-1.846	20.280		
165	kFeF +2	2.700	6.200		
166	kFeF2 +	4.800	10.800		
167	kFeF3 aq	5.400	14.000		
168	kCaHSO4 +		1.080		
169	kMn +3	25.800	-25.510		
170	kMnCl +		.610		
171	kMnCl2 aq		.250		
172	kMnCl3 -		-.310		
173	kMnOH +	14.400	-10.590		.040
174	kMn(OH)3 -		-34.800		
175	kMnF +		.840		
176	kMnSO4 aq	3.370	2.250		
177	kMn(NO3)2 aq	-.396	.600		
178	kMnHCO3 +		1.950		
179	kMnO4 -	176.620	-127.824		
180	kMnO4 -2	150.020	-118.440		
181	FeOH)2.7Cl.3		-3.040		
182	MnSO4	-15.480	2.669		
183	Pyrolusite	-65.110	41.380		
184	Birnessite		43.601		
185	Nsutite		42.564		
186	Bixbyite	-15.245	-.611		
187	Hausmannite	-100.640	61.030		
188	Pyrocroite		15.200		

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126	HF2	-1	3.5	39.0048
127	Cu	1	2.5	63.5460
128	CuCl2	-1	4.0	134.4520
129	CuCl3	-2	5.0	169.9050
130	Cu	2	6.0	63.5460
131	CuCO3 aq	0	.0	123.5554
132	Cu(CO3)2	-2	.0	183.5647
133	CuCl	1	4.0	98.9990
134	CuCl2 aq	0	.0	134.4520
135	CuCl3	-1	4.0	169.9050
136	CuCl4	-2	5.0	205.3580
137	CuF	1	.0	82.5444
138	CuOH	1	4.0	80.5534
139	Cu(OH)2	0	.0	97.5607
140	Cu(OH)3	-1	.0	114.5681
141	Cu(OH)4	-2	.0	131.5751
142	Cu2(OH)2	2	.0	161.1067
143	CuSO4 aq	0	.0	159.6076
144	Cu(HS)3	-1	.0	162.7619
145	Zn	2	6.0	65.3700
146	ZnCl	1	4.0	100.8230
147	ZnCl2 aq	0	.0	136.2760
148	ZnCl3	-1	4.0	171.7290
149	ZnCl4	-2	5.0	207.1820
150	ZnF	1	.0	84.3684
151	ZnOH	1	.0	82.3774
152	Zn(OH)2	0	.0	99.3847
153	Zn(OH)3	-1	.0	116.3921
154	Zn(OH)4	-2	.0	133.3995
155	ZnOHCl aq	0	.0	117.8304
156	Zn(HS)2	0	.0	131.5139
157	Zn(HS)3	-1	.0	164.5859
158	ZnSO4 aq	0	.0	161.4316
159	Zn(SO4)2	-2	.0	257.4932
160	Cd	2	.0	112.4000
161	CdCl	1	.0	147.8530
162	CdCl2 aq	0	.0	183.3060
163	CdCl3	-1	.0	218.7590
164	CdF	1	.0	131.3984
165	CdF2 aq	0	.0	150.3968
166	Cd(CO3)2	-2	.0	232.4188
167	CdOH	1	.0	129.4074
168	Cd(OH)2	0	.0	146.4147
169	Cd(OH)3	-1	.0	163.4221
170	Cd(OH)4	-2	.0	180.4295
171	Cd2OH	3	.0	241.8074
172	CdOHCl aq	0	.0	164.8604
173	CdNO3	1	.0	174.4049
174	CdSO4 aq	0	.0	208.4616
175	CdHS	1	.0	145.4720
176	Cd(HS)2	0	.0	178.5439
177	Cd(HS)3	-1	.0	211.6159
178	Cd(HS)4	-2	.0	244.6879
179	Fe2(OH)2	4	.0	145.7087
180	Fe3(OH)4	5	.0	235.5705
181	Al(OH)3	0	.0	78.0036
182	Pb	2	.0	207.1900
183	PbCl	1	.0	242.6430
184	PbCl2 aq	0	.0	278.0960
185	PbCl3	-1	.0	313.5490
186	PbCl4	-2	.0	349.0020
187	Pb(CO3)2	-2	.0	327.2087
188	PbF	1	.0	226.1884

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189	Manganite		25.340			189	PbF2 aq	0	.0	245.1868
190	Rhodochrs(a)		-10.390			190	PbF3	-1	.0	264.1852
191	MnCl2, 4H2O	17.380	2.710			191	PbF4	-2	.0	283.1836
192	MnS green	-5.790	3.800			192	PbOH	1	.0	224.1974
193	Mn3(PO4)2	2.120	-23.827			193	Pb(OH)2	0	.0	241.2047
194	MnHPO4		-12.947			194	Pb(OH)3	-1	.0	258.2121
195	a-Cryptomeln					195	Pb2OH	3	.0	431.3874
196	Hollandite					196	PbNO3	1	.0	269.1949
197	Psilomelane					197	PbSO4 aq	0	.0	303.2516
198	Todorokite					198	Pb(HS)2	0	.0	273.3339
199	Lithiophorit					199	Pb(HS)3	-1	.0	306.4059
200	Rancieite					200	Pb3(OH)4	2	.0	689.5995
201	kSiF6 -2	-16.260	30.180			201	BaSO4 aq	0	.0	233.4016
202	kHF aq	3.180	3.180	*	.010	202	NO2	-1	.0	46.0055
203	kHF2 -	4.550	3.760		.060	203	AlHSO4	2	.0	124.0511
204	Jarosite Na	-36.180	-5.280		1.000	204	Ni	2	.0	58.7100
205	Jarosite K	-31.280	-9.210		1.100	205	NiBr	1	.0	138.6140
206	kCuCl2 -	1.230	8.220			206	NiCl	1	.0	94.1630
207	kCuCl3 -2	1.910	8.420			207	NiF	1	.0	77.7084
208	kCu +2	1.650	2.720			208	NiOH	1	.0	75.7174
209	kCuCO3 aq		6.730		.050	209	Ni(OH)2	0	.0	92.7247
210	kCu(CO3)2 -2		9.830		.040	210	Ni(OH)3	-1	.0	109.7321
211	kCuCl +	8.650	.430			211	NiSO4 aq	0	.0	154.7716
212	kCuCl2 aq	10.560	.160			212	Ag	1	.0	107.8680
213	kCuCl3 -	13.690	-2.290			213	AgBr aq	0	.0	187.7720
214	kCuCl4 -2	17.780	-4.590			214	AgBr2	-1	.0	267.6760
215	kCuF +	1.620	1.260			215	AgCl aq	0	.0	143.3210
216	kCuOH +		-8.000			216	AgCl2	-1	.0	178.7740
217	kCu(OH)2 aq		-13.680			217	AgCl3	-2	.0	214.2270
218	kCu(OH)3 -		-26.900			218	AgCl4	-3	.0	249.6800
219	kCu(OH)4 -2		-39.600			219	AgF aq	0	.0	126.8664
220	kCu2(OH)2 +2	17.539	-10.359	*		220	AgHS aq	0	.0	140.9400
221	kCuSO4 aq	1.220	2.310			221	Ag(HS)2	-1	.0	174.0119
222	kCu(HS)3 -		25.900			222	AgI aq	0	.0	234.7724
223	Cu metal	17.130	-8.760			223	AgI2	-1	.0	361.6768
224	Nantokite	9.980	-6.760			224	AgOH aq	0	.0	124.8754
225	CuF	-12.370	7.080			225	Ag(OH)2	-1	.0	141.8827
226	Cuprite	6.245	-1.550			226	AgSO4	-1	.0	203.9296
227	Chalcocite	49.350	-34.619		.160	227	AgNO3 aq	0	.0	169.8729
228	Cu2SO4	-4.560	-1.950			228	Ag(NO2)2	-1	.0	199.8790
229	CuprousFerit	-3.800	-8.920			229	ZnBr	1	.0	145.2740
230	Melanothalit	-12.320	3.730			230	ZnBr2 aq	0	.0	225.1780
231	CuCO3		-9.630			231	ZnI	1	.0	192.2744
232	CuF2	-13.320	-.620			232	ZnI2 aq	0	.0	319.1788
233	CuF2, 2H2O	-3.650	-4.550			233	CdBr	1	.0	192.3040
234	Cu(OH)2	-15.250	8.640			234	CdBr2 aq	0	.0	272.2080
235	Malachite	-19.760	5.150		.080	235	CdI	1	.0	239.3044
236	Azurite	-30.870	3.750		.090	236	CdI2 aq	0	.0	366.2088
237	Atacamite	-18.690	7.340			237	PbBr	1	.0	287.0940
238	Cu2(OH)3NO3	-17.350	9.240			238	PbBr2 aq	0	.0	366.9980
239	Antlerite		8.290			239	PbI	1	.0	334.0944
240	Brochantite		15.340		.160	240	PbI2 aq	0	.0	460.9988
241	Langite	-39.610	16.790			241	PbCO3 aq	0	.0	267.1994
242	Tenorite	-15.240	7.620			242	Pb(OH)4	-2	.0	275.2195
243	CuOCuSO4	-35.575	11.530			243	Pb(SO4)2	-2	.0	399.3132
244	Cu3(PO4)2		-36.850			244	AgBr3	-2	.0	347.5800
245	Cu3(PO4)2,3w		-35.120			245	AgI3	-2	.0	488.5812
246	Covellite	24.010	-22.270		.300	246	AgI4	-3	.0	615.4856
247	CuSO4	-18.140	3.010			247	Fe(HS)2	0	.0	121.9909
248	Chalcanthite	1.440	-2.640			248	Fe(HS)3	-1	.0	155.0629
249	CupricFerrit	-38.690	5.880			249	As total	0	.0	74.9216
250	Chalcopyrite	35.480	-35.270			250	H3AsO3aq	0	.0	125.9437
251	kZnCl +	7.790	.430			251	H2AsO3	-1	.0	124.9357

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252	kZnCl2 aq	8.500	.450	
253	kZnCl3 -	9.560	.500	
254	kZnCl4 -2	10.960	.200	
255	kZnF +	2.220	1.150	
256	kZnOH +	13.400	-8.960	.050
257	kZn(OH)2 aq		-16.900	
258	kZn(OH)3 -		-28.400	.200
259	kZn(OH)4 -2		-41.200	.100
260	kZnOHCl aq		-7.480	
261	kZn(HS)2 aq		14.940	
262	kZn(HS)3 -		16.100	
263	kZnSO4 aq	1.360	2.370	
264	kZn(SO4)2 -2		3.280	
265	Zn metal	-36.780	25.757	
266	Zn(BO2)2		8.290	
267	ZnCl2	-17.480	7.030	
268	Smithsonite	-4.360	-10.000	
269	ZnCO3, 1H2O		-10.260	
270	ZnF2	-13.080	-1.520	
271	Zn(OH)2 (a)		12.450	
272	Zn(OH)2 (c)		12.200	
273	Zn(OH)2 (b)		11.750	.020
274	Zn(OH)2 (g)		11.710	
275	Zn(OH)2 (e)		11.500	.030
276	Zn2(OH)3Cl		15.200	
277	Zn5(OH)8Cl		38.500	
278	Zn2(OH)2SO4		7.500	
279	Zn4(OH)6SO4		28.400	
280	ZnNO3)2,6H2O	5.510	3.440	
281	ZnO (active)		11.310	
282	Zincite	-21.860	11.140	
283	Zn3O(SO4)2	-62.000	19.020	
284	Zn3(PO4)2,4w		-32.040	
285	ZnS (a)	3.670	-9.052	
286	Sphalerite	8.250	-11.618	
287	Wurtzite	5.060	-9.682	
288	ZnSiO3	-18.270	2.930	
289	Willemite	-33.370	15.330	
290	Zincosite	-19.200	3.010	
291	ZnSO4, 1H2O	-10.640	-.570	
292	Bianchite	-.160	-1.765	
293	Goslarite	3.300	-1.960	
294	kCdCl +	.590	1.980	.030
295	kCdCl2 aq	1.240	2.600	.100
296	kCdCl3 -	3.900	2.400	.100
297	kCdF +		1.100	
298	kCdF2 aq		1.500	
299	kCd(CO3)2 -2		6.400	
300	kCdOH +	13.100	-10.080	.100
301	kCd(OH)2 aq		-20.350	.200
302	kCd(OH)3 -		-33.300	
303	kCd(OH)4 -2		-47.350	.100
304	kCd2OH +3	10.900	-9.390	.050
305	kCdOHCl aq	4.355	-7.404	
306	kCdNO3 +	-5.200	.400	
307	kCdSO4 aq	1.080	2.460	
308	kCdHS +		10.170	
309	kCd(HS)2 aq		16.530	
310	kCd(HS)3 -		18.710	
311	kCd(HS)4 -2		20.900	
312	Cd metal	-18.000	13.490	
313	Gamma Cd	-18.140	13.590	
314	Cd(BO2)2		9.840	

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252	HAsO3	-2	.0	123.9278
253	AsO3	-3	.0	122.9198
254	H4AsO3	1	.0	126.9517
255	H3AsO4aq	0	.0	141.9431
256	H2AsO4	-1	.0	140.9351
257	HAsO4	-2	.0	139.9272
258	AsO4	-3	.0	138.9192
259	Cu(S4)2	-3	23.0	320.0580
260	CuS4S5	-3	25.0	352.1220
261	As3 tot	0	.0	74.9216
262	As5 tot	0	.0	74.9216
263	S2	-2	6.5	64.1280
264	S3	-2	8.0	96.1920
265	S4	-2	10.0	128.2560
266	S5	-2	12.0	160.3200
267	S6	-2	14.0	192.3840
268	Ag(S4)2	-3	22.0	364.3800
269	AgS4S5	-3	24.0	396.4440
270	Ag(HS)S4	-2	15.0	269.1960
271	CuHCO3	1	.0	124.5633
272	ZnHCO3	1	.0	126.3573
273	ZnCO3	0	.0	125.3794
274	Zn(CO3)2	-2	.0	185.3587
275	CdHCO3	1	.0	173.4173
276	CdCO3	0	.0	172.4094
277	Cd(SO4)2	-2	.0	208.4616
278	PbHCO3	1	.0	268.2073
279	NiCl2	0	.0	129.6160
280	NiHCO3	1	.0	119.7273
281	NiCO3	0	.0	118.7194
282	Ni(CO3)2	-2	.0	178.7287
283	Ni(SO4)2	-2	.0	250.8332
284	fulvate	-2	.0	650.0000
285	Humate	-2	.0	2000.0000
286	Hfulvate	-1	.0	651.0080
287	H Humate	-1	.0	2001.0080
288	Fefulvat	1	.0	705.8470
289	Fehumate	1	.0	2055.8470
290	Cufulvat	0	.0	713.5460
291	Cuhumate	0	.0	2063.5460
292	Cdfulvat	0	.0	762.4000
293	Cdhumate	0	.0	2112.4000
294	Agfulvat	-1	.0	757.8680
295	Aghumate	-1	.0	2107.8680
296	H2F2 aq	0	.0	40.0127
297	NaF aq	0	.0	41.9882
298	Se total	0	.0	78.9600
299	H2Se aq	0	.0	80.9759
300	Se4 tot	0	.0	78.9600
301	Se6 tot	0	.0	78.9600
302	HSe	-1	.0	79.9680
303	H2SeO3aq	0	.0	128.9741
304	HSeO3	-1	.0	127.9662
305	SeO3	-2	.0	126.9582
306	HSeO4	-1	.0	143.9656
307	SeO4	-2	.0	142.9576
308	FeF	1	.0	74.8454
309	FeHCO3	1	.0	116.8643
310	FeCO3 aq	0	.0	115.8564
311	MnCO3 aq	0	.0	114.9474
312	BaHCO3	1	.0	198.3573
313	BaCO3 aq	0	.0	197.3494
314	SrSO4 aq	0	.0	183.6816

I	Page2	dH	LogKto		Error
315	Otavite	-.019	-12.100		.100
316	CdCl2	-4.470	-.680		
317	CdCl2, 1H2O	-1.820	-1.710		
318	CdCl2,2.5H2O	1.710	-1.940		
319	CdF2	-9.720	-2.980		
320	Cd(OH)2 (a)	-20.770	13.730		
321	Cd(OH)2 (c)		13.650		.040
322	CdOHCl	-7.407	3.520		
323	Cd3(OH)4SO4		22.560		
324	Cd3OH)2SO4)2		6.710		
325	Cd4(OH)6SO4		28.400		
326	Monteponite	-24.760	13.770		
327	Cd3(PO4)2		-32.600		
328	CdSiO3	-16.630	9.060		
329	CdSO4	-14.740	-.100		
330	CdSO4, 1H2O	-7.520	-1.657		
331	CdSO4,2.7H2O	-4.300	-1.873		
332	Greenockite	16.360	-15.930		
333	kFe(SO4)2 -	4.600	5.380		
334	kFe2(OH)2 +4	13.500	-2.950		.050
335	kFe3(OH)4 +5	14.300	-6.300		.100
336	kAl(OH)3 aq	39.890	-16.900	*	
337	Jarosite H	-55.150	-5.390		
338	Alum k	7.220	-5.170		
339	Melanterite	4.910	-2.209	*	
340	Epsomite	2.820	-2.140		
341	kPbCl +	4.380	1.600		
342	kPbCl2 aq	1.080	1.800		
343	kPbCl3 -	2.170	1.700		
344	kPbCl4 2-	3.530	1.380		
345	kPb(CO3)2 -2		10.640		
346	kPbF +		1.250		
347	kPbF2 aq		2.560		
348	kPbF3 -		3.420		
349	kPbF4 -2		3.100		
350	kPbOH +		-7.710		.100
351	kPb(OH)2 aq		-17.120		.100
352	kPb(OH)3 -		-28.060		.050
353	kPb2OH +3		-6.360		.100
354	kPbNO3 +		1.170		.020
355	kPbSO4 aq		2.750		.100
356	kPb(HS)2 aq		15.270		
357	kPb(HS)3 -		16.570		
358	kPb3(OH)4 +2	26.500	-23.880		.200
359	kFeF +		1.000		
360	Pb metal	.400	4.270		
361	Pb(BO2)2	-5.800	7.610		
362	Cotunnite	5.600	-4.770		
363	Matlockite	7.950	-9.430		
364	Phosgenite		-19.810		
365	Cerrusite	4.860	-13.130		
366	PbF2	-.700	-7.440		
367	Massicot	-16.780	12.910		
368	Litharge	-16.380	12.720		
369	PbO, 0.3H2O		12.980		
370	Pb2OCO3	-11.460	-.500		
371	Larnakite	-6.440	-.280		
372	Pb3O2SO4	-20.750	10.400		
373	Pb4O3SO4	-35.070	22.100		
374	PbHPO4	7.040	-11.460		
375	Pb3(PO4)2	-1.670	-19.670		
376	Clpyromorph		-84.430		
377	Hxypyromorph		-62.790		

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315	FeCl	1	.0	91.3000
316	U total	0	.0	238.0290
317	U	4	.0	238.0290
318	UO2	2	.0	270.0278
319	U	3	.0	238.0290
320	UOH	3	.0	255.0364
321	U(OH)2	2	.0	272.0437
322	U(OH)3	1	.0	289.0511
323	U(OH)4	0	.0	306.0585
324	Blank	0	.0	.0000
325	U6(OH)15	9	.0	1683.2846
326	UF	3	.0	257.0274
327	UF2	2	.0	276.0258
328	UF3	2	.0	295.0242
329	UF4	0	.0	314.0226
330	UF5	-1	.0	333.0210
331	UF6	-2	.0	352.0194
332	UCl	3	.0	273.4820
333	USO4	2	.0	334.0906
334	U(SO4)2	0	.0	430.1522
335	U(CO3)4	-4	.0	478.0666
336	U(CO3)5	-6	.0	538.0760
337	Blank	0	.0	.0000
338	Blank	0	.0	.0000
339	UO2	1	.0	270.0278
340	UO2OH	1	.0	287.0352
341	UO2)2OH2	2	.0	574.0703
342	UO2)3OH5	1	.0	895.1203
343	UO2CO3	0	.0	330.0372
344	UO2CO3)2	-2	.0	390.0465
345	UO2CO3)3	-4	.0	450.0559
346	UO2F	1	.0	289.0262
347	UO2F2	0	.0	308.0246
348	UO2F3	-1	.0	327.0230
349	UO2F4	-2	.0	346.0214
350	UO2Cl	1	.0	305.4808
351	UO2SO4	0	.0	366.0894
352	UO2SO4)2	-2	.0	462.1510
353	UO2HPO4	0	.0	366.0072
354	UO2HPO42	-2	.0	461.9865
355	UO2H2PO4	1	.0	367.0151
356	U2H2P4)2	0	.0	464.0025
357	U2H2P4)3	-1	.0	560.9898
358	Blank	0	.0	.0000
359	U+6 tot	6	.0	238.0290
360	UBr	3	.0	317.9330
361	UI	3	.0	364.9334
362	UNO3	3	.0	300.0339
363	U(NO3)2	2	.0	362.0388
364	Blank	0	.0	.0000
365	UO2(OH)3	-1	.0	321.0500
366	UO2(OH)4	-2	.0	338.0574
367	(UO2)2OH	3	.0	557.0630
368	UO2)3OH4	2	.0	878.1130
369	UO2)3OH7	-1	.0	929.1352
370	UO2)4OH7	1	.0	1199.1630
371	UO2C12	0	.0	340.9338
372	UO2Br	1	.0	349.9318
373	UO2NO3	1	.0	332.0327
374	UO2H3PO4	2	.0	368.0232
375	UO23CO36	-6	.0	1170.1398
376	UO2PO4	-1	.0	364.9992
377	UO2CO3)3	-5	.0	450.0560

I	Page2	dH	LogKto	Error		I	Page1	Z	DHa	GFW
378	Pb3O2CO3	-26.430	11.020							
379	Plumbgummite		-32.790							
380	Hinsdalite		-2.500							
381	Tsumebite		-9.790							
382	PbSiO3	-9.260	7.320							
383	Pb2SiO4	-26.000	19.760							
384	Anglesite	2.150	-7.790	.020						
385	Galena	19.400	-12.780							
386	Plattnerite	-70.730	49.300							
387	Pb2O3		61.040							
388	Minium	-102.760	73.690							
389	Pb(OH)2 (c)	-13.990	8.150							
390	Laurionite		.623							
391	Pb2(OH)3Cl		8.793							
392	Hydcerrusite		-17.460							
393	Pb2O(OH)2		26.200							
394	Pb4(OH)6SO4		21.100							
395	SiO2 (a,N)	3.340	-2.710	*						
396	FCO3 Apatite	39.390	-114.400							
397	kAlHSO4 +2		.460							
398	BaF2	1.000	-5.760							
399	SrF2	1.250	-8.540							
400	kNO3/NO2	-43.760	28.570							
401	Dolomite (c)	-9.436	-17.090							
402	Sulfur	7.900	-15.026							
403	kNiBr +		.500							
404	kNiCl +		.400							
405	kNiF +		1.300							
406	kNiOH +	12.420	-9.860	.030						
407	kNi(OH)2 aq		-19.000	1.000						
408	kNi(OH)3 -		-30.000	.500						
409	kNiSO4 aq	1.520	2.290							
410	NiCO3	-9.940	-6.840							
411	Ni(OH)2	30.450	10.800	.100						
412	Ni4(OH)6SO4		32.000							
413	Bunsenite	-23.920	12.450							
414	Ni3(PO4)2		-31.300							
415	Millerite	2.500	-8.042							
416	Retgersite	1.100	-2.040							
417	Morenosite	2.940	-2.360							
418	Ni2SiO4	-33.360	14.540							
419	Fe3(OH)8		20.222							
420	Dioptase	-8.960	6.500							
421	kAgBr aq		4.240							
422	kAgBr2 -		7.280							
423	kAgCl aq	-2.680	3.270							
424	kAgCl2 -	-3.930	5.270							
425	kAgCl3 -2		5.290							
426	kAgCl4 -3		5.510							
427	kAgF aq	-2.830	.360							
428	kAgHS aq		14.050							
429	kAg(HS)2 -		18.450							
430	kAgI aq		6.600							
431	kAgI2 -		10.680							
432	kAgOH aq		-12.000	.300						
433	kAg(OH)2 -		-24.000	.050						
434	kAgSO4 -	1.490	1.290							
435	kAgNO3 aq		-.290							
436	kAg(NO2)2 -		2.220							
437	Ag metal	25.234	-13.510							
438	Bromyrite	20.170	-12.270							
439	Cerargyrite	15.652	-9.750							
440	Ag2CO3	9.530	-11.070							

I	Page2	dH	LogKto	Error	I	Page1	Z	DHa	GFW
441	AgF, 4H2O	4.270	.550						
442	Iodyrite	26.820	-16.070						
443	Ag2O	-10.430	12.580	.100					
444	Ag3PO4		-17.550						
445	Acanthite	53.300	-36.050						
446	Ag2SO4	4.250	-4.920						
447	kZnBr +		-.580						
448	kZnBr2 aq		-.980						
449	kZnI +		-2.910						
450	kZnI2 aq		-1.690						
451	kCdBr +	-.810	2.170						
452	kCdBr2 aq		2.900						
453	kCdI +	-2.370	2.150						
454	kCdI2 aq		3.590						
455	kPbBr +	2.880	1.770	.100					
456	kPbBr2 aq		1.440						
457	kPbI +		1.940						
458	kPbI2 aq		3.200						
459	CuBr	13.080	-8.210						
460	CuI	20.140	-11.890						
461	ZnBr2, 2H2O	-7.510	5.210						
462	ZnI2	-13.440	7.230						
463	CdBr2, 4H2O	7.230	-2.420						
464	CdI2	4.080	-3.610						
465	PbBr2	8.100	-5.180						
466	PbBrF		-8.490						
467	PbI2	15.160	-8.070						
468	kPbCO3 aq		7.240						
469	kPb(OH)4 -2		-39.700						
470	kPb(SO4)2 -2		3.470						
471	Jurbanite		-3.230						
472	Basaluminite		22.700						
473	kAgBr3 -2		8.710						
474	kAgI3 -2	-27.030	13.370						
475	kAgI4 -3		14.080						
476	kFe(HS)2 aq		8.950						
477	kFe(HS)3 -		10.987						
478	kH2AsO3 -	6.560	-9.228						
479	kHAsO3 -2	14.200	-21.330						
480	kAsO3 -3	20.250	-34.744						
481	kH4AsO3 +		-.305						
482	kH2AsO4 -	-1.690	-2.243						
483	kHAsO4 -2	-.920	-9.001						
484	kAsO4 -3	3.430	-20.597						
485	kCu(S4)2 -3		6.109						
486	kCuS4S5 -3		5.382						
487	kAs3/As5	30.015	-18.897						
488	As2O5	-5.405	6.699						
489	AlAsO4, 2H2O		-15.837						
490	Ca3AsO4)2,4w		-18.905						
491	Cu3AsO4)2,6w		-35.123						
492	Scorodite		-20.249						
493	Mn3AsO4)2,8w		-28.707						
494	Ni3AsO4)2,8w		-25.511						
495	Pb3(AsO4)2		-35.403						
496	Zn3AsO422.5w		-27.546						
497	Arsenolite	14.330	-2.801						
498	Claudetite	13.290	-3.065						
499	AsI3	1.875	4.155						
500	Orpiment	82.890	-60.971						
501	Realgar	30.545	-19.747						
502	kS2 -2	11.400	-14.528						
503	kS3 -2	10.400	-13.282						

I	Page2	dH	LogKto	Error		I	Page1	Z	DHa	GFW
504	kS4 -2	9.700	-9.829							
505	kS5 -2	9.300	-9.595							
506	kS6 -2		-9.881							
507	kAg(S4)2 -3		.991							
508	kAgS4S5 -3		.680							
509	kAg(HS)S4 -2		10.431							
510	kCuHCO3 +		2.700							
511	kZnHCO3 +		2.100							
512	kZnCO3 aq		5.300							
513	kZn(CO3)2 -2		9.630							
514	kCdHCO3 +		1.500							
515	kCdCO3 aq		2.900	.400						
516	kCd(SO4)2 -2		3.500							
517	kPbHCO3 +		2.900							
518	kNiCl2 aq		.960							
519	kNiHCO3 +		2.140							
520	kNiCO3 aq		6.870							
521	kNi(CO3)2 -2		10.110							
522	kNi(SO4)2 -2		1.020							
523	kH fulvate		4.270							
524	kh humate		4.270							
525	kFe fulvate		9.400							
526	kFe humate		9.400							
527	kCu fulvate		6.200							
528	kCu humate		6.200							
529	kCd fulvate		3.500							
530	kCd humate		3.500							
531	kAg fulvate		2.400							
532	kAg humate		2.400							
533	Blaublei I		-24.162	.150						
534	Blaublei II		-27.279	.150						
535	Anilite	43.535	-31.878	.150						
536	Djurleite	47.881	-33.920	.150						
537	kH2F2 aq		6.768							
538	kS(s)/H2S	-9.500	4.882							
539	Portlandite	-31.000	22.800							
540	kNaF aq		-.240	.050						
541	Ba3(AsO4)2	9.500	-50.110							
542	kFeCl +		.140							
543	kBaSO4 aq		2.700							
544	kH2Se aq	5.300	-3.800							
545	kH2SeO3 aq		11.250							
546	kHSeO3 -		8.500							
547	kHSeO4 -	4.910	1.660							
548	kSe4/Se6		-30.256							
549	kSe4/Se-2		42.514							
550	Se metal<Se=		-17.322							
551	Se metal<Se4		-59.836							
552	FeSe2		-18.580							
553	SeO2		-8.380							
554	CaSeO3		-5.600							
555	BaSeO3		-6.390							
556	Fe2(SeO3)3		-35.430							
557	kAs3/As		12.170							
558	kFeHCO3 +		2.000							
559	kFeCO3 aq		4.380							
560	kMnCO3 aq		4.900							
561	kBaHCO3 +	5.560	.982	*						
562	kBaCO3 aq	3.550	2.710	*						
563	kSrSO4 aq	2.080	2.290							
564	Rhodochrs(c)	-1.430	-11.130							
565	kU +4	-34.430	9.040	.040						
566	kU +3	24.400	-8.796							

I	Page2	dH	LogKto	Error	I	Page1	Z	DHa	GFW
567	kUOH +3	11.210	-.540	.060					
568	kU(OH)2 +2	17.730	-2.270						
569	kU(OH)3 +	22.645	-4.935						
570	kU(OH)4 aq	24.760	-8.498						
571	Na4UO2(CO3)3		-16.290	.160					
572	kU6(OH)15 +9		-17.200						
573	Uraninite(c)	-18.610	-4.800	.500					
574	UO2 (a)		.100	.700					
575	U4O9 (c)	-101.235	-3.384						
576	U3O8 (c)	-116.000	20.530	.310					
577	Coffinite	-11.600	-7.670						
578	kUF +3	-1.300	9.300	.100					
579	kUF2 +2	-.800	16.220	.190					
580	kUF3 +	.100	21.600	1.000					
581	kUF4 aq	-.870	25.500	1.000					
582	kUF5 -	4.850	27.010	.310					
583	kUF6 -2	3.300	29.100	.200					
584	UF4 (c)	-18.900	-18.606						
585	UF4,2.5H2O	-.588	-27.570						
586	kUCl +3	-4.540	1.720	.130					
587	kUSO4 +2	1.900	6.580	.190					
588	kU(SO4)2 aq	7.800	10.500	.200					
589	kU(CO3)4 -4		32.900	.900					
590	kU(CO3)5 -6	20.000	34.000	.900					
591	U(OH)2SO4 c		-3.200	.500					
592	UO2HPO4, 4w		-11.850	.090					
593	U(HPO4)2, 4w	3.840	-55.300	.150					
594	Ningyoite	-2.270	-53.906						
595	kUO2 +	-3.300	1.490	.020					
596	kUO2OH +	11.015	-5.200	.300					
597	kUO2)2OH)2+2	10.230	-5.620	.040					
598	kUO2)3OH)5 +	25.075	-15.550	.120					
599	UO3 (c)	-19.315	7.719						
600	Gummite	-23.015	10.403						
601	B-UO2(OH)2	-13.730	5.544						
602	Schoepite	-12.045	5.404						
603	kUO2CO3 aq	1.200	9.630	.050					
604	kUO2(CO3)2-2	4.420	17.000	.100					
605	kUO2(CO3)3-4	-9.130	21.630	.040					
606	Rutherfordin	-1.440	-14.450	.050					
607	kUO2F +	.410	5.090	.130					
608	kUO2F2 aq	.500	8.620	.040					
609	kUO2F3 -	.560	10.900	.400					
610	kUO2F4 -2	.070	11.700	.700					
611	kUO2Cl +	1.900	.170	.020					
612	kUO2SO4 aq	4.700	3.150	.020					
613	kUO2(SO4)2-2	8.400	4.140	.070					
614	kUO2HPO4 aq	-2.100	20.210	.120					
615	kUO2HPO4)2-2	-11.800	43.441						
616	kUO2H2PO4 +	-3.700	22.870	.060					
617	kUO2H2PO4)2a	-16.500	44.380	.050					
618	kUO2H2PO4)3-	-28.600	66.245						
619	UO2)3PO4)24w	41.500	-37.400	.300					
620	H-Autunite	-3.600	-47.931						
621	Na-Autunite	-.460	-47.409						
622	K-Autunite	5.860	-48.244						
623	Uramphite	9.700	-51.749						
624	Saleeite	-20.180	-43.646						
625	Autunite	-14.340	-43.927						
626	Sr-Autunite	-13.050	-44.457						
627	Uranocircite	-10.100	-44.631						
628	Bassetite	-19.900	-44.485						
629	Torbernite	-15.900	-45.279						

I	Page2	dH	LogKto	Error	I	Page1	Z	DHa	GFW
630	Przhevalskit	-11.000	-44.365						
631	Blank								
632	Uranophane		17.489						
633	kUBr +3		1.500	.200					
634	kUI +3		1.300	.300					
635	kUNO3 +3		1.470	.130					
636	kU(NO3)2 +2		2.300	.350					
637	Blank								
638	kUO2(OH)3 -		-19.200	.400					
639	kUO2(OH)4 -2		-33.000	2.000					
640	k(UO2)2OH +3		-2.700	1.000					
641	kUO2)3OH)4+2		-11.900	.300					
642	kUO2)3OH)7 -		-31.000	2.000					
643	kUO2)4OH)7 +		-21.900	1.000					
644	kUO2Cl2 aq	3.600	-1.100	.400					
645	kUO2Br +		.220	.020					
646	kUO2NO3 +		.300	.150					
647	kUO2H3PO4 +2		22.813	.060					
648	kUO2)3CO36-6		54.000	1.000					
649	kUO2PO4 -		13.690	.080					
650	kUO2(CO3)3 -	.005	8.920	.270					
651	Blank								
652	Blank								
653	Blank								

"*" Denotes that an analytical expression for Kt has been used

Summary of analytical expressions of the form Log K = A + B*T + C/T + D*T**2 + E/T**2 + F*LOG10(T)

I	React Product	A	B	C	D	E	F
12	Calcite	-171.9065	-.07799300	2839.3190			71.59500
13	kH3SiO4 -	-302.3724	-.05069800	15669.6900		-.111967E+07	108.18466
14	kH2SiO4 -2	-294.0184	-.07265000	11204.4900		-.111967E+07	108.18466
17	Anhydrite	197.5200		-8669.8000			-69.83500
18	Gypsum	68.2401		-3221.5100			-25.06270
20	Chrysotile	13.2480		10217.1000			-6.18940
21	Aragonite	-171.9773	-.07799300	2903.2930			71.59500
25	kH3BO3 aq	28.6059	.01207800	1573.2100			-13.22480
26	kNH3 aq	.6322	-.00122500	-2835.7600			
35	kH2CO3 aq	356.3094	.06091964	-21834.3700		.168492E+07	-126.83390
62	Fluorite	66.3480		-4298.2000			-25.27100
68	kHCO3 -	107.8871	.03252849	-5151.7900		.563714E+06	-38.92561
72	kKSO4 -	3.1060		-673.6000			
73	kMgCO3 aq	.9910	.00667000				
74	kMgHCO3 +	-59.2150		2537.4550			20.92298
77	kCaHCO3 +	1209.1200	.31294000	-34765.0500			-478.78200
78	kCaCO3 aq	-1228.7320	-.29944400	35512.7500			485.81800
79	kSrHCO3 +	-3.2480	.01486700				
80	kAlOH +2	-38.2530		-656.2700			14.32700
81	kAl(OH)2 +	88.5000		-9391.6000			-27.12100
82	kAl(OH)4 -	51.5780		-11168.9000			-14.86500
89	kHSO4 -	-56.8890	.00647300	2307.9000			19.88580
91	kH2S aq	11.1700	-.02386000	-3279.0000			
97	Chalcedony	-.0900		-1032.0000			
101	Quartz	.4100		-1309.0000			
135	kSrCO3 aq	-1.0190	.01282600				
137	kH2CO3 aq	108.3865	.01985076	-6919.5300		.669365E+06	-40.45154
142	Strontianite	155.0305		-7239.5940			-56.58638
143	Celestite	-14805.9622	-2.46609240	756968.5330		-.405536E+08	5436.35880
144	Barite	136.0350		7680.4100			-48.59500
145	Witherite	607.6420	.12109800	-20011.2500			-236.49480
152	kw	-283.9710	-.05069842	13323.0000		-.111967E+07	102.24447
157	Allophane(a)						
158	Allophane(f)						
202	kHF aq	-2.0330	.01264500	429.0100			
220	kCu2(OH)2 +2	2.4970		-3833.0000			
336	kAl(OH)3 aq	226.3740		-18247.8000			-73.59700
339	Melanterite	1.4470	-.00415300			-.214949E+06	
395	SiO2 (a,N)	-.2600		-731.0000			
561	kBaHCO3 +	-3.0938	.01366900				
562	kBaCO3 aq	.1130	.00872100				

Reference numbers for all possible numbered input constituents:

Number	Constituent	Z
0	Ca	2
1	Mg	2
2	Na	1
3	K	1
4	Cl	-1
5	SO4	-2
6	HCO3	-1
7	Fe	2
8	Fe	3
13	H2S aq	0
16	Fe total	2
17	CO3	-2
34	SiO2 tot	0
38	NH4	1
44	PO4	-3
48	Cs	1
50	Al	3
61	F	-1
80	Li	1
84	NO3	-1
86	B tot	0
87	Sr	2
89	Ba	2
94	Rb	1
96	I	-1
97	Br	-1
109	Mn	2
130	Cu	2
145	Zn	2
160	Cd	2
182	Pb	2
202	NO2	-1
204	Ni	2
212	Ag	1
249	As total	0
261	As3 tot	0
262	As5 tot	0
284	fulvate	-2
285	Humate	-2
298	Se total	0
299	H2Se aq	0
300	Se4 tot	0
301	Se6 tot	0
316	U total	0
317	U	4
359	U+6 tot	6

Attachment C. Program Listing of WATEQ4F

```
CWATEQ2 BEARBEITET VON D.W. ZACHMANN UND W. BAETHGE
C
C         UEBERSETZT IN FORTRAN (W.BAETHGE)
C
C         UNTERPROGRAMME :INTABL, PREP, SET, MAJEL, TREL, UEL,
C         SUMS, SOLUTS, PCTEST, RATIO, APCALC, ERRCLC, PHASES,
C         OUTPCH, OUTABL, INPUT
C
C         KANAL 1 -> EINLESEN DER DATENTABELLEN
C         KANAL 2 -> EINLESEN DER MESSWERTE UND STEUERDATEN
C         KANAL 3 -> AUSGABE DER ERGEBNISSE
C         KANAL 4 -> AUSGABE DER BATENTABELLEN MIT KOMMENTAR
C         KANAL 5 -> AUSGABE SUBROUTINE PUNCH (NOCH ANZUPASSEN)
C
C      UNIT NUMBERS CHANGED TO ACCOMMODATE IBM PC I/O REQUIREMENTS:
C
C         UNIT  5 -> INPUT OF THE WATER ANALYSIS DATA
C         UNIT  6 -> OUTPUT OF THE RESULTS
C         UNIT  7 -> OUTPUT OF SUBROUTINE OUTPCH (PLOT DATA)
C         UNIT  8 -> OUTPUT OF THE THERMODYNAMIC DATA (TABLES.OUT)
C         UNIT 11 -> INPUT OF TABLE1 DATA
C         UNIT 12 -> GENERAL USE SCRATCH FILE
C         UNIT 13 -> INPUT OF TABLE2 DATA
C         UNIT 14 -> INPUT OF TABLE3 OR TABL3A DATA
C         UNIT 15 -> INPUT OF TABLE4 DATA
C
C    ************************************************************************
C    ****                                                                ****
C    ****   Modifications installed on 12/15/87, by J W Ball:            ****
C    ****                                                                ****
C    ****   1. Parameter list passed to Subroutine INPUT has been        ****
C    ****      modified to pass LOGKTO instead of LOGKT.  Now works      ****
C    ****      as originally coded in WATEQ2.                            ****
C    ****                                                                ****
C    ****   2. Corrected input of the CORALK parameter.  Input was       ****
C    ****      previously a local floating point variable.  It is        ****
C    ****      now a global integer variable.  NOTE that program         ****
C    ****      WQ4FINPT was modified (also on 12/15/87), and that        ****
C    ****      old data sets are NOT compatible, i.e., the last data     ****
C    ****      item on record 5 must now be an integer.                  ****
C    ****                                                                ****
C    ****   Modifications installed on 3/3/88, by J W Ball:              ****
C    ****                                                                ****
C    ****   1. Uploaded version running on the PC using Microsoft        ****
C    ****      FORTRAN, Version 4.00 to the PRIME.  This is now          ****
C    ****      the primary version, replacing the IBM Professional       ****
C    ****      FORTRAN version.                                          ****
C    ****                                                                ****
C    ****   2. Log IAP/K output now prints blank fields, rather          ****
C    ****      than zeros, when no data are present.                     ****
C    ****                                                                ****
C    ****   3. The new calculation of Uematsu and Franck for the         ****
C    ****      dielectric constant of water between 0 and 100 C          ****
C    ****      has been added to Subroutine PREP.                        ****
C    ****                                                                ****
C    ****   4. The new analytical expression for Kw of Olofsson          ****
C    ****      and Olofsson has been added to Subroutine SET.            ****
C    ****                                                                ****
C    ****   5. Subroutine SUMS was modified to ensure that the           ****
C    ****      variable ANLCO3 does not ever go below zero.  ANLCO3      ****
C    ****      <0 causes the program to blow up, and would happen        ****
C    ****      whenever CORALK=0 and noncarbonate alkalinity>total       ****
C    ****      alkalinity (e.g., at very high pH).                       ****
C    ****                                                                ****
C    ****   6. Subroutine SOLUTS was modified to test the absolute       ****
```

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C   ****      value of EPMCAT-EPMAN, so that the warning message    ****
C   ****      is printed when the value is <-30% as well as >+30%.  ****
C   ************************************************************************
C   ************************************************************************
C   ****                                                                ****
C   ****************       WATEQ4F, VERSION 1.1       ****************
C   ****                                                                ****
C   ****                                                                ****
C   ****   Modifications installed on 3/16/88, by J W Ball:             ****
C   ****                                                                ****
C   ****   1. Added Selenium calculations to the model.  This           ****
C   ****      increased solute dimension from 297 to 307, and           ****
C   ****      thermo data dimension from 543 to 556.  Includes the      ****
C   ****      capability to speciate using either individual redox      ****
C   ****      species (Se 2-, Se 4+, Se 6+) or total Se + Eh input.     ****
C   ****                                                                ****
C   ****   2. Removed the following unused parameters from lists        ****
C   ****      passed to the following subroutines:                      ****
C   ****      a. ERRT and LOGKT from PREP parameter list.               ****
C   ****      b. CUNITS from MAJEL and RATIO parameter lists.           ****
C   ****      c. ENDE from INPUT parameter list (called from PREP).     ****
C   ****                                                                ****
C   ****   3. In subroutine SUMS, removed species 81 from summation     ****
C   ****      of noncarbonate alkalinity species molalities.  Spe-      ****
C   ****      cies used to be LiOH aq, but is now CaHSO4+.              ****
C   ****                                                                ****
C   ****   Modifications installed on 6/21/88, by J W Ball:             ****
C   ****                                                                ****
C   ****   1. In subroutine OUTPCH, added charge balance to the         ****
C   ****      quantities written into file CARDS.EQP, at end of         ****
C   ****      the file.                                                 ****
C   ****                                                                ****
C   ****   2. In subroutine APCALC, changed calculation of mineral      ****
C   ****      140, amorphous Al(OH)3, to be in terms of H+ and H2O      ****
C   ****      rather than OH-.  Changed TABLE 2 thermodynamic data.     ****
C   ****                                                                ****
C   ****   Modifications installed on 10/11/88, by J W Ball:            ****
C   ****                                                                ****
C   ****   1. Altered the charge balance calculation to read:           ****
C   ****                                                                ****
C   ****      DIFF=100.*(EPMCAT-EPMAN)/(EPMAN+EPMCAT)                   ****
C   ****                                                                ****
C   ****      This change divides the difference by the sum of the      ****
C   ****      cations + anions, rather than by their average.  The      ****
C   ****      effect of this modification is to make the charge         ****
C   ****      balance equal to half of its previous value.              ****
C   ****                                                                ****
C   ****   Modifications installed on 3/7/89, by J W Ball:              ****
C   ****                                                                ****
C   ****   1. Added the following solute species: FeF+, FeHCO3+,        ****
C   ****      FeCO3 aq, MnCO3 aq, BaHCO3+, BaCO3 aq and SrSO4 aq.       ****
C   ****                                                                ****
C   ****   2. Recoded the following reactions to match stoichiometry****
C   ****      of new thermodynamic data: MgOH+, CaOH+, SrOH+,           ****
C   ****      Brucite, Chrysotile, Kaolinite, Alunite, Pyrolusite       ****
C   ****      and Manganite.                                            ****
C   ****                                                                ****
C   ****   3. Revised TABLE2 data ONLY for the following solute         ****
C   ****      species and minerals: kFe+3, kFeSO4+, Siderite,           ****
C   ****      Dolomite, Brucite, kMgF+, kCaSO4 aq, Sepioline (c),       ****
C   ****      Kaolinite, Alunite, Gibbsite (c), kNaCO3-, kMgSO4 aq,     ****
C   ****      kCaOH+, kAlF +2, kAlF2 +, kAlF3 aq, kAlF4 -, kFeOH2 +,****
C   ****      kFeOH3 aq, kFeOH4 -, Goethite, kSrOH+, kBaOH+, AlOH3a,****
C   ****      kCaF+, kMn +3, kMnCl +, kMnCl2 aq, kMnCl3 -, kMnF+,       ****
C   ****      kMnSO4 aq, kMnHCO3 +, Pyrolusite, Birnessite, Nsutite,****
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C   ****      Hausmannite, Pyrochroite, Manganite, Rhodochrosite,    ****
C   ****      kHF2 -, kFe(SO4)2 -, kNaF aq.                          ****
C   ****                                                             ****
C   ****   4. Revised or added new analytical expressions for the    ****
C   ****      following: kH3SiO4 -, kH2SiO4 -2, Anhydrite, Gypsum,   ****
C   ****      Chrysotile, Fluorite, kMgHCO3 +, kAlOH +2, kAl(OH)2 +, ****
C   ****      kAl(OH)4-, kHSO4 -, Chalcedony, Quartz, kH2CO3 aq,     ****
C   ****      Celestite, Barite, Witherite, kw, kHF aq, kAl(OH)3 aq, ****
C   ****      Melanterite, SiO2 (a,M). Removed the analytical        ****
C   ****      expression for kMgOH + (reaction rewritten, no new     ****
C   ****      expression available). Revised subroutine INTABL to    ****
C   ****      print out the revised list of analytical expressions.  ****
C   ****                                                             ****
C   ****   Modifications installed on 9/27/89, by J W Ball:          ****
C   ****                                                             ****
C   ****   1. Altered the charge balance calculation to read:        ****
C   ****                                                             ****
C   ****      DIFF=200.*(EPMCAT-EPMAN)/(EPMAN+EPMCAT)                ****
C   ****                                                             ****
C   ****      This change divides the difference by the average of   ****
C   ****      the cations + anions, rather than by their sum. The    ****
C   ****      effect of this modification is to make the charge      ****
C   ****      balance equal to twice its previous value, and         ****
C   ****      restores the calculation to its pre-10/11/88 form.     ****
C   ****                                                             ****
C   ****   Modifications installed on 11/8/89, by J W Ball:          ****
C   ****                                                             ****
C   ****   1. Added 4 statements to subroutine MAJEL, to flag the    ****
C   ****      Se input species for omission from the total molality  ****
C   ****      calculations; the statements set LISTE(298), (299),    ****
C   ****      (300) and (301) to zero, starting at MAJEL line 32.    ****
C   ****                                                             ****
C   ****   Modifications installed on 11/29/89, by J W Ball:         ****
C   ****                                                             ****
C   ****   1. Added the following solute species: FeCl+, TABLE1      ****
C   ****      index number 315, TABLE2 index number 542.             ****
C   ****                                                             ****
C   ****   Modifications installed on 1/3/90, by J W Ball:           ****
C   ****                                                             ****
C   ****   1. Changed constants used in the calculation of the       ****
C   ****      DeBye-Huckel A and B parameters in lines WAT04000      ****
C   ****      and WAT04010, respectively, of PREP as follows:        ****
C   ****                                                             ****
C   ****         FOR CALC OF          FROM           TO             ****
C   ****         -----------        --------       ---------        ****
C   ****             A              1824600        1824827.7        ****
C   ****             B               50.29          50.2905         ****
C   ****                                                             ****
C   ****   Modifications installed on 2/10/90, by J W Ball:          ****
C   ****                                                             ****
C   ****   1. Restored the coding of the IAP calculation for         ****
C   ****      Halloysite, index number 47, to its earlier form,      ****
C   ****      to match its thermodynamic data. This corrects         ****
C   ****      an error that had been present since 3/7/89.           ****
C   ****                                                             ****
C   ****   2. Removed variable KT from parameter list passed from    ****
C   ****      WQ4FMAIN to SOLUTS. Replaced all occurrences of        ****
C   ****      DLOG10(KT(##)) with LOGKT(##).                         ****
C   ****                                                             ****
C   ****   3. Removed calculation of partial pressure of atmos-      ****
C   ****      pheric pCH4, replacing it with print of log pCO2.      ****
C   ****                                                             ****
C   *****************************************************************
C   *****************************************************************
C   ****                                                             ****
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C   ****************        WATEQ4F, VERSION 2.0        ****************
C   ****                                                              ****
C   ****                                                              ****
C   ****   Modifications installed on 3/14/90, by J W Ball:           ****
C   ****                                                              ****
C   ****   1. Split thermodynamic data output off from subroutine     ****
C   ****      INTABL, naming it OUTABL.  OUTABL can now be called     ****
C   ****      separately, and the thermodynamic data can be printed   ****
C   ****      out at run time with user option PRNT=4, 5, 6 or 7.     ****
C   ****                                                              ****
C   ****   2. Added nine Eh options.  User may now elect to have      ****
C   ****      redox calculations done using any input or calculated   ****
C   ****      Eh value.  The Eh value used is variable at different   ****
C   ****      parts of the program, as follows:                       ****
C   ****                                                              ****
C   ****         1.  Fe species distribution.                         ****
C   ****         2.  Mn species other than +2.                        ****
C   ****         3.  Cu +1 species.                                   ****
C   ****         4.  As species distribution.                         ****
C   ****         5.  Se species distribution.                         ****
C   ****         6.  IAP calculations.                                ****
C   ****         7.  PO2 calculation (in SOLUTS).                     ****
C   ****         8.  H2S (aq) activity calculation (in SOLUTS).       ****
C   ****         9.  U species distribution.                          ****
C   ****                                                              ****
C   ****         The Eh value selected may be any of the following:   ****
C   ****                                                              ****
C   ****         0.  Input (Pt electrode) Eh.                         ****
C   ****         1.  Eh calculated from Fe 2/3.                       ****
C   ****         2.  Eh calculated from H2O/O2 using Sato relation.   ****
C   ****         3.  Eh calculated from H2O2/O2.                      ****
C   ****         4.  Eh calculated from NH4/NO3.                      ****
C   ****         5.  Eh calculated from S=/SO4.                       ****
C   ****         6.  Eh calculated from NO2/NO3.                      ****
C   ****         7.  Eh calculated from S=/S(s).                      ****
C   ****         8.  Eh calculated from As 3/5.                       ****
C   ****         9.  Eh calculated from As(s)/As 3+.                  ****
C   ****        10.  Eh calculated from Se 4/6.                       ****
C   ****        11.  Eh calculated from Se(s)/Se 4+.                  ****
C   ****        12.  Eh calculated from Se=/Se(s).                    ****
C   ****        13.  Eh calculated from U 4/6.                        ****
C   ****                                                              ****
C   ****   Modifications installed on 4/25/90, by J W Ball:           ****
C   ****                                                              ****
C   ****     Changed the following TABLE2 data per DK Nordstrom:      ****
C   ****                                                              ****
C   ****       I    Species          dH     Log K                    ****
C   ****       ---------------------------------                      ****
C   ****       87   kAlSO4 +        2.29     3.5                      ****
C   ****       88   kAlSO42-       3.11     5.0                      ****
C   ****                                                              ****
C   ****   Modifications installed on 5/27/90, by J W Ball:           ****
C   ****                                                              ****
C   ****    1. Removed ppm uncom CO2 from printout, added ppm O2      ****
C   ****       calc, ppm pCO2, and H2S from SO4.                      ****
C   ****                                                              ****
C   ****    2. Removed Min and Max KT feature from WATEQ4F.           ****
C   ****                                                              ****
C   ****    3. Modified PRNT options to the following:                ****
C   ****       0 = Print minimum output                               ****
C   ****       1 = Include complete aqueous speciation/solubility     ****
C   ****       2 = Include mole ratios page                           ****
C   ****       3 = 1 plus 2                                           ****
C   ****       4 = 0 plus generate thermodynamic data table           ****
C   ****       5 = 1 plus generate thermodynamic data table           ****
```

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C   ****       6 = 2 plus generate thermodynamic data table          ****
C   ****       7 = 3 plus generate thermodynamic data table          ****
C   ****                                                             ****
C   ****    4. Added subroutine PCTEST, to test aqueous output       ****
C   ****       data for comprising >= 1% of the total input          ****
C   ****       concentration of the parent species.  If PRNT         ****
C   ****       option 0 or 2 is selected, only aqueous species       ****
C   ****       > 1% of the total will be printed out.                ****
C   ****                                                             ****
C   ****    5. Modified aqueous and mineral output to be printed     ****
C   ****       in alphabetical order throughout.                     ****
C   ****                                                             ****
C   ****    6. Added crystalline rhodochrosite, species #564, and    ****
C   ****       crystalline siderite, species #94.                    ****
C   ****                                                             ****
C   ****    7. Added uranium calculations to the model.  New         ****
C   ****       thermodynamic data and reactions, where available,    ****
C   ****       from Grenthe and others (1990); otherwise data        ****
C   ****       from Langmuir (1978).  See Ball and others (1991)     ****
C   ****       Open-File Report 91-183 for further details.          ****
C   ****                                                             ****
C   ****  Modifications installed on 8/10/90, by J W Ball:           ****
C   ****                                                             ****
C   ****    1. Changed log K for monteponite (CdO) from 15.12 to     ****
C   ****       13.77 (data from Dirkse, 1986).                       ****
C   ****                                                             ****
C   ****    2. Changed log K for covellite (CuS) from -23.038 to     ****
C   ****       -22.27 (data from Shea and Helz, 1989).               ****
C   ****                                                             ****
C   ****    3. Changed log K for galena (PbS) from -15.132 to        ****
C   ****       -12.78 (data from Shea and Helz, 1989).               ****
C   ****                                                             ****
C   ****    4. Modified element ratios printout to print a large     ****
C   ****       number of weight and molar ratios of the elements     ****
C   ****       to Cl, SO4, HCO3 and Fe.  Eliminated the log          ****
C   ****       activity ratios.                                      ****
C   ****                                                             ****
C   ****  Modifications installed on 3/6/91, by J W Ball:            ****
C   ****                                                             ****
C   ****    1. Changed log K for otavite (CdCO3) from -13.74 to      ****
C   ****       -12.1+/-0.1, delta-H from -0.58 to -0.019 (data       ****
C   ****       from Stipp, 1991).                                    ****
C   ****                                                             ****
C   ****    2. Changed species 166 (reaction 299) from Cd(CO3)3 -4   ****
C   ****       to Cd(CO3)2 -2 log K=6.4 (data from Stipp, 1991).     ****
C   ****                                                             ****
C   ****    3. Changed log K for species 514 (CdHCO3 +) from 2.1     ****
C   ****       to 1.5 (data from Stipp, 1991).                       ****
C   ****                                                             ****
C   ****    4. Changed log K for species 515 (CdCO3 aq) from 5.4     ****
C   ****       to 2.9 +/- 0.4 (Data from Stipp, 1991).               ****
C   ****                                                             ****
C   ****  Modifications installed on 4/26/91, by J W Ball:           ****
C   ****                                                             ****
C   ****    1. Added an input option for analytical data in MMOL     ****
C   ****       (millimoles per liter); per D. K. Nordstrom.          ****
C   ****                                                             ****
C   ****  Modifications installed on 7/12/91, by J W Ball:           ****
C   ****                                                             ****
C   ****    1. Corrected several minor errors in subroutine UEL:     ****
C   ****         a) Set all UTEMP to +78 prior to calculations,      ****
C   ****            lines 12-14.                                     ****
C   ****         b) Removed all other statements setting UTEMP to    ****
C   ****            +78, throughout the subroutine.                  ****
C   ****         c) Added test for PE when calculating U +3 (species ****
```

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C   ****          319, line 20), UO2 + (species 339, line 66), and ****
C   ****          UO2(CO3)3 -5 (species 377, line 85).             ****
C   ****                                                           ****
C   ****     2. In subroutine SUMS:                                ****
C   ****        a) Added species 375 and 377 to summation of the   ****
C   ****           carbonate species, lines 42 and 53.             ****
C   ****        b) Added calculation of TENMPE, line 166, before   ****
C   ****           its use, line 167.                              ****
C   ****        c) Increased DO loop value from 36 to 38 in        ****
C   ****           carbonate molality and activity calculations,   ****
C   ****           line 196.                                       ****
C   ****        d) Corrected spacing on FORMAT statement # 1020,   ****
C   ****           lines 519-521.                                  ****
C   ****        e) Changed minimum number of iterations allowed    ****
C   ****           by WATEQ4F from 2 to 3, line 526.               ****
C   ****                                                           ****
C   ****   Modifications installed on 7/14/91, by J W Ball:        ****
C   ****                                                           ****
C   ****     1. In subroutine PCTEST, added multiplier NPOLY to    ****
C   ****        accurately reflect presence of polynuclear master  ****
C   ****        species when calculating percent of total, lines   ****
C   ****        2, 46, 47 and 61.                                  ****
C   ****                                                           ****
C   ***************************************************************
C
      REAL*8 ALFA(0:377),ANALMI(0:377),AP(0:653),CUNITS(0:377),DH(0:653)
     *,DHA(0:377),ERR(0:653),ERRT(0:653),GAMMA(0:377),GFW(0:377),
     *KT(0:653),LOGKT(0:653),LOGKTO(0:653),
     *MI(0:377),SIGMA(0:377),V(0:377)
C
      INTEGER ANAL(0:377),Z(0:377)
C
      CHARACTER*12 PAGE2(0:653)
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*1 DEST
C
$INCLUDE:'COMMON.BLK'
C
C**** THE FOLLOWING SUPPRESSES UNDERFLOW ERRORS
C
C     IERRN = 208
C     CALL ERRSET(IERRN,256,-1,1,1,IERRN)
C
      D = 377
      E = 653
C
      CALL INTABL(PAGE1,PAGE2,Z,DHA,GFW,V,DH,LOGKTO,ERRT)
      DO 5 I = 1 , D
      SIGMA(I) = 0.0
    5 CONTINUE
      NMBR=0
      OPEN (UNIT=5,FILE='WATEQ4F.DAT',STATUS='OLD')
      K=6
      OPEN (UNIT=K,FILE='WATEQ4F.OUT')
 1000 CONTINUE
      NMBR=NMBR+1
      ENDE = 0
      CALL PREP (PAGE1,PAGE2,ANAL,Z,DHA,ANALMI,CUNITS,DH,GFW,
     *LOGKTO,MI,SIGMA,V,ENDE,ERRT)
      IF (ENDE .NE. 0) GOTO 60
      CALL SET(DH,GAMMA,KT,LOGKT,LOGKTO,MI)
      ITER = 0
      RBIT = 1
      DO 7 I = 0 , D
      ALFA(I) = 0.0
```

```
    7 CONTINUE
   10 ITER = ITER + 1
      CALL MAJEL(ALFA,DHA,GAMMA,KT,LOGKT,MI,Z)
      CALL TREL(ALFA,GAMMA,KT,LOGKT,MI)
      CALL UEL(ALFA,GAMMA,LOGKT,MI)
      CALL SUMS(ALFA,GAMMA,KT,LOGKT,MI)
      IF (RBIT .NE. 0) GOTO 10
      CALL SOLUTS(ANAL,Z,PAGE1,ALFA,ANALMI,CUNITS,GAMMA,GFW,MI,LOGKT
     *,SIGMA,ERR)
      IF (PRNT .GE. 2) CALL RATIO(PAGE1,ANALMI,CUNITS)
      CALL APCALC(AP,ALFA,GAMMA,MI)
      DO 40 I = 0 , E
      ERR(I) = 2.0E7
   40 CONTINUE
      CALL ERRCLC(CUNITS,SIGMA,ERR)
      IF (PUNCH .EQ. 0) CALL OUTPCH(ALFA,AP,CUNITS,LOGKT)
      CALL PHASES(PAGE2,AP,LOGKT,ERR,ERRT)
      GOTO 1000
   60 CLOSE(5)
      CLOSE(K)
      STOP
      END
      SUBROUTINE INTABL(PAGE1,PAGE2,Z,DHA,GFW,V,DH,LOGKTO,
     *ERRT)
C
      REAL*8 DH(0:653),DHA(0:377),ERRT(0:653),GFW(0:377),V(0:377),
     *LOGKTO(0:653)
      INTEGER Z(0:377)
      CHARACTER*12 PAGE2(0:653)
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*2 MARKE
C
$INCLUDE:'COMMON.BLK'
C
      DO 100 I = 0 , D
      V(I)     = 1.0
      GFW(I)   = 1.0
      Z(I)     = 1
      DHA (I)  = 1.0
  100 CONTINUE
      DO 110 I = 0 , E
      LOGKTO(I) = 1.0
      DH (I)    = 1.0
      ERRT(I)   = 0.1
  110 CONTINUE
      OPEN (UNIT=11,FILE='TABLE1',STATUS='OLD')
      DO 120 N = 0 , D
      READ (11,9000)I,PAGE1(I),Z(I),GFW(I),DHA(I)
 9000 FORMAT(I4,1X,A8,I3,F9.4,F4.1)
  120 CONTINUE
      CLOSE(11)
      OPEN (UNIT=13,FILE='TABLE2',STATUS='OLD')
      DO 130 N = 0 , E
      READ (13,9010)I,PAGE2(I),DH(I),LOGKTO(I),ERRT(I)
  130 CONTINUE
 9010 FORMAT(I4,1X,A12,2(F9.3),F5.2)
      CLOSE(13)
C
      DO 140  I = 0 , D
      V(I) = 1.0
      IF (Z(I).EQ. 0) GOTO 140
      V(I) = ABS(Z(I))
  140 CONTINUE
      PRNT    = 0
      PUNCH   = 0
```

```
      DO 145 I=1,9
        EHOPT(I) = 0
  145 CONTINUE
      SIGMDO = 0.0
      SIGMEH = 0.0
      SIGMPH = 0.0
C
      C = 2.302585093
      F = 23.0603
      R = 1.98719E-3
      RETURN
      END
      SUBROUTINE OUTABL(PAGE1,PAGE2,Z,DHA,GFW,DH,LOGKTO,ERRT)
C
      REAL*8 DH(0:653),DHA(0:377),ERRT(0:653),GFW(0:377),
     *LOGKTO(0:653),COEF(0:6,41)
      INTEGER Z(0:377),LISTE2(46)
      CHARACTER*15 CCOEF
      CHARACTER*13 CCOEFF(4)
      CHARACTER*12 CC0E
      CHARACTER*12 PAGE2(0:653)
      CHARACTER*10 SC(2)
      CHARACTER*8 SSC
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*2 MARKE
C
$INCLUDE:'COMMON.BLK'
C
      DATA COEF/12.,-171.9065D0,-0.077993D0,2839.319D0,2*0.D0,71.595D0,
     *13.,-302.3724D0,-0.050698D0,15669.69D0,0.,-1119669.D0,108.18466D0,
     *14.,-294.0184D0,-0.07265D0,11204.49D0,0.,-1119669.D0,108.18466D0,
     *17.,197.52D0,0.,-8669.8D0,2*0.,-69.835D0,
     *18.,68.2401D0,0.,-3221.51D0,2*0.,-25.0627D0,
     *20.,13.248D0,0.,10217.1D0,2*0.,-6.1894D0,
     *21.,-171.9773D0,-0.077993D0,2903.293D0,2*0.,71.595D0,
     *25.,28.6059D0,0.012078D0,1573.21D0,2*0.,-13.2248D0,
     *26.,0.6322D0,-0.001225D0,-2835.76D0,3*0.,
     *35.,356.3094D0,0.06091964D0,-21834.37D0,0.,1684915.D0,-126.8339D0,
     *62.,66.348D0,0.,-4298.2D0,2*0.,-25.271D0,
     *68.,107.8871D0,0.03252849D0,-5151.79D0,0.,563713.9D0,-38.92561D0,
     *72.,3.106D0,0.,-673.6D0,3*0.,
     *73.,0.991D0,0.00667D0,4*0.,
     *74.,-59.215D0,0.,2537.455D0,2*0.,20.92298D0,
     *77.,1209.12D0,0.31294D0,-34765.05D0,2*0.,-478.782D0,
     *78.,-1228.732D0,-0.299444D0,35512.75D0,2*0.,485.818D0,
     *79.,-3.248D0,0.014867D0,4*0.,
     *80.,-38.253D0,0.,-656.27D0,2*0.,14.327D0,
     *81.,88.5D0,0.,-9391.6D0,2*0.,-27.121D0,
     *82.,51.578D0,0.,-11168.9D0,2*0.,-14.865D0,
     *89.,-56.889D0,0.006473D0,2307.9D0,2*0.,19.8858D0,
     *91.,11.17D0,-0.02386D0,-3279.D0,3*0.,
     *97.,-0.09D0,0.,-1032D0,3*0.,
     *101.,0.41D0,0.,-1309D0,3*0.,
     *135.,-1.019D0,0.012826D0,4*0.,
     *137.,108.3865D0,0.01985076D0,-6919.53D0,0.,669365.D0,-40.45154D0,
     *142.,155.0305D0,0.,-7239.594D0,2*0.,-56.58638D0,
     *143.,-1.48059622D4,-2.4660924D0,7.56968533D5,0.,
     *     -4.0553604D7,5436.3588D0,
     *144.,136.035D0,0.,7680.41D0,2*0.,-48.595D0,
     *145.,607.642D0,0.121098D0,-20011.25D0,2*0.,-236.4948D0,
     *152.,-283.971D0,-0.05069842D0,13323.D0,0.,-1119669D0,102.24447D0,
     *157.,6*0.,158.,6*0.,
     *202.,-2.033D0,0.012645D0,429.01D0,3*0.,
     *220.,2.497D0,0.,-3833.D0,3*0.,
     *336.,226.374D0,0.,-18247.8D0,2*0.,-73.597D0,
```

```
     *339.,1.447D0,-0.004153D0,2*0.,-214949.D0,0.,
     *395.,-0.26D0,0.,-731.D0,3*0.,
     *561.,-3.0938D0,0.013669D0,4*0.,
     *562.,0.113D0,0.008721D0,4*0. /
      DATA LISTE2/0,1,2,3,4,5,6,7,8,13,16,17,34,38,44,48,50,61,80,84,
     *86,87,89,94,96,97,109,130,145,160,182,202,204,212,249,261,262,
     *284,285,298,299,300,301,316,317,359/
C
      NEQU=41
      OPEN (UNIT=12,STATUS='NEW')
      OPEN (UNIT=8,FILE='TABLES.OUT',STATUS='NEW')
      WRITE(8,9025)
 9025 FORMAT (1H1,'  I   Page2            dH      LogKto     Error',9X,
     *'I   Page1     Z  DHa     GFW')
      IN=0
      DO 170 I = 0 , E
      MARKE = '  '
      DO 150 J = 1 , NEQU
      IF(I.EQ.INT(COEF(0,J))) MARKE = ' *'
  150 CONTINUE
      REWIND 12
      IF(ABS(DH(I)) .GT. 1D-78) THEN
        WRITE(12,1120) DH(I)
      ELSE
        WRITE(12,1130)
      END IF
      IF(ABS(LOGKTO(I)) .GT. 1D-78) THEN
        WRITE(12,1120) LOGKTO(I)
      ELSE
        WRITE(12,1130)
      END IF
      IF(ABS(ERRT(I)) .GT. 1D-78) THEN
        WRITE(12,1140) ERRT(I)
      ELSE
        WRITE(12,1150)
      END IF
      REWIND 12
      DO 155 L=1,2
        READ(12,1160)SC(L)
  155 CONTINUE
      READ(12,1170)SSC
 1120 FORMAT(F10.3)
 1130 FORMAT('          ')
 1140 FORMAT(F8.3)
 1150 FORMAT('        ')
 1160 FORMAT(A10)
 1170 FORMAT(A8)
      IF (I.GT.D) GOTO 160
      WRITE(8,9030)I,PAGE2(I),SC(1),SC(2),
     *MARKE,SSC,I,PAGE1(I),Z(I),DHA(I),GFW(I)
      GOTO 165
  160 WRITE(8,9030)I,PAGE2(I),SC(1),SC(2),
     *MARKE,SSC
 9030 FORMAT(1H ,I3,2X,A12,2A10,A2,A8,I10,2X,A8,I4,F5.1,F10.4)
  165 IN=IN+1
      IF (IN.LT.59) GOTO 170
      IN=0
      WRITE(8,9025)
  170 CONTINUE
C
      WRITE(8,9040)
 9040 FORMAT(/,'  "*" Denotes that an analytical expression for Kt has',
     *' been used'/1H1,'Summary of analytical expressions of the form',
     *' Log K = A + B*T + C/T + D*T**2 + E/T**2 + F*LOG10(T)'//
     *'   I  React Product         A             B             C
```

```
     *   D              E              F')
C
      DO 180 L = 1, NEQU
      I = INT(COEF(0,L))
      REWIND 12
      IF(ABS(COEF(1,L)) .GT. 1D-78) THEN
        WRITE(12,1180) COEF(1,L)
      ELSE
        WRITE(12,1190)
      END IF
      IF(ABS(COEF(2,L)) .GT. 1D-78) THEN
        WRITE(12,1200) COEF(2,L)
      ELSE
        WRITE(12,1190)
      END IF
      IF(ABS(COEF(3,L)) .GT. 1D-78) THEN
        WRITE(12,1180) COEF(3,L)
      ELSE
        WRITE(12,1190)
      END IF
      IF(ABS(COEF(4,L)) .GT. 1D-78) THEN
        WRITE(12,1210) COEF(4,L)
      ELSE
        WRITE(12,1190)
      END IF
      IF(ABS(COEF(5,L)) .GT. 1D-78) THEN
        WRITE(12,1220) COEF(5,L)
      ELSE
        WRITE(12,1230)
      END IF
      IF(ABS(COEF(6,L)) .GT. 1D-78) THEN
        WRITE(12,1240) COEF(6,L)
      ELSE
        WRITE(12,1250)
      END IF
      REWIND 12
      DO 185 J=1,4
        READ(12,1260)CCOEFF(J)
  185 CONTINUE
      READ(12,1270)CCOEF
      READ(12,1280)CCOE
      WRITE(8,9050) I,PAGE2(I),(CCOEFF(J),J=1,4),CCOEF,CCOE
  180 CONTINUE
 1180 FORMAT(F13.4)
 1190 FORMAT('              ')
 1200 FORMAT(F13.8)
 1210 FORMAT(1PE13.5)
 1220 FORMAT(E15.6)
 1230 FORMAT('                ')
 1240 FORMAT(0PF12.5)
 1250 FORMAT('             ')
 1260 FORMAT(A13)
 1270 FORMAT(A15)
 1280 FORMAT(A12)
C9050 FORMAT(I4,2X,A12,2X,F13.4,F13.8,F13.4,2X,1PE13.5,E15.6,0PF12.5)
 9050 FORMAT(I4,2X,A12,2X,3A13,2X,A13,A15,A12)
      WRITE(8,9060)
 9060 FORMAT(1H1,'Reference numbers for all possible numbered input cons
     *tituents:')
      WRITE(8,9070)
 9070 FORMAT(/,'    Number   Constituent   Z')
C
      DO 190 J = 1 , 46
      I = LISTE2(J)
      WRITE(8,9080)I,PAGE1(I),Z(I)
```

```
  190 CONTINUE
 9080 FORMAT('    ',I4,10X,A8,I3)
      CLOSE(8)
      PRNT=PRNT-4
      RETURN
      END
      SUBROUTINE PREP (PAGE1,PAGE2,ANAL,Z,DHA,ANALMI,CUNITS,DH,GFW,
     *LOGKTO,MI,SIGMA,V,ENDE,ERRT)
C
      INTEGER ANAL(0:377),Z(0:377)
      REAL*8 ANALMI(0:377),CUNITS(0:377),DH(0:653),V(0:377),GFW(0:377),
     *LOGKTO(0:653),MI(0:377),SIGMA(0:377),DHA(0:377),ERRT(0:653)
      CHARACTER*12 PAGE2(0:653)
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*4 CHECK,START
      CHARACTER*2 MARKE
C
$INCLUDE:'COMMON.BLK'
C
      DATA START/'****'/
C
      DO 120 I = 0 , D
      CUNITS(I) = 0.0
      MI(I) = 0.0
      ANALMI(I) = 1.0
      ANAL(I) = 0
  120 CONTINUE
      CORALK  = 0
      EMPOX   = 0.0
      FULFLG = 0
      HUMFLG = 0
      DO 130 I=0,13
        EH(I) = 9.9
        PE(I) = 100.
  130 CONTINUE
      DOX     = -1.0
      DENS    =  1.0
      READ(5,2222,END=140)CHECK
 2222 FORMAT(A4)
      IF (CHECK .EQ. START) GOTO 150
  140 ENDE = 1
      RETURN
C
  150 CALL INPUT(PAGE1,CUNITS,SIGMA,LOGKTO)
C
      IF(PRNT.GE.4) CALL OUTABL(PAGE1,PAGE2,Z,DHA,GFW,DH,LOGKTO,ERRT)
C
      T = TEMP + 273.16E0
      DO 160 I = 0, D
      IF (CUNITS(I) .GE. 0.0) GOTO 160
      ANAL(I)   = 1
      CUNITS(I) = 0.0
  160 CONTINUE
      IF (EH(0) .GT. 9.0) PE(0) = 100.
      IF (EH(0) .LE. 9.0) PE(0) = EH(0)/(C*R*T/F)
      IF (CUNITS(284) .LE. 0.0) GOTO 170
      IF (GFW(284) .NE. 650.0) GOTO 170
      FULFLG = 1
      WRITE(K,970)
  970 FORMAT(/,' NO GFW INPUT WITH CONC VALUE FOR FULVIC ACID.',/,
     *' RESULTS WILL BE FLAGGED WITH ASTERISKS',
     *' TO SIGNIFY THAT THEY ARE PURELY QUALITATIVE.')
  170 IF (CUNITS(285) .LE. 0.0 ) GOTO 180
      IF ( GFW(285) .NE. 2000.0) GOTO 180
      HUMFLG = 1
```

```
      WRITE(K,980)
  980 FORMAT (/,' NO GFW INPUT WITH CONC VALUE FOR HUMIC ACID.',
     *' RESULTS WILL BE FLAGGED WITH ASTERISKS TO SIGNIFY THAT',
     *' THEY ARE PURELY QUALITATIVE.')
  180 WRITE(K,990)
  990 FORMAT(///,' ITER  S1-AnalCO3     S2-AnalSO4',
     *'      S3-AnalF      S4-AnalPO4     S5-AnalCL ',
     *'     S6-AnalH2S    S7-AnalFULV     S8-AnalHUM')
C
C****  FE SPECIES INPUT ADJUSTMENT
C
      IF (CUNITS(16).GT.0.) THEN
        IF (CUNITS(8).LT.1D-78) THEN
          IF (CUNITS(7).GT.0.) CUNITS(8)=DMAX1(0D0,CUNITS(16)-CUNITS(7))
        ELSE
         IF(CUNITS(7).LT.1D-78)CUNITS(7)=DMAX1(0D0,CUNITS(16)-CUNITS(8))
        END IF
      END IF
      IF (CUNITS(7).GT.0. .OR. CUNITS(8).GT.0.) CUNITS(16)=0.
C
C****  AS SPECIES INPUT ADJUSTMENT
C
      IF (CUNITS(249).GT.0.) THEN
        IF (CUNITS(262).LT.1D-78) THEN
          IF (CUNITS(261).GT.0.)
     *      CUNITS(262)=DMAX1(0D0,CUNITS(249)-CUNITS(261))
        ELSE
          IF (CUNITS(261).LT.1D-78)
     *      CUNITS(261)=DMAX1(0D0,CUNITS(249)-CUNITS(262))
        END IF
      END IF
      IF (CUNITS(261).GT.0. .OR. CUNITS(262).GT.0.) CUNITS(249)=0.
C
C****  U SPECIES INPUT ADJUSTMENT
C
      IF (CUNITS(316).GT.0.) THEN
        IF (CUNITS(359).LT.1D-78) THEN
          IF (CUNITS(317).GT.0.)
     *      CUNITS(359)=DMAX1(0D0,CUNITS(316)-CUNITS(317))
        ELSE
          IF (CUNITS(317).LT.1D-78)
     *      CUNITS(317)=DMAX1(0D0,CUNITS(316)-CUNITS(359))
        END IF
      END IF
      IF (CUNITS(317).GT.0. .OR. CUNITS(359).GT.0.) CUNITS(316)=0.
C
C****           CALCULATION OF ANALYZED MOLALITY
C
      IF (FLAG .NE.4) GOTO 200
C                                          4 -> 'MMOL/L'
      DO 190 I = 0, D
      CUNITS(I) = CUNITS(I) * GFW(I)
  190 CONTINUE
      FLAG = 2
C                                          FLAG='MG/L'
  200 IF (FLAG .NE.1) GOTO 220
C                                          1 -> 'MEQ/L'
      DO 210 I = 0, D
      CUNITS(I) = CUNITS(I) * GFW(I) / V(I)
  210 CONTINUE
      FLAG = 2
C                                          FLAG='MG/L'
  220 IF (FLAG .NE.2) GOTO 240
C                                          2 -> 'MG/L'
      DO 230 I = 0, D
```

```
      CUNITS(I) = CUNITS(I) /DENS
  230 CONTINUE
      FLAG = 3
C                                          FLAG='PPM'
  240 IF (FLAG .NE.3) GOTO 270
C                                          3 -> 'PPM'
      C1=0.0
      DO 250 I = 0 , D
      C1 = C1 + CUNITS(I)
  250 CONTINUE
      DO 260 I = 0 , D
      IF(GFW(I) .GT. 0.) MI(I) = CUNITS(I) * (1./ (1.-1E-6 * C1)) /
     *                           (1000.* GFW(I))
  260 CONTINUE
  270 IF (FLAG .NE.5) GOTO 290
C                                          5 -> 'MOLAL'
      DO 280 I = 0 , D
      MI(I) = CUNITS(I)
      CUNITS(I) =MI(I) * 1E3 * GFW(I) * (1-1E-6*C1)
  280 CONTINUE
  290 DO 300 I = 0 , D
      ANALMI(I) = MI(I)
  300 CONTINUE
      EPMCAT = 0.0
      EPMAN  = 0.0
C
C**** CALCULATION OF CATION-ANION BALANCE *
C
      MI(63)=1D1**(-PH)
      DO 310 I = 0 , D
      IF (Z(I) .GT. 0) EPMCAT = EPMCAT + Z(I) * MI(I)
      IF (Z(I) .LT. 0) EPMAN  = EPMAN  - Z(I) * MI(I)
  310 CONTINUE
      IF (MI(26) .LT. 1D-78) THEN
        KW=LOGKTO(152)-DH(152)*((298.16-T)/(298.16*T*C*R))
        EPMAN = EPMAN+1E1**(PH+KW)
      END IF
      DIFF = 0.0
      IF (ABS(EPMAN+EPMCAT) .GT. 0.0)
     *DIFF = 2.0*ABS((EPMAN - EPMCAT) / (EPMAN+EPMCAT))
      IF (DIFF .LE. 0.3) GOTO 320
      WRITE(*,1000)
      WRITE(K,1000)
 1000 FORMAT(/' DIFFERENCE IN INPUT CHARGE BALANCE GREATER THAN 30 PERCE
     *NT.  CHECK INPUT DATA.')
      EPCAT1 = EPMCAT * 1000.
      EPMAN1 = EPMAN * 1000.
      WRITE(*,1010)EPCAT1,EPMAN1
      WRITE(K,1010)EPCAT1,EPMAN1
 1010 FORMAT(' ANAL EPMCAT = ',F12.4,'   ANAL EPMAN =',F12.4)
C
C****  Calculation of total ionic strength (from initial input data)
C
  320 XMUSAV=0E0
      DO 330 I=0,D
      IF (MI(I).GT.1D-78) XMUSAV=XMUSAV+0.5E0*MI(I)*Z(I)*Z(I)
  330 CONTINUE
C
C****  TEMP. AFFECTS ON DEBYE-HUCKEL SOLVENT CONSTANTS
C
      S1 = 374.11 - TEMP
      S2 = S1**.333333
      S3 = SQRT((1.0 +.1342489E0 * S2 - 3.946263E-3 * S1)/
     *(3.1975E0 -.3151548E0 *S2 -1.203374E-3 *S1+ 7.48908E-13 *S1**4))
      IF (T .LT. 373.16)
```

```
C     *C1 = 87.74 -TEMP *(TEMP *(1.41E-6 *TEMP -9.398E -4)+.4008)
C
C    Dielectric constant calc for 0 to 100 deg C added on 1/6/87:
C      Uematsu & Franck (1980) J. Phys. Chem. Ref. Data 9, 1291.
C      Nordstrom & Others (1984) WRI 84-4186.
C
      *C1 = 2727.586+0.6224107*T-466.9151*ALOG(T)-52000.87/T
       IF (T .GE. 373.16)
      *C1 = 5321 / T+233.76 -T *(T* (8.292E-7 *T-1.417E-3) +.9297E0)
       C1 = SQRT ( C1 * T )
       A = 18248.277E2 * S3 / C1**3
       B = 50.2905 * S3 / C1
       RETURN
       END
       SUBROUTINE SET (DH,GAMMA,KT,LOGKT,LOGKTO,MI)
C
       REAL*8 DH(0:653),GAMMA(0:377),KT(0:653),LOGKT(0:653),LOGKTO(0:653)
      *,MI(0:377)
C
$INCLUDE:'COMMON.BLK'
C
       INTEGER LISTE1(41)
       DATA LISTE1 /12,13,14,17,18,20,21,25,26,35,62,68,72,73,74,77,78,
      *79,80,81,82,89,91,97,101,135,137,142,143,144,145,152,157,158,202,
      *220,336,339,395,561,562/
C
       DO 10 I = 0 , E
       KT(I)= 1.0
       LOGKT(I) = 1.0
   10 CONTINUE
       DO 20 I = 0 , D
       GAMMA(I) = 1.0
   20 CONTINUE
C
C**** INITIALIZE STARTING VALUES FOR ITERATIVE LOOP AND CONSTANT GAMMAS
C
       ANLCO3  = MI(6) + 2. * MI (17)
       CO2TIT  = MI(6) + 2. * MI(17)
       SITOT   = MI(34)
       IF (CORALK .EQ. 2) CO2TIT=MI(6) + MI(17) + MI(85)
       CATOT   = MI(0)
       MGTOT   = MI(1)
       NATOT   = MI(2)
       KTOT    = MI(3)
       SO4TOT  = MI(5)
       FETOTL  = MI(16)
       FE2TOT  = MI(7)
       FE3TOT  = MI(8)
       NO2TOT  = MI(202)
       AGTOT   = MI(212)
       PTOT    = MI(44)
       MI(46)  = MI(44)
       ALTOT   = MI(50)
       FTOT    = MI(61)
       BTOT    = MI(86)
       LITOT   = MI(80)
       NH4TOT  = MI(38)
       H2STOT  = MI(13)
       SRTOT   = MI(87)
       BATOT   = MI(89)
       NITOT   = MI(204)
       CSTOT   = MI(48)
       CLTOT   = MI(4)
       HCO3TT  = MI(6)
       PBTOT   = MI(182)
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```
      MNTOT   = MI(109)
      CUTOT   = MI(130)
      ZNTOT   = MI(145)
      CDTOT   = MI(160)
      AS3TOT  = MI(261)
      AS5TOT  = MI(262)
      ASTOTL  = MI(249)
      FULVTT  = MI(284)
      HUMTOT  = MI(285)
      SETOTL  = MI(298)
      H2SETT  = MI(299)
      SEO3TT  = MI(300)
      SEO4TT  = MI(301)
      U4TOT   = MI(317)
      U6TOT   = MI(359)
      UTOTAL  = MI(316)
      MI(249) = 0.0
      MI(261) = 0.0
      MI(262) = 0.0
      MI(298) = 0.0
      MI(299) = 0.0
      MI(300) = 0.0
      MI(301) = 0.0
      MI(316) = 0.0
      MI(359) = 0.0
      MI(34)  = 0.0
      MI(16)  = 0.0
      MI(86)  = 0.0
      TENPH   = 10**PH
C
C**** VANT HOFF EQN. FOR EFFECT OF T ON K
C
      C1 = (298.16 - T) / (298.16 * T * C * R)
      DO 340 I = 0 , E
      LOGKT(I) = LOGKTO(I) - DH(I) * C1
      IF (ABS(LOGKT(I)).LT. 78.) KT(I) = 10**LOGKT(I)
  340 CONTINUE
C
C**** ANALYTICAL EXPRS. FOR EFFECT OF T ON K */
C
C
C     NEW ANALYTICAL EXPR FOR KW ADDED 1/6/87:
C       (Olofsson & Olofsson (1981) J. Chem. Thermo. 13, 437.)
C
C      KT(152) = EXP (-204.52+800.18/T-0.066246*T+28.7918*ALOG(T)
C     *               +5.4822*ALOG(T-197.))
C
C 2/22/89:
C     New and revised analytical expressions added by J.W. Ball, from
C       Nordstrom, Plummer, Langmuir, Busenberg, May, Jones and Parkhurst
C       (1989) for the following reactions:
C
C       13, 14, 17, 18, 62, 74, 80, 81, 82, 89, 97, 101, 137,
C       143, 144, 145, 152, 202, 336, 339, 395
C
      KT(152) = 10. **(-283.971+13323./T-0.05069842*T
     *                +102.24447*DLOG10(T)-1119669./(T*T))
      KW = KT(152)
      C1 = ALOG10(T)
      KT(12) = 1D1 ** (-171.9065-0.077993*T+2839.319/T+71.595*C1)
C     KT(13) = 1D1 ** (6.368E0-1.6346E-2*T-3405.9E0/T)
      KT(13) = 10. ** (-302.3724-0.050698*T+15669.69/T+108.18466*C1
     *                 -1119669./(T*T))
C     KT(14) = 1D1 ** (39.478D0-6.5927D-2*T-12355.1D0/T)
      KT(14) = 10. ** (-294.0184-0.07265*T+11204.49/T+108.18466*C1
```

```
     *                 -1119669./(T*T))
      KT(17) = 10. ** (197.52-8669.8/T-69.835*C1)
      KT(18) = 10. ** (68.2401-3221.51/T-25.0627*C1)
      KT(20) = 10. ** (13.248+10217.1/T-6.1894*C1)
      KT(21) = 1D1 ** (-171.9773-0.077993*T+2903.293/T+71.595*C1)
C     KT(24) = 1D1 ** (.684+.0051*T)
      KT(25) = KW*1D1**(28.6059+0.012078*T+1573.21/T-13.2248*C1)
      KT(26) = 1D1 ** (0.6322D0-1.225D-3*T-2835.76D0/T)
      KT(35) = 1D1**(356.3094+.06091964*T-21834.37/T-126.8339*C1
     *                +1684915./T**2)
C     KT(62) = 1D1 ** (109.25+.0024*T-3120.98/T-37.62424*C1
C    *                -2088.47/(T*T)-4.9D-7*T*T-(298.4/SQRT(T)))
      KT(62) = 10. ** (66.348-4298.2/T-25.271*C1)
      KT(68) = 1D1 ** (107.8871+.03252849*T-5151.79/T-38.92561*C1
     *                +563713.9/T**2)
      KT(72) = 1D1 ** (3.106D0-673.6D0/T)
      KT(73) = 1D1 ** (0.991+0.00667*T)
C     KT(74) = 1D1 ** (2.319-.011056*T+2.29812D-5*T*T)
      KT(74) = 10. ** (-59.215+2537.455/T+20.92298*C1)
      KT(77) = 1D1 ** (1209.12+0.31294*T-34765.05/T-478.782*C1)
      KT(78) = 1D1 ** (-1228.732-0.299444*T+35512.75/T+485.818*C1)
      KT(79) = 1D1 ** (-3.248+0.014867*T)
      KT(80) = 10. ** (-38.253-656.27/T+14.327*C1)
      KT(81) = 10. ** (88.5-9391.6/T-27.121*C1)
      KT(82) = 10. ** (51.578-11168.9/T-14.865*C1)
C     KT(89) = 10. ** (-5.3505+0.0183412*T+557.2467/T)
      KT(89) = 10. ** (-56.889+0.006473*T+2307.9/T+19.8858*C1)
      KT(91) = 10. ** (11.17-0.02386*T-3279.0/T)
      KT(97) = 10. ** (-0.09-1032./T)
      KT(101) = 10. ** (0.41-1309./T)
      KT(135) = 1D1 ** (-1.019+0.012826*T)
      KT(137) = 10. ** (108.3865+0.01985076*T-6919.53/T-40.45154*C1
     *                 +669365./(T*T))
      KT(142) = 1D1 ** (155.0305 -7239.594/T-56.58638*C1)
      KT(143) = 10. ** (-14805.9622-2.4660924*T+756968.533/T
     *                 -40553604./(T*T)+5436.3588*C1)
      KT(144) = 10. ** (136.035-7680.41/T-48.595*C1)
      KT(145) = 10. ** (607.642+0.121098*T-20011.25/T-236.4948*C1)
      KT(157) = 10. ** (-5.7 +1.68 *PH)
      KT(158) = 10. ** (-5.4 +1.52 *PH)
      KT(202) = 10. ** (-2.033+0.012645*T+429.01/T)
      KT(220) = 10. ** (2.497 -3833./T)
      KT(336) = 10. ** (226.374-18247.8/T-73.597*C1)
      KT(339) = 10. ** (1.447-0.004153*T-214949./(T*T))
      KT(395) = 10. ** (-0.26-731./T)
      KT(561) = 10. ** (-3.0938+0.013669*T)
      KT(562) = 10. ** (0.113+0.008721*T)
C
C     LISTE1
C
      DO 350 J = 1 , 41
      I = LISTE1(J)
      LOGKT(I) = DLOG10 (KT(I))
  350 CONTINUE
      RETURN
      END
      SUBROUTINE MAJEL(ALFA,DHA,GAMMA,KT,LOGKT,MI,Z)
C
      REAL*8 ALFA(0:377),DHA(0:377),GAMMA(0:377),LOGKT(0:653),
     *KT(0:653),LGAMMA,MI(0:377)
      INTEGER Z(0:377)
      INTEGER LISTE(0:377),LISTE1(15),LISTE2(18),LISTE3(34),LISTE4(19)
C
$INCLUDE:'COMMON.BLK'
C
```

```
      DATA LISTE1/6,17,63,68,88,259,260,263,264,265,266,267,268,269,270/
      DATA LISTE2/8,9,12,14,15,27,32,76,77,78,98,105,106,107,108,123,
     *288,289/
      DATA LISTE3/7,8,9,10,11,12,14,15,27,32,33,64,76,77,78,79,98,99,
     *105,106,107,108,122,123,179,180,247,248,288,289,308,309,310,315/
      DATA LISTE4/9,12,14,15,27,32,76,77,78,98,105,106,107,108,123,179,
     *180,288,289/
C
      DO 355 I = 0 , D
      LISTE(I) = 1
  355 CONTINUE
      LISTE(16) = 0
      LISTE(34) = 0
      LISTE(65) = 0
      LISTE(69) = 0
      LISTE(70) = 0
      LISTE(71) = 0
      LISTE(83) = 0
      LISTE(86) = 0
      LISTE(249)= 0
      LISTE(261)= 0
      LISTE(262)= 0
      LISTE(298)= 0
      LISTE(299)= 0
      LISTE(300)= 0
      LISTE(301)= 0
      LISTE(316)= 0
      LISTE(359)= 0
C
C**** CALC. OF TOTAL MOLALITY & AH2O */
C
      C1=0.0
      DO 360 I = 0 , D
      IF (LISTE(I).EQ.0) GOTO 360
      C1 = C1 + MI(I)
  360 CONTINUE
      AH2O = 1. - 1.7E-2 * C1
      IF (AH2O .LT. 0.0 ) GOTO 370
      LH2O = ALOG10(AH2O)
      GOTO 380
  370 LH2O = 0.0
  380 CONTINUE
C
C**** CALC. OF ACTIVITY COEFFICIENTS
C
      XMU = 0.0
      DO 390 I = 0 , D
      IF (LISTE(I) .EQ. 0) GOTO 390
      XMU = XMU + 0.5 *MI(I) *Z(I) *Z(I)
  390 CONTINUE
      XMUHL = SQRT(XMU)
      C1 = -A * 4. * XMUHL
      GAMMA(0) = 10. **(C1  /(1. + B * 5. * XMUHL) + 0.165 * XMU)
      GAMMA(1) = 10. **(C1  /(1. + B * 5.5 * XMUHL) + 0.2 * XMU)
      GAMMA(2) = 10. **(-A * XMUHL / (1. + B * 4. *XMUHL) +0.075 *XMU)
      GAMMA(3) = 10. **(-A * XMUHL / (1. + B * 3.5*
     *XMUHL) + 0.015 * XMU)
      GAMMA(4) = GAMMA(3)
      GAMMA(5) = 10.  ** (C1  /(1. + B * 5. * XMUHL) - 0.04 * XMU)
C
C**** DAVIES EQUATION FOR MOST ACTIVITY COEFFS.
C
      DO 400  I = 6 , D
      IF (Z(I) .NE. 0) GOTO 410
      LGAMMA = .1 * XMU
```

```
      IF(LGAMMA.LT.80) GAMMA(I) = 10.**LGAMMA
      GOTO 400
  410 LGAMMA = -A * Z(I) * Z(I) * (XMUHL / (1. + XMUHL) - 0.3 * XMU)
      IF(LGAMMA.LT.80) GAMMA(I) = 10.**LGAMMA
  400 CONTINUE
C
C**** DEBYE-HUCKEL EQN FOR POLYSULFIDE SPECIES(DHA FROM CLOKE,1963),
C****  CARBONATES, H+, AND Sr SPECIES
C
      DO 420 J = 1 , 15
      I = LISTE1(J)
      IF (DHA(I).GT. 0.0) GAMMA(I) = 10. ** (-A * Z(I) * Z(I) *
     *XMUHL / (1.0 + DHA(I) * B * XMUHL))
  420 CONTINUE
      GAMMA(85) = 10.**(XMU* (170.01/T -.8798 +.0013935*T)+
     * XMU * XMU* (28.81 / T - .2108 + .0003641 * T))
      GAMMA(87)= 10.  ** (C1  /(1. + B * 5.26 * XMUHL) + 0.121 * XMU)
      GAMMA(95)= 10. ** (-0.5 * XMU)
C
C**** CALC OF MINOR ANION ACTIVITIES */
C
      ALFA(84) = MI(84) * GAMMA(84)
      ALFA(96) = MI(96) * GAMMA(96)
      ALFA(97) = MI(97) * GAMMA(97)
      ALFA(202)= MI(202)* GAMMA(202)
      IF (ALFA(202)*ALFA(84) .LE. 0.0) GOTO 425
      PE(6) = (LOGKT(400) + DLOG10(ALFA(84))-DLOG10(ALFA(202))
     *-LH2O-2*PH)/2E0
      EH(6) = PE(6) * C*R*T/F
C
C**** CALC. OF PE & EHDO
C
  425 IF (DOX .LE. 0.0) GOTO 430
      PE(2)= -(DLOG10(KT(136))+ PH+ 0.5 *LH2O -0.25 * ALOG10(DOX/32E3))
      PE(3)= -(DLOG10(KT(151))+ PH+ 0.5 *LH2O -0.25 * ALOG10(DOX/32E3))
      EH(2) = PE(2) * C * R * T / F
      EH(3) = PE(3) * C * R * T / F
  430 CONTINUE
C
C**** ACTIVITIES OF OH & H+ SPECIES */
C
      ALFA(26) = AH2O * KW * TENPH
      MI(26) = ALFA(26) / GAMMA(26)
      ALFA(63) = 10**(-PH)
      MI(63) = 1. / (TENPH * GAMMA(63))
C
      IF (ITER .NE. 1) GOTO 560
C
C**** INITIAL CO2 SPECIES */
C
      IF (CORALK .EQ. 2) GOTO 460
      C1 = 2.0 * TENPH / (KT(68) * GAMMA(17))
      MI(6) = CO2TIT /(1.0 + GAMMA(6) * C1)
      ALFA(6) = MI(6) * GAMMA(6)
      C2 = KT(35) / (TENPH * GAMMA(85))
      MI(17) = C1 * ALFA(6) / 2.0
      MI(85) = C2 * ALFA(6)
      ALFA(17) = MI(17) * GAMMA(17)
      ALFA(85) = MI(85) * GAMMA(85)
      GOTO480
  460 MI(6)=CO2TIT/(1E0 + GAMMA(6)*((KT(35)/(TENPH*GAMMA(85)))+TENPH/
     *(KT(68)*GAMMA(17))))
      ALFA(6)=MI(6)*GAMMA(6)
      MI(17)=ALFA(6)*TENPH/(GAMMA(17)*KT(68))
      MI(85)=ALFA(6)*KT(35)/(TENPH*GAMMA(85))
```

```
      ALFA(17) = MI(17) * GAMMA(17)
      ALFA(85) = MI(85) * GAMMA(85)
C
C**** INITIAL SULFATE SPECIES */
C
  480 IF (SO4TOT .LE. 0.0) GOTO 490
      MI(62)=KT(89)/(TENPH*GAMMA(62))
      MI(5)=SO4TOT/(1E0 + GAMMA(5)*MI(62))
      C1 = MI(5) * GAMMA(5)
      ALFA(5) = C1
      MI(62)=C1 * MI(62)
      ALFA(62) = MI(62) * GAMMA(62)
C
C**** INITIAL FLUORIDE SPECIES */
C
  490 IF (FTOT .LE. 0.0) GOTO 500
      MI(125) = KT(202) / (TENPH * GAMMA(125))
      MI(126) = KT(203) * MI(61) * GAMMA(61) / (TENPH * GAMMA(126))
      MI(296) = KT(537) * MI(61) * GAMMA(61) / (TENPH**2 * GAMMA(296))
      MI(61)  = FTOT / (1 + GAMMA(61) * (MI(125) + MI(126) + MI(296)))
      ALFA(61) = MI(61) * GAMMA(61)
      C1 = MI(61) * GAMMA(61)
C
      MI(125) = C1 * MI(125)
      ALFA(125) = MI(125) * GAMMA(125)
      MI(126) = C1 * MI(126)
      ALFA(126) = MI(126)* GAMMA(126)
      MI(296) = C1 * MI(296)
      ALFA(296) = MI(296) * GAMMA(296)
C
C**** INITIAL PHOSPHATE SPECIES */
C
  500 IF (PTOT .LE. 0.0) GOTO 520
      MI(46) = KT(15) / (TENPH * GAMMA(46))
      MI(47) = KT(16) / (TENPH**2 * GAMMA(47))
      MI(44) = PTOT/(1E0 + GAMMA(44) * (MI(46) + MI(47)))
      ALFA(44) = MI(44) * GAMMA(44)
      C1 =  MI(44) * GAMMA(44)
      DO 510 I = 46 , 47
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  510 CONTINUE
C
C**** INITIAL CHLORIDE */
C
  520 ALFA(4) = MI(4) * GAMMA(4)
C
C**** INITIAL SULFIDE SPECIES */
C
      IF (H2STOT .LE. 0.0) GOTO 540
      MI(13) = 1 / (KT(91) * TENPH * GAMMA(13))
      MI(67) = KT(92) * TENPH / GAMMA(67)
      MI(263) = KT(502) * TENPH / GAMMA(263)
      MI(264) = KT(503) * TENPH / GAMMA(264)
      MI(265) = KT(504) * TENPH / GAMMA(265)
      MI(266) = KT(505) * TENPH / GAMMA(266)
      MI(267) = KT(506) * TENPH / GAMMA(267)
      MI(66) = H2STOT / (1.0 + GAMMA(66) * (MI(13) + MI(67) + MI(263)
     *+ MI(264) + MI(265) + MI(266) + MI(267)))
      C1 = MI(66) * GAMMA(66)
      ALFA(66) = C1
      MI(13) = C1 * MI(13)
      ALFA(13) = MI(13) * GAMMA(13)
      MI(67) = C1 * MI(67)
      ALFA(67) = MI(67) * GAMMA(67)
```

```
      DO 530 I= 263 , 267
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  530 CONTINUE
      IF (ALFA(5)*ALFA(13) .LE. 0.0) GOTO 535
      PE(5) = 0.125 * LOGKT(90)+0.125 * DLOG10(ALFA(5))-1.25*PH
     *-0.125 * DLOG10(ALFA(13))-0.5*LH2O
      EH(5) = PE(5)* C*R*T / F
  535 IF (ALFA(13) .LE. 0.0) GOTO 540
      PE(7) = (LOGKT(538)-DLOG10(ALFA(13)))/2E0-PH
      EH(7) = PE(7) * C*R*T/F
C
C**** INITIAL ORGANIC LIGANDS */
C
  540 IF (FULVTT .LE. 0.0) GOTO 550
      MI(286) = KT(523) / (TENPH * GAMMA(286))
      MI(284) = FULVTT / (1 + GAMMA(284) * MI(286))
      C1=MI(284) * GAMMA(284)
      ALFA(284) = C1
      MI(286) = C1 * MI(286)
      ALFA(286) = MI(286) * GAMMA(286)
C
  550 IF (HUMTOT .LE. 0.0) GOTO 580
      MI(287)=KT(524)/(TENPH*GAMMA(287))
      MI(285)=HUMTOT/(1 + GAMMA(285)*MI(287))
      C1 = MI(285) * GAMMA(285)
      ALFA(285) = C1
      MI(287) = C1 * MI(287)
      ALFA(287) = MI(287) * GAMMA(287)
      GOTO 580
  560 ALFA(4) = MI(4) * GAMMA(4)
      ALFA(5) = MI(5) * GAMMA(5)
      ALFA(6) = MI(6) * GAMMA(6)
      ALFA(17) = MI(17) * GAMMA(17)
      ALFA(44) = MI(44) * GAMMA(44)
      ALFA(46) = MI(46) * GAMMA(46)
      ALFA(47) = MI(47) * GAMMA(47)
      ALFA(61) = MI(61) * GAMMA(61)
      ALFA(66) = MI(66) * GAMMA(66)
      ALFA(284) = MI(284) * GAMMA(284)
      ALFA(285) = MI(285) * GAMMA(285)
C
C**** SILICA SPECIES */
C
  580 C1 = KT(13) * TENPH   /  GAMMA(24)
      C2 = KT(14) * TENPH**2 / GAMMA(25)
      C3 = KT(201) * ALFA(61)**6 / (GAMMA(124) * TENPH**4 * AH2O**4)
      C4=0
      IF (ITER.GT.1) THEN
        IF (ALFA(318).GT.1D-78) C4=KT(631)*ALFA(318)*TENPH/GAMMA(358)
      END IF
      MI(23) = SITOT / (1E0 + GAMMA(23) * (C1 + C2 + C3 + C4))
      ALFA(23) = MI(23) * GAMMA(23)
      MI(24) = ALFA(23) * C1
      MI(25) = ALFA(23) * C2
      MI(124) = ALFA(23) * C3
      MI(358) = ALFA(23) * C4
      ALFA(24) = MI(24) * GAMMA(24)
      ALFA(25) = MI(25) * GAMMA(25)
      ALFA(124)=MI(124)*GAMMA(124)
      ALFA(358)=MI(358)*GAMMA(358)
C
C**** BORON SPECIES */
C
      IF (BTOT .LE. 0.0) GOTO 600
```

```
      MI(36) = KT(25) * TENPH / GAMMA(36)
      MI(101)= KT(161)* ALFA(61) / GAMMA(101)
      MI(102)= KT(162)* ALFA(61)**2 / (GAMMA(102) * AH2O * TENPH)
      MI(103)= KT(163)* ALFA(61)**3 / (GAMMA(103) * (AH2O * TENPH)**2)
      MI(104)= KT(164)* ALFA(61)**4 / (GAMMA(104) * (AH2O * TENPH)**3)
      MI(35) = BTOT / (1+GAMMA(35) * (MI(36) + MI(101) + MI(102)+
     *MI(103) + MI(104)))
      C1 = MI(35) * GAMMA(35)
      ALFA(35) = C1
      MI(36) = C1 * MI(36)
      ALFA(36) = MI(36) * GAMMA(36)
      DO 590 I = 101 , 104
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  590 CONTINUE
C
C**** NITROGEN SPECIES */
C
  600 C1 = TENPH * KT(26) / GAMMA(37)
      C2 = ALFA(5) * KT(131) / GAMMA(91)
      MI(38) = NH4TOT / (1.0 + GAMMA(38) * (C1 + C2))
      ALFA(38) = MI(38) * GAMMA(38)
      MI(37) = ALFA(38) * C1
      ALFA(37) = MI(37) * GAMMA(37)
      MI(91) = ALFA(38) * C2
      ALFA(91) = MI(91) * GAMMA(91)
      IF (ALFA(38)*ALFA(84) .LE. 0.0) GOTO 605
      PE(4)=(-LOGKT(127)+DLOG10(ALFA(84))- 10.0 * PH - DLOG10(ALFA(38))
     *-3E0*LH2O)/8E0
      EH(4) = PE(4)* C*R*T / F
C
C**** MG SPECIES */
C
  605 MI(18) = AH2O*TENPH * KT(24) / GAMMA(18)
      MI(19) = ALFA(61) * KT(22) / GAMMA(19)
      MI(20) = ALFA(17) * KT(73) / GAMMA(20)
      MI(21) = ALFA(6)  * KT(74) / GAMMA(21)
      MI(22) = ALFA(5)  * KT(75) / GAMMA(22)
      MI(39) = ALFA(44) * KT(123) / GAMMA(39)
      MI(40) = ALFA(47) * KT(124) / GAMMA(40)
      MI(72) = ALFA(46) * KT(33) / GAMMA(72)
      MI(1) = MGTOT / (1.0 + GAMMA(1) * (MI(18) + MI(19) + MI(20)+
     *MI(21) + MI(22) + MI(39) + MI(40) + MI(72)))
      C1 = MI(1) * GAMMA(1)
      ALFA(1) = C1
      DO 610 I = 18 , 22
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  610 CONTINUE
      MI(39) = C1 * MI(39)
      ALFA(39) = MI(39) * GAMMA(39)
      MI(40) = C1 * MI(40)
      ALFA(40) = MI(40) * GAMMA(40)
      MI(72) = C1 * MI(72)
      ALFA(72) = MI(72) * GAMMA(72)
C
C**** CA SPECIES */
C
      MI(28)  = AH2O*TENPH * KT(76)/ GAMMA(28)
      MI(29)  = ALFA(6)  * KT(77)  / GAMMA(29)
      MI(30)  = ALFA(17) * KT(78)  / GAMMA(30)
      MI(31)  = ALFA(5)  * KT(23)  / GAMMA(31)
      MI(73)  = ALFA(46) * KT(34)  / GAMMA(73)
      MI(74)  = ALFA(44) * KT(121) / GAMMA(74)
      MI(75)  = ALFA(47) * KT(122) / GAMMA(75)
```

```
      MI(81)  = ALFA(62) * KT(168) / GAMMA(81)
      MI(100) = ALFA(61) * KT(160) / GAMMA(100)
      MI(0) = CATOT / (1.0 + GAMMA(0) * (MI(28) +MI(29) +MI(30)+
     * MI(31) +MI(73) +MI(74) +MI(75) +MI(81) +MI(100)))
      C1=MI(0)*GAMMA(0)
      ALFA(0) = C1
      MI(28) = C1 * MI(28)
      ALFA(28) = MI(28) * GAMMA(28)
      MI(29) = C1 * MI(29)
      ALFA(29) = MI(29) * GAMMA(29)
      MI(30) = C1 * MI(30)
      ALFA(30) = MI(30) * GAMMA(30)
      MI(31) = C1 * MI(31)
      ALFA(31) = MI(31) * GAMMA(31)
      MI(73) = C1 * MI(73)
      ALFA(73) = MI(73) * GAMMA(73)
      MI(74) = C1 * MI(74)
      ALFA(74) = MI(74) * GAMMA(74)
      MI(75) = C1 * MI(75)
      ALFA(75) = MI(75) * GAMMA(75)
      MI(81) = C1 * MI(81)
      ALFA(81) = MI(81) * GAMMA(81)
      MI(100)= C1 * MI(100)
      ALFA(100)= MI(100)* GAMMA(100)
C
C**** NA SPECIES */
C
      MI(41) = ALFA(17) * KT(69) / GAMMA(41)
      MI(42) = ALFA(6)  * KT(70) / GAMMA(42)
      MI(43) = ALFA(5)  * KT(71) / GAMMA(43)
      MI(49) = ALFA(46) * KT(30) / GAMMA(49)
      MI(297) = ALFA(61)* KT(540)/ GAMMA(297)
      MI(2) = NATOT /(1.0 +GAMMA(2) *(MI(41)+MI(42)+MI(43)+MI(49)
     *        +MI(297)))
      C1 = MI(2) * GAMMA(2)
      ALFA(2) = C1
      MI(41) = C1 * MI(41)
      ALFA(41) = MI(41) * GAMMA(41)
      MI(42) = C1 * MI(42)
      ALFA(42) = MI(42) * GAMMA(42)
      MI(43) = C1 * MI(43)
      ALFA(43) = MI(43) * GAMMA(43)
      MI(49) = C1 * MI(49)
      ALFA(49) = MI(49) * GAMMA(49)
      MI(297)= C1 * MI(297)
      ALFA(297)= MI(297)* GAMMA(297)
C
C**** K SPECIES */
C
      MI(45) = ALFA(5)  * KT(72) / GAMMA(45)
      MI(60) = ALFA(46) * KT(32) / GAMMA(60)
      MI(3) = KTOT /(1.0 +GAMMA(3) * (MI(45) + MI(60)))
      C1 = MI(3) * GAMMA(3)
      ALFA(3) = C1
      MI(45) = C1 * MI(45)
      ALFA(45) = MI(45) * GAMMA(45)
      MI(60) = C1 * MI(60)
      ALFA(60) = MI(60) * GAMMA(60)
C
C**** AL SPECIES */
C
      IF (ALTOT .LE. 0.0) GOTO 630
      MI(51)=AH2O*TENPH*KT(80)/GAMMA(51)
      MI(52)=(AH2O*TENPH)**2*KT(81)/GAMMA(52)
      MI(53)=(AH2O*TENPH)**4*KT(82)/GAMMA(53)
```

```
      MI(54)=ALFA(61)*KT(83)/GAMMA(54)
      MI(55)=ALFA(61)**2*KT(84)/GAMMA(55)
      MI(56)=ALFA(61)**3*KT(85)/GAMMA(56)
      MI(57)=ALFA(61)**4*KT(86)/GAMMA(57)
      MI(58)=ALFA(5)*KT(87)/GAMMA(58)
      MI(59)=ALFA(5)**2*KT(88)/GAMMA(59)
      MI(181)=KT(336)*(AH2O*TENPH)**3/GAMMA(181)
      MI(203)=ALFA(62)*KT(397)/GAMMA(203)
      MI(50)=ALTOT/(1E0+GAMMA(50)*(MI(51)+MI(52)+MI(53)+MI(54)+MI(55)
     *+MI(56)+MI(57)+MI(58)+MI(59)+MI(181)+MI(203)))
      C1 = MI(50) * GAMMA(50)
      ALFA(50) = C1
      DO 620 I = 51 , 59
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  620 CONTINUE
      MI(181) = C1 * MI(181)
      ALFA(181) = MI(181) * GAMMA(181)
      MI(203) = C1 * MI(203)
      ALFA(203) = MI(203) * GAMMA(203)
      GOTO 650
  630 DO 640 I = 51 , 59
      MI(I) = 0.0
  640 CONTINUE
      MI(181) = 0.0
      MI(203) = 0.0
C
C**** FE SPECIES */
C
  650 IF( FE2TOT + FE3TOT .GT. 0.0) GOTO 660
      IF( EH(EHOPT(1)) .LT. 9.9 .AND. FETOTL .GT. 0.0)GOTO 660
      GOTO 730
C
C**** FE +2 SPECIES */
C
  660 MI(10)  = KT(2)   * AH2O*TENPH          / GAMMA(10)
      MI(11)  = KT(3)   * AH2O**3 * TENPH**3  / GAMMA(11)
      MI(33)  = KT(8)   * ALFA(5)             / GAMMA(33)
      MI(64)  = KT(120) * ALFA(47)            / GAMMA(64)
      MI(79)  = KT(105) * (AH2O*TENPH)**2     / GAMMA(79)
      MI(99)  = KT(138) * ALFA(46)            / GAMMA(99)
      MI(122) = KT(148) * ALFA(62)            / GAMMA(122)
      MI(247) = KT(476) * ALFA(66)**2         / GAMMA(247)
      MI(248) = KT(477) * ALFA(66)**3         / GAMMA(248)
      MI(308) = KT(359) * ALFA(61)            / GAMMA(308)
      MI(309) = KT(558) * ALFA(6)             / GAMMA(309)
      MI(310) = KT(559) * ALFA(17)            / GAMMA(310)
      MI(315) = KT(542) * ALFA(4)             / GAMMA(315)
C
C**** FE +3 SPECIES */
C
      MI(9)   = KT(1)  * AH2O*TENPH     / GAMMA(9)
      MI(12)  = KT(139)* ALFA(46)       / GAMMA(12)
      MI(14)  = KT(4)  * ALFA(5)        / GAMMA(14)
      MI(15)  = KT(5)  * ALFA(4)        / GAMMA(15)
      MI(27)  = KT(6)  * ALFA(4)**2     / GAMMA(27)
      MI(32)  = KT(7)  * ALFA(4)**3     / GAMMA(32)
      MI(76)  = KT(102)*(AH2O*TENPH)**2/ GAMMA(76)
      MI(77)  = KT(103)*(AH2O*TENPH)**3/ GAMMA(77)
      MI(78)  = KT(104)*(AH2O*TENPH)**4/ GAMMA(78)
      MI(98)  = KT(156)     * ALFA(47)  / GAMMA(98)
      MI(105) = ALFA(61)    * KT(165)   / GAMMA(105)
      MI(106) = ALFA(61)**2 * KT(166)   / GAMMA(106)
      MI(107) = ALFA(61)**3 * KT(167)   / GAMMA(107)
      MI(108) = KT(333)* ALFA(5)**2     / GAMMA(108)
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      MI(123) = KT(159)* ALFA(62)      / GAMMA(123)
      MI(179) = KT(334)*(AH2O*TENPH)**2 *MI(8)*GAMMA(8) / GAMMA(179)
      MI(180) = KT(335)*(AH2O*TENPH)**4 *(MI(8)*GAMMA(8))**2 /GAMMA(180)
      MI(288) = KT(525)     * ALFA(284) / GAMMA(288)
      MI(289) = KT(526)     * ALFA(285) / GAMMA(289)
C
      IF (FE2TOT + FE3TOT .LE. 0.0) GOTO 680
C
C****  SPLIT IRON      FE +2 SPECIES
C
      MI(7) = FE2TOT / (1.+ GAMMA(7) * (MI(10) + MI(11) + MI(33) +
     *MI(64) + MI(79) + MI(99) + MI(122) + MI(247) + MI(248) + MI(308) +
     *MI(309) + MI(310) + MI(315)))
      C1 = MI(7) * GAMMA(7)
      ALFA(7) = C1
C
      MI(10) = C1 * MI(10)
      MI(11) = C1 * MI(11)
      MI(33) = C1 * MI(33)
      MI(64) = C1 * MI(64)
      MI(79) = C1 * MI(79)
      MI(99) = C1 * MI(99)
      MI(122)= C1 * MI(122)
      MI(247)= C1 * MI(247)
      MI(248)= C1 * MI(248)
      MI(308)= C1 * MI(308)
      MI(309)= C1 * MI(309)
      MI(310)= C1 * MI(310)
      MI(315)= C1 * MI(315)
C
C****  SPLIT IRON       FE +3 SPECIES
C
      MI(8) = FE3TOT / (1.+ GAMMA(8) * (MI(9) +MI(12) +MI(14) +MI(15)
     *+MI(27) + MI(32)  + MI(76)  + MI(77) + MI(78) + MI(98) + MI(105)+
     *MI(106) + MI(107) + MI(108) + MI(123) + 2 *MI(179) + 3 *MI(180)+
     *MI(288) + MI(289)))
      C1 = MI(8) * GAMMA(8)
      ALFA(8) = C1
C
      DO 670 J = 1 , 19
      I = LISTE4(J)
      MI(I) = C1 * MI(I)
  670 CONTINUE
      GOTO 710
C
  680 MI(8) = 1.0 / GAMMA(8)
      C1 = KT(0) / 10.**(-PE(EHOPT(1)))
C
      DO 690 J = 1 ,18
      I = LISTE2(J)
      MI(I) = C1 * MI(I)
  690 CONTINUE
      MI(179)=KT(334)*C1**2*(AH2O*TENPH)**2*MI(7)*GAMMA(7)
     */GAMMA(179)
      MI(180)=KT(335)*C1**3*(AH2O*TENPH)**4*(MI(7)*GAMMA(7))**2
     */GAMMA(180)
      MI(7)=FETOTL/(1.0+GAMMA(7)*(MI(8)+MI(9)+MI(10)+MI(11)+MI(12)+
     *MI(14)+MI(15)+MI(27)+MI(32)+MI(33)+MI(64)+MI(76)+MI(77)+
     *MI(78)+MI(79)+MI(98)+MI(99)+MI(105)+MI(106)+MI(107)+
     *MI(108)+MI(122)+MI(123)+2*MI(179)+3*MI(180)+MI(247)+MI(248)+
     *MI(288)+MI(289)+MI(308)+MI(309)+MI(310)))
      C1 = MI(7) * GAMMA(7)
      ALFA(7) = C1
C
      DO 700 J = 2 ,34
```

```
      I =LISTE3(J)
      MI(I)=C1*MI(I)
  700 CONTINUE
      ALFA(8)=MI(8)*GAMMA(8)
  710 CONTINUE
C
      DO 720 J = 3 , 34
      I = LISTE3(J)
      ALFA(I)=MI(I)*GAMMA(I)
  720 CONTINUE
      GOTO 745
C
  730 DO 740 J = 1 , 34
      I = LISTE3(J)
      MI(I) = 0.0
  740 CONTINUE
  745 IF (ALFA(7) * ALFA(8) .LE. 0.0) GOTO 750
      PE(1) = -DLOG10(KT(0) * ALFA(7) / ALFA(8))
      EH(1) = PE(1) * C*R*T/F
  750 CONTINUE
C
C**** LI, SR, BA, CS, RB SPECIES */
C
      C2 = KT(126) * ALFA(5)/GAMMA(82)
      MI(80) = LITOT/(1E0+GAMMA(80)*C2)
      ALFA(80) = MI(80)*GAMMA(80)
      MI(82)=C2 * ALFA(80)
      C1=KT(129) * AH2O*TENPH/GAMMA(88)
      C2=KT(79) * ALFA(6)/GAMMA(68)
      C3=KT(135)* ALFA(17)/GAMMA(95)
      C4=KT(563)*ALFA(5)/GAMMA(314)
      MI(87) = SRTOT/(1E0+GAMMA(87)*(C1+C2+C3+C4))
      MI(88) = GAMMA(87)*MI(87)*C1
      MI(68) = GAMMA(87)*MI(87)*C2
      MI(95) = GAMMA(87)*MI(87)*C3
      MI(314)= GAMMA(87)*MI(87)*C4
      C1=KT(130)*AH2O*TENPH/GAMMA(90)
      C2=KT(543)*ALFA(5)/GAMMA(201)
      C3=KT(561)*ALFA(6)/GAMMA(312)
      C4=KT(562)*ALFA(17)/GAMMA(313)
      MI(89)=BATOT/(1E0+GAMMA(89)*(C1+C2+C3+C4))
      ALFA(89)=MI(89)*GAMMA(89)
      MI(90)=ALFA(89)*C1
      MI(201)=ALFA(89)*C2
      MI(312)=ALFA(89)*C3
      MI(313)=ALFA(89)*C4
      ALFA(48) = MI(48) * GAMMA(48)
      ALFA(68) = MI(68) * GAMMA(68)
      ALFA(82) = MI(82) * GAMMA(82)
      ALFA(87) = MI(87) * GAMMA(87)
      ALFA(88) = MI(88) * GAMMA(88)
      ALFA(90) = MI(90) * GAMMA(90)
      ALFA(94) = MI(94) * GAMMA(94)
      ALFA(95) = MI(95) * GAMMA(95)
      ALFA(201)= MI(201)* GAMMA(201)
      ALFA(312)= MI(312)* GAMMA(312)
      ALFA(313)= MI(313)* GAMMA(313)
      ALFA(314)= MI(314)* GAMMA(314)
      RETURN
      END
      SUBROUTINE TREL(ALFA,GAMMA,KT,LOGKT,MI)
C
      REAL*8 ALFA(0:377),GAMMA(0:377),KT(0:653),LOGKT(0:653),MI(0:377)
      INTEGER LISTE1(23),LISTE2(22),LISTE3(28),LISTE4(27),LISTE5(13),
     *LISTE6(25)
```

```
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE1/130,127,128,129,131,132,133,134,135,136,137,138,139
     *,140,141,142,143,144,259,260,271,290,291/
      DATA LISTE2/145,146,147,148,149,150,151,152,153,154,155,156,157
     *,158,159,229,230,231,232,272,273,274/
      DATA LISTE3/160,161,162,163,164,165,166,167,168,169,170,171,172
     *,173,174,175,176,177,178,233,234,235,236,275,276,277,292,293/
      DATA LISTE4/182,183,184,185,186,187,188,189,190,191,192,193,194
     *,195,196,197,198,199,200,237,238,239,240,241,242,243,278/
      DATA LISTE5/204,205,206,207,208,209,210,211,279,280,281,282,283/
      DATA LISTE6/212,213,214,215,216,217,218,219,220,221,222,223,224
     *,225,226,227,228,244,245,246,268,269,270,294,295/
C
C**** MN SPECIES */
C
      IF(MNTOT .LE. 0.0) GOTO 30
C
C**** MN +2 SPECIES */
C
      MI(111)=KT(170)*ALFA(4)/GAMMA(111)
      MI(112)=KT(171)*ALFA(4)**2/GAMMA(112)
      MI(113)=KT(172)*ALFA(4)**3/GAMMA(113)
      MI(114)=KT(173)*AH2O*TENPH/GAMMA(114)
      MI(115)=KT(174)*(AH2O*TENPH)**3/GAMMA(115)
      MI(116)=KT(175)*ALFA(61)/GAMMA(116)
      MI(117)=KT(176)*ALFA(5)/GAMMA(117)
      MI(118)=KT(177)*ALFA(84)**2/GAMMA(118)
      MI(119)=KT(178)*ALFA(6)/GAMMA(119)
      MI(311)=KT(560)*ALFA(17)/GAMMA(311)
C
      IF (EH(EHOPT(2)) .GE. 9.9) GOTO 10
C
C**** MN +3, +6, +7 SPECIES */
C
      C1=10.**(-PE(EHOPT(2)))
      MI(110) = KT(169)/(GAMMA(110)*C1)
      XMI120 = LOGKT(179) +4. *LH2O-(DLOG10(GAMMA(120)) -8.*PH -5.*
     *PE(EHOPT(2)))
      IF (XMI120 .GT. -70.) MI(120)= 10**XMI120
      IF (XMI120 .LE. -70.) MI(120)= 0.0
      XMI121 = LOGKT(180)+ 4. * LH2O- (DLOG10(GAMMA(121)) -8.*PH -4.*
     *PE(EHOPT(2)))
      IF (XMI121 .GT. -70.) MI(121)=10**XMI121
      IF (XMI121 .LE. -70.) MI(121) = 0.0
   10 CONTINUE
      MI(109)=MNTOT/(1.+GAMMA(109)*(MI(110)+MI(111)+MI(112)+MI(113)+
     *MI(114)+MI(115)+MI(116)+MI(117)+MI(118)+MI(119)+MI(120)
     *+MI(121)+MI(311)))
      C1 = MI(109) * GAMMA(109)
      ALFA(109) = C1
      DO 20  I = 110 , 121
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
   20 CONTINUE
      MI(311) = C1 * MI(311)
      ALFA(311) = MI(311) * GAMMA(311)
      GOTO 50
   30 DO 40 I = 109 , 121
      MI(I) = 0.0
   40 CONTINUE
      MI(311) = 0.0
C
C**** CU SPECIES */
```

```
C
   50 IF (CUTOT .LE. 0.0) GOTO 80
      IF (EH(EHOPT(3)) .GE. 9.9)  GOTO 60
C
C**** CU +1 SPECIES */
C
      C1=10.**(-PE(EHOPT(3)))
      MI(127) = KT(208) * C1 / GAMMA(127)
      MI(128) =KT(206) * ALFA(4)**2 * C1 / GAMMA(128)
      MI(129) =KT(207) * ALFA(4)**3 * C1 / GAMMA(129)
      MI(259) =KT(485) * (ALFA(66) * TENPH)**2 * C1 / GAMMA(259)
      MI(260) =KT(486) * (ALFA(66) * TENPH)**2 * C1 / GAMMA(260)
   60 CONTINUE
C
C**** CU +2 SPECIES */
C
      MI(131)=KT(209)*ALFA(17)/GAMMA(131)
      MI(132)=KT(210)*ALFA(17)**2/GAMMA(132)
      MI(133)=KT(211)*ALFA(4)/GAMMA(133)
      MI(134)=KT(212)*ALFA(4)**2/GAMMA(134)
      MI(135)=KT(213)*ALFA(4)**3/GAMMA(135)
      MI(136)=KT(214)*ALFA(4)**4/GAMMA(136)
      MI(137)=KT(215)*ALFA(61)/GAMMA(137)
      MI(138)=KT(216)*AH2O*TENPH/GAMMA(138)
      MI(139)=KT(217)*(AH2O*TENPH)**2/GAMMA(139)
      MI(140)=KT(218)*(AH2O*TENPH)**3/GAMMA(140)
      MI(141)=KT(219)*(AH2O*TENPH)**4/GAMMA(141)
      MI(142)=KT(220)*MI(130)*GAMMA(130)*(AH2O*TENPH)**2/GAMMA(142)
      MI(143)=KT(221)*ALFA(5)/GAMMA(143)
      MI(144)=KT(222)*ALFA(66)**3/GAMMA(144)
      MI(271)=KT(510)*ALFA(6)/GAMMA(271)
      MI(290)=KT(527)*ALFA(284)/GAMMA(290)
      MI(291)=KT(528)*ALFA(285)/GAMMA(291)
C
      MI(130)=CUTOT/(1.+GAMMA(130)*(MI(127)+MI(128)+MI(129)+MI(131)
     *+MI(132)+MI(133)+MI(134)+MI(135)+MI(136)+MI(137)
     *+MI(138)+MI(139)+MI(140)+MI(141)+2.*MI(142)+MI(143)
     *+MI(144)+MI(259)+MI(260)+MI(271)+MI(290)+MI(291)))
      C1 = MI(130) * GAMMA(130)
      ALFA(130) = C1
C
      DO 70 J = 2 , 23
      I = LISTE1(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
   70 CONTINUE
      GOTO 100
C
   80 DO 90 J = 1 , 23
      I = LISTE1(J)
      MI(I) = 0.0
   90 CONTINUE
C
C**** ZN SPECIES */
C
  100 IF (ZNTOT .LE. 0.0) GOTO 120
      MI(146)=KT(251)*ALFA(4)/GAMMA(146)
      MI(147)=KT(252)*ALFA(4)**2/GAMMA(147)
      MI(148)=KT(253)*ALFA(4)**3/GAMMA(148)
      MI(149)=KT(254)*ALFA(4)**4/GAMMA(149)
      MI(150)=KT(255)*ALFA(61)/GAMMA(150)
      MI(151)=KT(256)*AH2O*TENPH/GAMMA(151)
      MI(152)=KT(257)*(AH2O*TENPH)**2/GAMMA(152)
      MI(153)=KT(258)*(AH2O*TENPH)**3/GAMMA(153)
      MI(154)=KT(259)*(AH2O*TENPH)**4/GAMMA(154)
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      MI(155)=KT(260)*AH2O*TENPH*ALFA(4)/GAMMA(155)
      MI(156)=KT(261)*ALFA(66)**2/GAMMA(156)
      MI(157)=KT(262)*ALFA(66)**3/GAMMA(157)
      MI(158)=KT(263)*ALFA(5)/GAMMA(158)
      MI(159)=KT(264)*ALFA(5)**2/GAMMA(159)
      MI(229)=KT(447)*ALFA(97)/GAMMA(229)
      MI(230)=KT(448)*ALFA(97)**2/GAMMA(230)
      MI(231)=KT(449)*ALFA(96)/GAMMA(231)
      MI(232)=KT(450)*ALFA(96)**2/GAMMA(232)
      MI(272)=KT(511)*ALFA(6)/GAMMA(272)
      MI(273)=KT(512)*ALFA(17)/GAMMA(273)
      MI(274)=KT(513)*ALFA(17)**2/GAMMA(274)
      MI(145)=ZNTOT/(1+GAMMA(145)*(MI(146)+MI(147)+MI(148)+MI(149)+
C
     *MI(150)+MI(151)+MI(152)+MI(153)+MI(154)+MI(155)+MI(156)
     *+MI(157)+MI(158)+MI(159)+MI(229)+MI(230)+MI(231)
     *+MI(232)+MI(272)+MI(273)+MI(274)))
      C1 = MI(145) * GAMMA(145)
      ALFA(145)= C1
C
      DO 110 J = 2 , 22
      I = LISTE2(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  110 CONTINUE
      GOTO 140
C
  120 DO 130 J = 1 , 22
      I = LISTE2(J)
      MI(I) = 0.0
  130 CONTINUE
C
C**** CD SPECIES */
C
  140 IF (CDTOT .LE. 0.0) GOTO 175
      MI(161)=KT(294)*ALFA(4)/GAMMA(161)
      MI(162)=KT(295)*ALFA(4)**2/GAMMA(162)
      MI(163)=KT(296)*ALFA(4)**3/GAMMA(163)
      MI(164)=KT(297)*ALFA(61)/GAMMA(164)
      MI(165)=KT(298)*ALFA(61)**2/GAMMA(165)
      MI(166)=KT(299)*ALFA(17)**2/GAMMA(166)
      MI(167)=KT(300)*AH2O*TENPH/GAMMA(167)
      MI(168)=KT(301)*(AH2O*TENPH)**2/GAMMA(168)
      MI(169)=KT(302)*(AH2O*TENPH)**3/GAMMA(169)
      MI(170)=KT(303)*(AH2O*TENPH)**4/GAMMA(170)
      MI(171)=KT(304)*MI(160)*GAMMA(160)*AH2O*TENPH/GAMMA(171)
      MI(172)=KT(305)*AH2O*TENPH*ALFA(4)/GAMMA(172)
      MI(173)=KT(306)*ALFA(84)/GAMMA(173)
      MI(174)=KT(307)*ALFA(5)/GAMMA(174)
      MI(175)=KT(308)*ALFA(66)/GAMMA(175)
      MI(176)=KT(309)*ALFA(66)**2/GAMMA(176)
      MI(177)=KT(310)*ALFA(66)**3/GAMMA(177)
C
      IF (ALFA(66) .LE. 0.0) GOTO 150
      XMI178 = LOGKT(311) + 4E0 * DLOG10(ALFA(66)) - DLOG10(GAMMA(178))
      IF (XMI178 .GT. -70) MI(178) = 10**XMI178
      GOTO 160
  150 MI(178) = 0.0
  160 MI(233)=KT(451)*ALFA(97)/GAMMA(233)
      MI(234)=KT(452)*ALFA(97)**2/GAMMA(234)
      MI(235)=KT(453)*ALFA(96)/GAMMA(235)
      MI(236)=KT(454)*ALFA(96)**2/GAMMA(236)
      MI(275)=KT(514)*ALFA(6)/GAMMA(275)
      MI(276)=KT(515)*ALFA(17)/GAMMA(276)
      MI(277)=KT(516)*ALFA(5)**2/GAMMA(277)
```

```
      MI(292)=KT(529)*ALFA(284)/GAMMA(292)
      MI(293)=KT(530)*ALFA(285)/GAMMA(293)
C
      MI(160)=CDTOT/(1+GAMMA(160)*(MI(161)+MI(162)+MI(163)+MI(164)+
     *MI(165)+MI(166)+MI(167)+MI(168)+MI(169)+MI(170)+2*MI(171)
     *+MI(172)+MI(173)+MI(174)+MI(175)+MI(176)+MI(177)+
     *MI(178)+MI(233)+MI(234)+MI(235)+MI(236)+MI(275)+MI(276)+
     *MI(277)+MI(292)+MI(293)))
      C1=MI(160)*GAMMA(160)
      ALFA(160) = C1
C
      DO 170J = 2 , 28
      I = LISTE3(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  170 CONTINUE
      GOTO 190
C
  175 DO 180 J = 1 , 28
      I = LISTE3(J)
      MI(I) = 0.0
  180 CONTINUE
C
C**** PB SPECIES */
C
  190 IF (PBTOT .LE. 0.0) GOTO 210
      MI(183)=KT(341)*ALFA(4)/GAMMA(183)
      MI(184)=KT(342)*ALFA(4)**2/GAMMA(184)
      MI(185)=KT(343)*ALFA(4)**3/GAMMA(185)
      MI(186)=KT(344)*ALFA(4)**4/GAMMA(186)
      MI(187)=KT(345)*ALFA(17)**2/GAMMA(187)
      MI(188)=KT(346)*ALFA(61)/GAMMA(188)
      MI(189)=KT(347)*ALFA(61)**2/GAMMA(189)
      MI(190)=KT(348)*ALFA(61)**3/GAMMA(190)
      MI(191)=KT(349)*ALFA(61)**4/GAMMA(191)
      MI(192)=KT(350)*AH2O*TENPH/GAMMA(192)
      MI(193)=KT(351)*(AH2O*TENPH)**2/GAMMA(193)
      MI(194)=KT(352)*(AH2O*TENPH)**3/GAMMA(194)
      MI(195)=KT(353)*AH2O*TENPH*MI(182)*GAMMA(182)/GAMMA(195)
      MI(196)=KT(354)*ALFA(84)/GAMMA(196)
      MI(197)=KT(355)*ALFA(5)/GAMMA(197)
      MI(198)=KT(356)*ALFA(66)**2/GAMMA(198)
      MI(199)=KT(357)*ALFA(66)**3/GAMMA(199)
      MI(200)=KT(358)*(MI(182)*GAMMA(182))**2*(AH2O*TENPH)**4/GAMMA(200)
      MI(237)=KT(455)*ALFA(97)/GAMMA(237)
      MI(238)=KT(456)*ALFA(97)**2/GAMMA(238)
      MI(239)=KT(457)*ALFA(96)/GAMMA(239)
      MI(240)=KT(458)*ALFA(96)**2/GAMMA(240)
      MI(241)=KT(468)*ALFA(17)/GAMMA(241)
      MI(242)=KT(469)*(AH2O*TENPH)**4/GAMMA(242)
      MI(243)=KT(470)*ALFA(5)**2/GAMMA(243)
      MI(278)=KT(517)*ALFA(6)/GAMMA(278)
C
      MI(182)=PBTOT/(1+GAMMA(182)*(MI(183)+MI(184)+MI(185)+MI(186)+
     *MI(187)+MI(188)+MI(189)+MI(190)+MI(191)+MI(192)+MI(193)+
     *MI(194)+2*MI(195)+MI(196)+MI(197)+MI(198)+MI(199)+3*MI(200)+
     *MI(237)+MI(238)+MI(239)+MI(240)+MI(241)+MI(242)+
     *MI(243)+MI(278)))
      C1 = MI(182) * GAMMA(182)
      ALFA(182) = C1
C
      DO 200 J = 2 , 27
      I = LISTE4(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
```

```
  200 CONTINUE
      GOTO 230
C
  210 DO 220 J = 1 , 27
      I = LISTE4(J)
      MI(I) = 0.0
  220 CONTINUE
C
C**** NI SPECIES */
C
  230 IF (NITOT .LE. 0.0) GOTO 250
      MI(205)=KT(403)*ALFA(97)/GAMMA(205)
      MI(206)=KT(404)*ALFA(4)/GAMMA(206)
      MI(207)=KT(405)*ALFA(61)/GAMMA(207)
      MI(208)=KT(406)*AH2O*TENPH/GAMMA(208)
      MI(209)=KT(407)*(AH2O*TENPH)**2/GAMMA(209)
      MI(210)=KT(408)*(AH2O*TENPH)**3/GAMMA(210)
      MI(211)=KT(409)*ALFA(5)/GAMMA(211)
      MI(279)=KT(518)*ALFA(4)**2/GAMMA(279)
      MI(280)=KT(519)*ALFA(6)/GAMMA(280)
      MI(281)=KT(520)*ALFA(17)/GAMMA(281)
      MI(282)=KT(521)*ALFA(17)**2/GAMMA(282)
      MI(283)=KT(522)*ALFA(5)**2/GAMMA(283)
      MI(204)=NITOT/(1+GAMMA(204)*(MI(205)+MI(206)+MI(207)+MI(208)+
     *MI(209)+MI(210)+MI(211)+MI(279)+MI(280)+MI(281)+MI(282)+
     *MI(283)))
      C1 = MI(204) * GAMMA(204)
      ALFA(204)= C1
C
      DO 240J = 2 , 13
      I = LISTE5(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  240 CONTINUE
      GOTO 270
C
  250 DO 260 J = 1 , 13
      I = LISTE5(J)
      MI(I) = 0.0
  260 CONTINUE
C
C**** AG SPECIES */
C
  270 IF (AGTOT .LE. 0.0) GOTO 290
      MI(213)=KT(421)*ALFA(97)/GAMMA(213)
      MI(214)=KT(422)*ALFA(97)**2/GAMMA(214)
      MI(215)=KT(423)*ALFA(4)/GAMMA(215)
      MI(216)=KT(424)*ALFA(4)**2/GAMMA(216)
      MI(217)=KT(425)*ALFA(4)**3/GAMMA(217)
      MI(218)=KT(426)*ALFA(4)**4/GAMMA(218)
      MI(219)=KT(427)*ALFA(61)/GAMMA(219)
      MI(220)=KT(428)*ALFA(66)/GAMMA(220)
      MI(221)=KT(429)*ALFA(66)**2/GAMMA(221)
      MI(222)=KT(430)*ALFA(96)/GAMMA(222)
      MI(223)=KT(431)*ALFA(96)**2/GAMMA(223)
      MI(224)=KT(432)*AH2O*TENPH/GAMMA(224)
      MI(225)=KT(433)*(AH2O*TENPH)**2/GAMMA(225)
      MI(226)=KT(434)*ALFA(5)/GAMMA(226)
      MI(227)=KT(435)*ALFA(84)/GAMMA(227)
      MI(228)=KT(436)*ALFA(202)**2/GAMMA(228)
      MI(244)=KT(473)*ALFA(97)**3/GAMMA(244)
      MI(245)=KT(474)*ALFA(96)**3/GAMMA(245)
      MI(246)=KT(475)*ALFA(96)**4/GAMMA(246)
      MI(268)=KT(507)*(ALFA(66)*TENPH)**2/GAMMA(268)
      MI(269)=KT(508)*(ALFA(66)*TENPH)**2/GAMMA(269)
```

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      MI(270)=KT(509)*ALFA(66)**2*TENPH/GAMMA(270)
      MI(294)=KT(531)*ALFA(284)/GAMMA(294)
      MI(295)=KT(532)*ALFA(285)/GAMMA(295)
C
      MI(212)=AGTOT/(1+GAMMA(212)*(MI(213)+MI(214)+MI(215)+MI(216)+
     *MI(217)+MI(218)+MI(219)+MI(220)+MI(221)+MI(222)+MI(223)+
     *MI(224)+MI(225)+MI(226)+MI(227)+MI(228)+MI(244)+MI(245)+
     *MI(246)+MI(268)+MI(269)+MI(270)+MI(294)+MI(295)))
      C1 = MI(212) * GAMMA(212)
      ALFA(212) = C1
C
      DO 280 J = 2 , 25
      I = LISTE6(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  280 CONTINUE
      GOTO 310
C
  290 DO 300 J = 1 , 25
      I = LISTE6(J)
      MI(I) = 0.0
  300 CONTINUE
C
C**** AS SPECIES */
C
  310 IF (AS3TOT + AS5TOT .GT. 0.0) GOTO 420
      IF (EH(EHOPT(4)) .LT. 9.9 .AND. ASTOTL .GT. 0.0) GOTO 420
      GOTO 370
  420 MI(251)=KT(478)*TENPH/GAMMA(251)
      MI(252)=KT(479)*TENPH**2/GAMMA(252)
      MI(253)=KT(480)*TENPH**3/GAMMA(253)
      MI(254)=KT(481)/(TENPH*GAMMA(254))
      MI(256)=KT(482)*TENPH/GAMMA(256)
      MI(257)=KT(483)*TENPH**2/GAMMA(257)
      MI(258)=KT(484)*TENPH**3/GAMMA(258)
      IF (AS3TOT + AS5TOT .LE. 0.0) GOTO320
C
C     SPLIT-ARSENIC
C
C**** AS +3 SPECIES */
C
      MI(250) = AS3TOT/(1E0 + GAMMA(250) * (MI(251) + MI(252) +
     *MI(253) + MI(254)))
      C1 = MI(250) * GAMMA(250)
      ALFA(250) = C1
      DO 400  I = 251 , 254
      MI(I) = C1 * MI(I)
  400 CONTINUE
C
C**** AS +5 SPECIES */
C
      MI(255) = AS5TOT/ (1E0 + GAMMA(255) * (MI(256) + MI(257) +
     *MI(258)))
      C1 = MI(255) * GAMMA(255)
      ALFA(255) = C1
      DO 410 I = 256 , 258
      MI(I) = C1 * MI(I)
  410 CONTINUE
      GOTO 350
C
C     END SPLIT-ARSENIC
C
  320 MI(255) = 1.0 / GAMMA(255)
      C2=10.**(-PE(EHOPT(4)))
      C1 = KT(487) * AH2O * TENPH**2 / C2**2
```

```
      DO 330  I = 255 , 258
      MI(I) = C1 * MI(I)
  330 CONTINUE
      MI(250)=ASTOTL/(1E0 + GAMMA(250)*(MI(251)+MI(252)+MI(253)+
     *MI(254)+MI(255)+MI(256)+MI(257)+MI(258)))
      C1 = MI(250) * GAMMA(250)
      ALFA(250) = C1
      DO 340 I = 251 , 258
      MI(I) = C1 * MI(I)
  340 CONTINUE
      ALFA(255) = MI(255) * GAMMA(255)
C
  350 ALFA(251) = MI(251) * GAMMA(251)
      ALFA(252) = MI(252) * GAMMA(252)
      ALFA(253) = MI(253) * GAMMA(253)
      ALFA(254) = MI(254) * GAMMA(254)
      ALFA(256) = MI(256) * GAMMA(256)
      ALFA(257) = MI(257) * GAMMA(257)
      ALFA(258) = MI(258) * GAMMA(258)
      IF (ALFA(250)*ALFA(255) .LE. 0.0) GOTO 360
      PE(8) = (DLOG10(ALFA(255)/ALFA(250)) - LOGKT(487)-LH2O)/2E0-PH
      EH(8) = PE(8) * C*R*T/F
  360 IF (ALFA(250) .LE. 0.0) GOTO 390
      PE(9) = (LOGKT(557) + DLOG10(ALFA(250)))/3E0-LH2O-PH
      EH(9) = PE(9) * C*R*T/F
      GOTO 390
  370 DO 380 I = 250 , 258
      MI(I) = 0.0
  380 CONTINUE
C
C**** SE SPECIES */
C
  390 IF (H2SETT + SEO3TT + SEO4TT .GT. 0.0) GOTO 450
      IF (EH(EHOPT(5)) .LT. 9.9 .AND. SETOTL .GT. 0.0) GOTO 450
      GOTO 480
  450 MI(299) = 1 / (KT(544) * TENPH * GAMMA(299))
      MI(303) = KT(545) / (TENPH**2  * GAMMA(303))
      MI(304) = KT(546) / (TENPH     * GAMMA(304))
      MI(306) = KT(547) / (TENPH     * GAMMA(306))
      IF (H2SETT + SEO3TT + SEO4TT .LE. 0.0) GOTO 460
C
C     SPLIT-SELENIUM
C
C**** SELENIDE SPECIES */
C
      MI(302) = H2SETT / (1.0 + GAMMA(302) * MI(299))
      C1 = MI(302) * GAMMA(302)
      ALFA(302) = C1
      MI(299) = C1 * MI(299)
C
C**** SELENITE SPECIES */
C
      MI(305)=SEO3TT/(1E0 + GAMMA(305)*(MI(303)+MI(304)))
      C1 = MI(305) * GAMMA(305)
      ALFA(305) = C1
      MI(303)=C1 * MI(303)
      MI(304)=C1 * MI(304)
C
C**** SELENATE SPECIES */
C
      MI(307)=SEO4TT/(1E0 + GAMMA(307)*MI(306))
      ALFA(307) = MI(307) * GAMMA(307)
      C1 = ALFA(307)
      MI(306)= C1 * MI(306)
      GOTO 470
```

```
C
C     END SPLIT-SELENIUM
C
  460 MI(302) = 1.0 / GAMMA(302)
      C2=10.**(-PE(EHOPT(5)))
      C1 = KT(549) * C2**6 / (AH2O**3 * TENPH**7)
      MI(299) = C1 * MI(299)
      MI(302) = C1 * MI(302)
      MI(307) = 1.0 / GAMMA(307)
      C1 = KT(548) * AH2O * TENPH**2 / C2**2
      MI(306) = C1 * MI(306)
      MI(307) = C1 * MI(307)
      MI(305) = SETOTL/(1E0 + GAMMA(305) * (MI(299)+MI(302)+MI(303)+
     *                  MI(304)+MI(306)+MI(307)))
      ALFA(305) = MI(305) * GAMMA(305)
      C1 = ALFA(305)
      MI(299) = C1 * MI(299)
      MI(302) = C1 * MI(302)
      MI(303) = C1 * MI(303)
      MI(304) = C1 * MI(304)
      MI(306) = C1 * MI(306)
      MI(307) = C1 * MI(307)
      ALFA(302) = MI(302) * GAMMA(302)
      ALFA(307) = MI(307) * GAMMA(307)
C
  470 ALFA(299) = MI(299) * GAMMA(299)
      ALFA(303) = MI(303) * GAMMA(303)
      ALFA(304) = MI(304) * GAMMA(304)
      ALFA(306) = MI(306) * GAMMA(306)
      IF (ALFA(305)*ALFA(307) .LE. 0.0) GOTO 472
      PE(10) = (DLOG10(ALFA(307)/ALFA(305)) - LOGKT(548)-LH2O)/2E0-PH
      EH(10) = PE(10) * C*R*T/F
C      END
  472 IF (ALFA(305) .LE. 0.0) GOTO 474
      PE(11) = (DLOG10(ALFA(305)) + LOGKT(551)-3*LH2O-6*PH)/4E0
      EH(11) = PE(11) * C*R*T/F
C      END
  474 IF (ALFA(302) .LE. 0.0) GOTO 500
      PE(12) = (LOGKT(550)- DLOG10(ALFA(302)) - PH)/2E0
      EH(12) = PE(12) * C*R*T/F
      GOTO 500
  480 DO 490 I = 298 , 307
      MI(I) = 0.0
  490 CONTINUE
  500 RETURN
      END
      SUBROUTINE UEL(ALFA,GAMMA,LOGKT,MI)
C
$INCLUDE:'COMMON.BLK'
C
      REAL*8 ALFA(0:377),GAMMA(0:377),LOGKT(0:653),MI(0:377),
     *UTEMP(316:377),XA4,XA5,XA17,XA44,XA61,XA84,XA96,XA97,XA318,PEU
C
C  /**  URANIUM MASS ACTION AND MASS BALANCE **/
C
      IF ((U4TOT+U6TOT.GT.0E0) .OR. (EH(EHOPT(9)).LT.9.9 .AND.
     *    UTOTAL.GT.0E0))THEN
         DO 1 I=316,377
           UTEMP(I)=78.
    1    CONTINUE
         PEU=PE(EHOPT(9))
         IF(PEU.LT.100) TENMPE = 10.**(-PEU)
C
C        /*U+4 SPECIES*/
C
```

```
      IF(PEU.LT.100.) UTEMP(319)=LOGKT(566)-PEU-DLOG10(GAMMA(319))
      UTEMP(320)=LOGKT(567)+LH2O+PH-DLOG10(GAMMA(320))
      UTEMP(321)=LOGKT(568)+2*(LH2O+PH)-DLOG10(GAMMA(321))
      UTEMP(322)=LOGKT(569)+3*(LH2O+PH)-DLOG10(GAMMA(322))
      UTEMP(323)=LOGKT(570)+4*(LH2O+PH)-DLOG10(GAMMA(323))
      IF (MI(317)*GAMMA(317).GT.1D-78) UTEMP(325)=LOGKT(572)+
     *    15*(PH+LH2O)+5*DLOG10(MI(317)*GAMMA(317))-DLOG10(GAMMA(325))
      IF (ALFA(17).GT.1D-78) THEN
        XA17=DLOG10(ALFA(17))
        UTEMP(335)=LOGKT(589)+4*XA17-DLOG10(GAMMA(335))
        UTEMP(336)=LOGKT(590)+5*XA17-DLOG10(GAMMA(336))
      END IF
      IF (ALFA(61).GT.1D-78) THEN
        XA61=DLOG10(ALFA(61))
        UTEMP(326)=LOGKT(578)+XA61-DLOG10(GAMMA(326))
        UTEMP(327)=LOGKT(579)+2*XA61-DLOG10(GAMMA(327))
        UTEMP(328)=LOGKT(580)+3*XA61-DLOG10(GAMMA(328))
        UTEMP(329)=LOGKT(581)+4*XA61-DLOG10(GAMMA(329))
        UTEMP(330)=LOGKT(582)+5*XA61-DLOG10(GAMMA(330))
        UTEMP(331)=LOGKT(583)+6*XA61-DLOG10(GAMMA(331))
      END IF
      IF (ALFA(4).GT.1D-78) THEN
        XA4=DLOG10(ALFA(4))
        UTEMP(332)=LOGKT(586)+XA4-DLOG10(GAMMA(332))
      END IF
      IF (ALFA(5).GT.1D-78) THEN
        XA5=DLOG10(ALFA(5))
        UTEMP(333)=LOGKT(587)+XA5-DLOG10(GAMMA(333))
        UTEMP(334)=LOGKT(588)+2*XA5-DLOG10(GAMMA(334))
      END IF
      IF (ALFA(97).GT.1D-78) THEN
        XA97=DLOG10(ALFA(97))
        UTEMP(360)=LOGKT(633)+XA97-DLOG10(GAMMA(360))
      END IF
      IF (ALFA(96).GT.1D-78) THEN
        XA96=DLOG10(ALFA(96))
        UTEMP(361)=LOGKT(634)+XA96-DLOG10(GAMMA(361))
      END IF
      IF (ALFA(84).GT.1D-78) THEN
        XA84=DLOG10(ALFA(84))
        UTEMP(362)=LOGKT(635)+XA84-DLOG10(GAMMA(362))
        UTEMP(363)=LOGKT(636)+2*XA84-DLOG10(GAMMA(363))
      END IF
C
C     /*U+6 SPECIES*/
C
      IF(PEU.LT.100) UTEMP(339)=LOGKT(595)-PEU-DLOG10(GAMMA(339))
      UTEMP(340)=LOGKT(596)+LH2O+PH-DLOG10(GAMMA(340))
      UTEMP(365)=LOGKT(638)+3*(LH2O+PH)-DLOG10(GAMMA(365))
      UTEMP(366)=LOGKT(639)+4*(LH2O+PH)-DLOG10(GAMMA(366))
      IF (MI(318)*GAMMA(318).GT.1D-78) THEN
        XA318=DLOG10(MI(318)*GAMMA(318))
        UTEMP(341)=LOGKT(597)+XA318+2*(LH2O+PH)-DLOG10(GAMMA(341))
        UTEMP(342)=LOGKT(598)+2*XA318+5*(LH2O+PH)-DLOG10(GAMMA(342))
        UTEMP(367)=LOGKT(640)+XA318+LH2O+PH-DLOG10(GAMMA(367))
        UTEMP(368)=LOGKT(641)+2*XA318+4*(LH2O+PH)-DLOG10(GAMMA(368))
        UTEMP(369)=LOGKT(642)+2*XA318+7*(LH2O+PH)-DLOG10(GAMMA(369))
        UTEMP(370)=LOGKT(643)+3*XA318+7*(LH2O+PH)-DLOG10(GAMMA(370))
      END IF
      IF (ALFA(17).GT.1D-78) THEN
        XA17=DLOG10(ALFA(17))
        UTEMP(343)=LOGKT(603)+XA17-DLOG10(GAMMA(343))
        UTEMP(344)=LOGKT(604)+2*XA17-DLOG10(GAMMA(344))
        UTEMP(345)=LOGKT(605)+3*XA17-DLOG10(GAMMA(345))
        IF(PEU.LT.100)
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```
*       UTEMP(377)=LOGKT(650)+3*XA17-PEU-DLOG10(GAMMA(377))
        IF (MI(318)*GAMMA(318).GT.1D-78) THEN
          XA318=DLOG10(MI(318)*GAMMA(318))
          UTEMP(375)=LOGKT(648)+2*XA318+6*XA17-DLOG10(GAMMA(375))
        END IF
      END IF
      IF (ALFA(61).GT.1D-78) THEN
        XA61=DLOG10(ALFA(61))
        UTEMP(346)=LOGKT(607)+XA61-DLOG10(GAMMA(346))
        UTEMP(347)=LOGKT(608)+2*XA61-DLOG10(GAMMA(347))
        UTEMP(348)=LOGKT(609)+3*XA61-DLOG10(GAMMA(348))
        UTEMP(349)=LOGKT(610)+4*XA61-DLOG10(GAMMA(349))
      END IF
      IF (ALFA(4).GT.1D-78) THEN
        XA4=DLOG10(ALFA(4))
        UTEMP(350)=LOGKT(611)+XA4-DLOG10(GAMMA(350))
        UTEMP(371)=LOGKT(644)+2*XA4-DLOG10(GAMMA(371))
      END IF
      IF (ALFA(5).GT.1D-78) THEN
        XA5=DLOG10(ALFA(5))
        UTEMP(351)=LOGKT(612)+XA5-DLOG10(GAMMA(351))
        UTEMP(352)=LOGKT(613)+2*XA5-DLOG10(GAMMA(352))
      END IF
      IF (ALFA(44).GT.1D-78) THEN
        XA44=DLOG10(ALFA(44))
        UTEMP(353)=LOGKT(614)+XA44-PH-DLOG10(GAMMA(353))
        UTEMP(354)=LOGKT(615)+2*(XA44-PH)-DLOG10(GAMMA(354))
        UTEMP(355)=LOGKT(616)+XA44-2*PH-DLOG10(GAMMA(355))
        UTEMP(356)=LOGKT(617)+2*(XA44-2*PH)-DLOG10(GAMMA(356))
        UTEMP(357)=LOGKT(618)+3*(XA44-2*PH)-DLOG10(GAMMA(357))
        UTEMP(374)=LOGKT(647)+XA44-3*PH-DLOG10(GAMMA(374))
        UTEMP(376)=LOGKT(649)+XA44-DLOG10(GAMMA(376))
      END IF
      IF (ALFA(97).GT.1D-78)
*       UTEMP(372)=LOGKT(645)+DLOG10(ALFA(97))-LOG10(GAMMA(372))
      IF (ALFA(84).GT.1D-78)
*       UTEMP(373)=LOGKT(646)+DLOG10(ALFA(84))-LOG10(GAMMA(373))
      DO 90 I=319, 357
        IF (ABS(UTEMP(I)).LT.78) THEN
          MI(I)=1E1**UTEMP(I)
        ELSE
          MI(I)=0
        END IF
90      CONTINUE
      DO 95 I=360, 377
        IF (ABS(UTEMP(I)).LT.78) THEN
          MI(I)=1E1**UTEMP(I)
        ELSE
          MI(I)=0
        END IF
95      CONTINUE
      IF (U4TOT+U6TOT .GT. 0E0) THEN
C
C       /* FOLLOWING IS MARK CANTRELL'S VERSION OF SPLIT_U */
C
        MI(317)=U4TOT/(1+GAMMA(317)*(MI(319)+MI(320)+MI(321)+MI(322)+
*                                    MI(323)+6*MI(325)+MI(326)+
*                                    MI(327)+MI(328)+MI(329)+MI(330)+
*                                    MI(331)+MI(332)+MI(333)+MI(334)+
*                                    MI(335)+MI(336)+MI(360)+MI(361)+
*                                    MI(362)+MI(363)))
        ALFA(317)=MI(317)*GAMMA(317)
        C1=ALFA(317)
        DO 100 I=319, 336
          MI(I)=C1*MI(I)
```

```
  100     CONTINUE
          DO 105 I=360, 363
            MI(I)=C1*MI(I)
  105     CONTINUE
          MI(318)=U6TOT/(1+GAMMA(318)*(MI(339)+MI(340)+2*MI(341)+
     *                                 3*MI(342)+MI(343)+MI(344)+
     *                                 MI(345)+MI(346)+MI(347)+MI(348)+
     *                                 MI(349)+MI(350)+MI(351)+MI(352)+
     *                                 MI(353)+MI(354)+MI(355)+MI(356)+
     *                                 MI(357)+MI(365)+MI(366)+
     *                                 2*MI(367)+3*MI(368)+3*MI(369)+
     *                                 4*MI(370)+MI(371)+MI(372)+
     *                                 MI(373)+MI(374)+3*MI(375)+
     *                                 MI(376)+MI(377)))
          ALFA(318)=MI(318)*GAMMA(318)
          C1=ALFA(318)
          DO 110 I=339, 357
            MI(I)=C1*MI(I)
  110     CONTINUE
          DO 115 I=365, 377
            MI(I)=C1*MI(I)
  115     CONTINUE
        ELSE
C
C         /* IF UTOT AND Eh BUT U4TOT AND U6TOT NOT SPECIFIED */
C
          MI(317)=1E0/GAMMA(317)
          C1=10.**LOGKT(565)*TENMPE**2/(AH2O**2*TENPH**4)
          MI(317)=C1*MI(317)
          DO 120 I=319, 336
            MI(I)=C1*MI(I)
  120     CONTINUE
          DO 125 I=360, 363
            MI(I)=C1*MI(I)
  125     CONTINUE
          C1=MI(317)
          DO 130 I=319, 357
            C1=C1+MI(I)
  130     CONTINUE
          C1=C1+5*MI(325)+MI(341)+2*MI(342)
          DO 135 I=360, 377
            C1=C1+MI(I)
  135     CONTINUE
          C1=C1+MI(367)+2*MI(368)+2*MI(369)+3*MI(370)+2*MI(375)
          MI(318)=UTOTAL/(1E0+GAMMA(318)*C1)
          ALFA(318)=MI(318)*GAMMA(318)
          C1=ALFA(318)
          MI(317)=MI(317)*C1
          DO 140 I=319, 357
            MI(I)=MI(I)*C1
  140     CONTINUE
          DO 145 I=360, 377
            MI(I)=MI(I)*C1
  145     CONTINUE
          ALFA(317)=MI(317)*GAMMA(317)
        END IF
        DO 150 I=319, 357
          ALFA(I)=MI(I)*GAMMA(I)
  150   CONTINUE
        DO 155 I=360, 377
          ALFA(I)=MI(I)*GAMMA(I)
  155   CONTINUE
        IF (ALFA(317).GT.1D-78 .AND. ALFA(318).GT.1D-78) THEN
          PE(13) = -0.5*(-LOGKT(565)+DLOG10(ALFA(317))+2.*LH2O-
     *             DLOG10(ALFA(318))+4.*PH)
```

```
          EH(13)=PE(13)*C*R*T/F
        END IF
C
C
      ELSE
        DO 160 I=317, 377
          MI(I)=0E0
  160   CONTINUE
      END IF
      RETURN
      END
      SUBROUTINE SUMS(ALFA,GAMMA,KT,LOGKT,MI)
C
      REAL*8 ALFA(0:377),GAMMA(0:377),KT(0:653),MI(0:377),LOGKT(0:653)
      REAL*8 S1,S2,S3,S4,S5,S6,S7,S8,M1,M2,M3,M4,M5,M6,M7,M8
      INTEGER LISTE1(38),LISTE2(33),LISTE3(40),LISTE4(21),LISTE5(35),
     *LISTE6(25)
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE1/6,20,21,29,30,41,42,68,85,95,119,131,132,166,187,241,
     * 271,272,273,274,275,276,278,280,281,282,309,310,311,312,313,335,
     * 336,343,344,345,375,377/
      DATA LISTE2/14,22,31,33,43,45,58,59,62,81,82,91,108,117,122,123,
     *143,158,159,174,197,201,203,211,226,243,277,283,314,333,334,351,
     *352/
      DATA LISTE3/19,54,55,56,57,100,101,102,103,104,105,106,107,116,
     *124,125,126,137,150,164,165,188,189,190,191,207,219,296,297,308,
     *326,327,328,329,330,331,346,347,348,349/
      DATA LISTE4/12,39,40,46,47,49,60,64,72,73,74,75,98,99,
     *353,354,355,356,357,374,376/
      DATA LISTE5/15,27,32,111,112,113,128,129,133,134,135,136,146,147,
     *148,149,155,161,162,163,172,183,184,185,186,206,215,216,217,
     *218,279,315,332,350,371/
      DATA LISTE6/13,67,247,248,144,156,157,175,176,177,178,198,199,
     *220,221,259,260,263,264,265,266,267,268,269,270/
C
C**** SUMMATION OF ANION SPECIES */
C
C**** HCO3
C
      M1 = MI(6)
      IF (CORALK .NE. 2) GOTO 10
      S1 =   MI(17)  +      MI(20)  +      MI(21)  +      MI(29)
     *+      MI(30)  +      MI(41)  +      MI(42)  +      MI(68)
     *+      MI(85)  +      MI(95)  +      MI(119) +      MI(131)
     *+ 2. * MI(132) + 2. * MI(166) + 2. * MI(187) +      MI(241)
     *+      MI(271) +      MI(272) +      MI(273) + 2. * MI(274)
     *+      MI(275) +      MI(276) +      MI(278) +      MI(280)
     *+      MI(281) + 2. * MI(282) +      MI(309) +      MI(310)
     *+      MI(311) +      MI(312) +      MI(313) + 4. * MI(335)
     *+ 5. * MI(336) +      MI(343) + 2. * MI(344) + 3. * MI(345)
     *+ 6. * MI(375) + 3. * MI(377)
      GOTO 20
   10 S1 = 2.* MI(17)+ 2. * MI(20)  +      MI(21)  +      MI(29)
     *+ 2. * MI(30)  + 2. * MI(41)  +      MI(42)  +      MI(68)
     *               + 2. * MI(95)  +      MI(119) + 2. * MI(131)
     *+ 4. * MI(132) + 4. * MI(166) + 4. * MI(187) + 2. * MI(241)
     *+      MI(271) +      MI(272) + 2. * MI(273) + 4. * MI(274)
     *+      MI(275) + 2. * MI(276) +      MI(278) +      MI(280)
     *+ 2. * MI(281) + 4. * MI(282) +      MI(309) + 2. * MI(310)
     *+ 2. * MI(311) +      MI(312) + 2. * MI(313) + 8. * MI(335)
     *+10. * MI(336) + 2. * MI(343) + 4. * MI(344) + 6. * MI(345)
     *+12. * MI(375) + 6. * MI(377)
C
```

```
C**** SO4
C
   20 M2 = MI(5)
      S2 =   MI(14)  +      MI(22)  +      MI(31)  +      MI(43)
     *+      MI(45)  +      MI(58)  + 2. * MI(59)  +      MI(62)
     *+      MI(81)  +      MI(82)  +      MI(91)  +      MI(33)
     *+      MI(117) +      MI(122) +      MI(123) +      MI(143)
     *+ 2. * MI(108) +      MI(158) + 2. * MI(159) +      MI(174)
     *+      MI(197) +      MI(201) +      MI(203) +      MI(211)
     *+      MI(226) + 2. * MI(243) + 2. * MI(277) + 2. * MI(283)
     *+      MI(314) +      MI(333) + 2. * MI(334) +      MI(351)
     *+ 2. * MI(352)
C
C**** F
C
      M3 = MI(61)
      S3 =   MI(54)  + 2. * MI(55)  + 3. * MI(56)  + 4. * MI(57)
     *+      MI(19)  +      MI(100) +      MI(101) + 2. * MI(102)
     *+ 3. * MI(103) + 4. * MI(104) +      MI(105) + 2. * MI(106)
     *+ 3. * MI(107) +      MI(116) + 6. * MI(124) +      MI(125)
     *+ 2. * MI(126) +      MI(137) +      MI(150) +      MI(164)
     *+ 2. * MI(165) +      MI(188) + 2. * MI(189) + 3. * MI(190)
     *+ 4. * MI(191) +      MI(207) +      MI(219) + 2. * MI(296)
     *+      MI(297) +      MI(308) +      MI(326) + 2. * MI(327)
     *+ 3. * MI(328) + 4. * MI(329) + 5. * MI(330) + 6. * MI(331)
     *+      MI(346) + 2. * MI(347) + 3. * MI(348) + 4. * MI(349)
C
C**** PO4
C
      M4 = MI(44)
      S4 =   MI(12)  +      MI(39)  +      MI(40)  +      MI(46)
     *+      MI(47)  +      MI(49)  +      MI(60)  +      MI(64)
     *+      MI(72)  +      MI(73)  +      MI(74)  +      MI(75)
     *+      MI(98)  +      MI(99)  +      MI(353) + 2. * MI(354)
     *+      MI(355) + 2. * MI(356) + 3. * MI(357) +      MI(374)
     *+      MI(376)
C
C**** CL
C
      M5 = MI(4)
      S5 =   MI(15)  + 2. * MI(27)  + 3. * MI(32)  + 2. * MI(128)
     *+ 3. * MI(129) +      MI(133) + 2. * MI(134) + 3. * MI(135)
     *+ 4. * MI(136) +      MI(146) + 2. * MI(147) + 3. * MI(148)
     *+ 4. * MI(149) +      MI(155) +      MI(161) + 2. * MI(162)
     *+ 3. * MI(163) +      MI(172) +      MI(183) + 2. * MI(184)
     *+ 3. * MI(185) + 4. * MI(186) +      MI(111) + 2. * MI(112)
     *+ 3. * MI(113) +      MI(206) +      MI(215) + 2. * MI(216)
     *+ 3. * MI(217) + 4. * MI(218) + 2. * MI(279) +      MI(315)
     *+      MI(332) +      MI(350) + 2. * MI(371)
C
C**** H2S
C
      M6 = MI(13)
      S6 =   MI(66)  +      MI(67)  + 2. * MI(247) + 3. * MI(248)
     *+ 3. * MI(144) + 2. * MI(156) + 3. * MI(157) +      MI(175)
     *+ 2. * MI(176) + 3. * MI(177) + 4. * MI(178) + 2. * MI(198)
     *+ 3. * MI(199) +      MI(220) + 2. * MI(221) + 2. * MI(259)
     *+ 2. * MI(260) +      MI(263) +      MI(264) +      MI(265)
     *+      MI(266) +      MI(267) + 2. * MI(268) + 2. * MI(269)
     *+ 2. * MI(270)
C
C**** FULVATE
C
      M7 = MI(284)
      S7 =   MI(286) + MI(288) + MI(290) + MI(292) + MI(294)
```

```
C
C**** HUMATE
C
      M8 = MI(285)
      S8 = MI(287) + MI(289) + MI(291) + MI(293) + MI(295)
C
C**** ANION MASS BALANCE CALCULATIONS */
C
C**** MASS BALANCE ON CARBON */
C
      IF (CO2TIT .LE. 0.0) GOTO 60
      MI(6)   = KT(68)  / (TENPH    * GAMMA(6))
      MI(20)  = KT(73)  * ALFA(1)   / GAMMA(20)
      MI(21)  = KT(74)  * KT(68)    * ALFA(1) / (TENPH * GAMMA(21))
      MI(29)  = KT(77)  * KT(68)    * ALFA(0) / (TENPH * GAMMA(29))
      MI(30)  = KT(78)  * ALFA(0)   / GAMMA(30)
      MI(41)  = KT(69)  * ALFA(2)   / GAMMA(41)
      MI(42)  = KT(70)  * KT(68)    * ALFA(2) / (TENPH * GAMMA(42))
      MI(68)  = KT(79)  * KT(68)    * ALFA(87)/ (TENPH * GAMMA(68))
      MI(85)  = KT(35)  * KT(68)    / (TENPH**2 * GAMMA(85))
      MI(95)  = KT(135) * ALFA(87)  / GAMMA(95)
      MI(119) = KT(178) * KT(68)    * ALFA(109) / (TENPH * GAMMA(119))
      MI(131) = KT(209) * ALFA(130) / GAMMA(131)
      MI(132) = KT(210) * ALFA(130) * ALFA(17)  / GAMMA(132)
      MI(166) = KT(299) * ALFA(160) * ALFA(17)  / GAMMA(166)
      MI(187) = KT(345) * ALFA(182) * ALFA(17)  / GAMMA(187)
      MI(241) = KT(468) * ALFA(182) / GAMMA(241)
      MI(271) = KT(510) * KT(68)    * ALFA(130) / (TENPH * GAMMA(271))
      MI(272) = KT(511) * KT(68)    * ALFA(145) / (TENPH * GAMMA(272))
      MI(273) = KT(512) * ALFA(145) / GAMMA(273)
      MI(274) = KT(513) * ALFA(145) * ALFA(17)  / GAMMA(274)
      MI(275) = KT(514) * KT(68)    * ALFA(160) / (TENPH * GAMMA(275))
      MI(276) = KT(515) * ALFA(160) / GAMMA(276)
      MI(278) = KT(517) * KT(68)    * ALFA(182) / (TENPH * GAMMA(278))
      MI(280) = KT(519) * KT(68)    * ALFA(204) / (TENPH * GAMMA(280))
      MI(281) = KT(520) * ALFA(204) / GAMMA(281)
      MI(282) = KT(521) * ALFA(204) * ALFA(17)  / GAMMA(282)
      MI(309) = KT(558) * KT(68)    * ALFA(7)   / (TENPH * GAMMA(309))
      MI(310) = KT(559) * ALFA(7)   / GAMMA(310)
      MI(311) = KT(560) * ALFA(109) / GAMMA(311)
      MI(312) = KT(561) * KT(68)    * ALFA(89)  / (TENPH * GAMMA(312))
      MI(313) = KT(562) * ALFA(89)  / GAMMA(313)
      MI(343) = KT(603) * ALFA(318) / GAMMA(343)
      MI(344) = KT(604) * ALFA(318) * ALFA(17) / GAMMA(344)
      MI(345) = KT(605) * ALFA(318) * ALFA(17)**2 / GAMMA(345)
      MI(375) = KT(648) * ALFA(318)**3 * ALFA(17)**5 / GAMMA(375)
      TENMPE=1E1**(-PE(EHOPT(9)))
      MI(377) = KT(650) * ALFA(318) * ALFA(17)**2 * TENMPE / GAMMA(377)
C
      IF (CORALK .NE. 2) GOTO 30
      MI(17) = ANLCO3 / (1.0 + GAMMA(17) * (MI(6)  + MI(20)
     *+ MI(21) + MI(29)  + MI(30) + MI(41) + MI(42) + MI(68) + MI(85)
     *+ MI(95) + MI(119) + MI(131) + 2. * MI(132) + 2. * MI(166)
     *+ 2. * MI(187) + MI(241) + MI(271) + MI(272) + MI(273)
     *+ 2. * MI(274) + MI(275) + MI(276) + MI(278) + MI(280)
     *+ MI(281) + 2. * MI(282) + MI(309) + MI(310) + MI(311) + MI(312)
     *+ MI(313) + MI(343) + 2. * MI(344) + 3. * MI(345) + 6. * MI(375)
     *+ 3. * MI(377)))
      GOTO 40
C
   30 NONCRB = MI(24) + 2. * MI(25) + MI(26) + MI(36) + 2. * MI(44)
     *+ MI(46) + MI(53) + MI(66) + 2. * MI(67)
      IF (CORALK .EQ. 0) ANLCO3 = DMAX1(0.0D0,(DBLE(CO2TIT) - NONCRB))
C
      MI(17) = ANLCO3 / (2.0 + GAMMA(17) * (MI(6) + 2. * MI(20)
```

```
     *+MI(21) + MI(29) + 2. * MI(30) + 2. * MI(41) + MI(42)
     *+MI(68) + 2. * MI(95) + MI(119)
     *+ 2. * MI(131) + 4. * MI(132) + 4. * MI(166) + 4. * MI(187)
     *+ 2. * MI(241) + MI(271) + MI(272) + 2 * MI(273) + 4. * MI(274)
     *+ MI(275) + 2. * MI(276) + MI(278) + MI(280) + 2. * MI(281)
     *+ 4. * MI(282) + MI(309) + 2. * MI(310) + 2. * MI(311) + MI(312)
     *+ 2. * MI(313) + 2. * MI(343) + 4. * MI(344) + 6. * MI(345)
     *+ 12. * MI(375) + 6. * MI(377)))
C
   40 C1 = MI(17) * GAMMA(17)
      ALFA(17) = C1
      DO 50 J = 1 , 38
      I = LISTE1(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
   50 CONTINUE
C
C**** MASS BALANCE ON SULFATE */
C
   60 IF (SO4TOT .LE. 0.0) GOTO 80
      MI(14)  = KT(4)   * ALFA(8)   / GAMMA(14)
      MI(22)  = KT(75)  * ALFA(1)   / GAMMA(22)
      MI(31)  = KT(23)  * ALFA(0)   / GAMMA(31)
      MI(33)  = KT(8)   * ALFA(7)   / GAMMA(33)
      MI(43)  = KT(71)  * ALFA(2)   / GAMMA(43)
      MI(45)  = KT(72)  * ALFA(3)   / GAMMA(45)
      MI(58)  = KT(87)  * ALFA(50)  / GAMMA(58)
      MI(59)  = KT(88)  * ALFA(50)  * ALFA(5)  / GAMMA(59)
      MI(62)  = KT(89)  / (TENPH * GAMMA(62))
      MI(81)  = KT(168) * KT(89) * ALFA(0) / (TENPH * GAMMA(81))
      MI(82)  = KT(126) * ALFA(80)  / GAMMA(82)
      MI(91)  = KT(131) * ALFA(38)  / GAMMA(91)
      MI(108) = KT(333) * ALFA(8)   * ALFA(5)  / GAMMA(108)
      MI(117) = KT(176) * ALFA(109) / GAMMA(117)
      MI(122) = KT(148) * KT(89) * ALFA(7) / (TENPH * GAMMA(122))
      MI(123) = KT(159) * KT(89) * ALFA(8) / (TENPH * GAMMA(123))
      MI(143) = KT(221) * ALFA(130) / GAMMA(143)
      MI(158) = KT(263) * ALFA(145) / GAMMA(158)
      MI(159) = KT(264) * ALFA(145) * ALFA(5)  / GAMMA(159)
      MI(174) = KT(307) * ALFA(160) / GAMMA(174)
      MI(197) = KT(355) * ALFA(182) / GAMMA(197)
      MI(201) = KT(543) * ALFA(89) / GAMMA(201)
      MI(203) = KT(397) * KT(89) * ALFA(50) / (TENPH * GAMMA(203))
      MI(211) = KT(409) * ALFA(204) / GAMMA(211)
      MI(226) = KT(434) * ALFA(212) / GAMMA(226)
      MI(243) = KT(470) * ALFA(182) * ALFA(5)  / GAMMA(243)
      MI(277) = KT(516) * ALFA(160) * ALFA(5)  / GAMMA(277)
      MI(283) = KT(522) * ALFA(204) * ALFA(5)  / GAMMA(283)
      MI(314) = KT(563) * ALFA(87)  / GAMMA(314)
      MI(333) = KT(587) * ALFA(317) / GAMMA(333)
      MI(334) = KT(588) * ALFA(317) * ALFA(5) / GAMMA(334)
      MI(351) = KT(612) * ALFA(318) / GAMMA(351)
      MI(352) = KT(613) * ALFA(318) * ALFA(5) / GAMMA(352)
      MI(5)=SO4TOT/(1E0 + GAMMA(5)*(MI(14)+MI(22)+MI(31)+MI(33)+MI(43)+
     *MI(45)+MI(58)+2.*MI(59)+MI(62)+MI(81)+MI(82)+MI(91)+2.*MI(108)+
     *MI(117)+MI(122)+MI(123)+MI(143)+MI(158)+2.*MI(159)+MI(174)+
     *MI(197)+MI(201)+MI(203)+MI(211)+MI(226)+2*MI(243)+
     *2.*MI(277)+2.*MI(283)+MI(314)+MI(333)+2.*MI(334)+MI(351)+
     *2.*MI(352)))
      ALFA(5)=MI(5)*GAMMA(5)
      C1=ALFA(5)
C
      DO 70 J = 1 , 33
      I = LISTE2(J)
      MI(I) = C1 * MI(I)
```

```
      ALFA(I) = MI(I) * GAMMA(I)
   70 CONTINUE
C
C**** MASS BALANCE ON FLUORIDE */
C
   80 IF (FTOT .LE. 0.0) GOTO 100
      MI(19)=KT(22)*ALFA(1)/GAMMA(19)
      MI(54)=KT(83)*ALFA(50)/GAMMA(54)
      MI(55)=KT(84)*ALFA(50)*ALFA(61)/GAMMA(55)
      MI(56)=KT(85)*ALFA(50)*ALFA(61)**2/GAMMA(56)
      MI(57)=KT(86)*ALFA(50)*ALFA(61)**3/GAMMA(57)
      MI(100)=KT(160)*ALFA(0)/GAMMA(100)
      MI(101)=KT(161)*ALFA(35)/GAMMA(101)
      MI(102)=KT(162)*ALFA(35)*ALFA(61)/(AH2O*TENPH*GAMMA(102))
      MI(103)=KT(163)*ALFA(35)*ALFA(61)**2/((AH2O*TENPH)**2*GAMMA(103))
      MI(104)=KT(164)*ALFA(35)*ALFA(61)**3/((AH2O*TENPH)**3*GAMMA(104))
      MI(105)=KT(165)*ALFA(8)/GAMMA(105)
      MI(106)=KT(166)*ALFA(8)*ALFA(61)/GAMMA(106)
      MI(107)=KT(167)*ALFA(8)*ALFA(61)**2/GAMMA(107)
      MI(116)=KT(175)*ALFA(109)/GAMMA(116)
      MI(124)=KT(201)*ALFA(23)*ALFA(61)**5/((TENPH*AH2O)**4*GAMMA(124))
      MI(125)=KT(202)/(TENPH*GAMMA(125))
      MI(126)=KT(203)*ALFA(61)/(TENPH*GAMMA(126))
      MI(137)=KT(215)*ALFA(130)/GAMMA(137)
      MI(150)=KT(255)*ALFA(145)/GAMMA(150)
      MI(164)=KT(297)*ALFA(160)/GAMMA(164)
      MI(165)=KT(298)*ALFA(160)*ALFA(61)/GAMMA(165)
      MI(188)=KT(346)*ALFA(182)/GAMMA(188)
      MI(189)=KT(347)*ALFA(182)*ALFA(61)/GAMMA(189)
      MI(190)=KT(348)*ALFA(182)*ALFA(61)**2/GAMMA(190)
      MI(191)=KT(349)*ALFA(182)*ALFA(61)**3/GAMMA(191)
      MI(207)=KT(405)*ALFA(204)/GAMMA(207)
      MI(219)=KT(427)*ALFA(212)/GAMMA(219)
      MI(296)=KT(537)*ALFA(61)/(TENPH**2*GAMMA(296))
      MI(297)=KT(540)*ALFA(2)/GAMMA(297)
      MI(308)=KT(359)*ALFA(7)/GAMMA(308)
      MI(326)=KT(578)*ALFA(317)/GAMMA(326)
      MI(327)=KT(579)*ALFA(317)*ALFA(61)/GAMMA(327)
      MI(328)=KT(580)*ALFA(317)*ALFA(61)**2/GAMMA(328)
      MI(329)=KT(581)*ALFA(317)*ALFA(61)**3/GAMMA(329)
      MI(330)=KT(582)*ALFA(317)*ALFA(61)**4/GAMMA(330)
      MI(331)=KT(583)*ALFA(317)*ALFA(61)**5/GAMMA(331)
      MI(346)=KT(607)*ALFA(318)/GAMMA(346)
      MI(347)=KT(608)*ALFA(318)*ALFA(61)/GAMMA(347)
      MI(348)=KT(609)*ALFA(318)*ALFA(61)**2/GAMMA(348)
      MI(349)=KT(610)*ALFA(318)*ALFA(61)**3/GAMMA(349)
      MI(61)=FTOT/(1.+GAMMA(61)*(MI(19)+MI(54)+2.*MI(55)+3.*MI(56)+
     *4.*MI(57)+MI(100)+MI(101)+2.*MI(102)+3.*MI(103)+4.*MI(104)+
     *MI(105)+2.*MI(106)+3.*MI(107)+MI(116)+6.*MI(124)+MI(125)+
     *2.*MI(126)+MI(137)+MI(150)+MI(164)+2.*MI(165)+MI(188)+
     *2.*MI(189)+3.*MI(190)+4.*MI(191)+MI(207)+MI(219)+2.*MI(296)+
     *MI(297)+MI(308)+MI(326)+2.*MI(327)+3.*MI(328)+4.*MI(329)+
     *5.*MI(330)+6.*MI(331)+MI(346)+2.*MI(347)+3.*MI(348)+
     *4.*MI(349)))
      C1 = MI(61) * GAMMA(61)
      ALFA(61) = C1
C
      DO 90 J = 1 , 40
      I = LISTE3(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
   90 CONTINUE
C
C**** MASS BALANCE ON PHOSPHATE */
C
```

```
  100 IF (PTOT .LE. 0.0) GOTO 120
      MI(12)=KT(139)*KT(15)*ALFA(8)/(TENPH*GAMMA(12))
      MI(39)=KT(123)*ALFA(1)/GAMMA(39)
      MI(40)=KT(124)*KT(16)*ALFA(1)/(TENPH**2*GAMMA(40))
      MI(46)=KT(15)/(TENPH*GAMMA(46))
      MI(47)=KT(16)/(TENPH**2*GAMMA(47))
      MI(49)=KT(30)*KT(15)*ALFA(2)/(TENPH*GAMMA(49))
      MI(60)=KT(32)*KT(15)*ALFA(3)/(TENPH*GAMMA(60))
      MI(64)=KT(120)*KT(16)*ALFA(7)/(TENPH**2*GAMMA(64))
      MI(72)=KT(33)*KT(15)*ALFA(1)/(TENPH*GAMMA(72))
      MI(73)=KT(34)*KT(15)*ALFA(0)/(TENPH*GAMMA(73))
      MI(74)=KT(121)*ALFA(0)/GAMMA(74)
      MI(75)=KT(122)*KT(16)*ALFA(0)/(TENPH**2*GAMMA(75))
      MI(98)=KT(156)*KT(16)*ALFA(8)/(TENPH**2*GAMMA(98))
      MI(99)=KT(138)*KT(15)*ALFA(7)/(TENPH*GAMMA(99))
      MI(353)=KT(614)*ALFA(318)/(TENPH*GAMMA(353))
      MI(354)=KT(615)*ALFA(318)*ALFA(44)/(TENPH**2*GAMMA(354))
      MI(355)=KT(616)*ALFA(318)/(TENPH**2*GAMMA(355))
      MI(356)=KT(617)*ALFA(318)*ALFA(44)/(TENPH**4*GAMMA(356))
      MI(357)=KT(618)*ALFA(318)*ALFA(44)**2/(TENPH**6*GAMMA(357))
      MI(374)=KT(647)*ALFA(318)/(TENPH**3*GAMMA(374))
      MI(376)=KT(649)*ALFA(318)/GAMMA(376)
      MI(44)=PTOT/(1.+ GAMMA(44)*(MI(12)+MI(39)+MI(40)+MI(46)+MI(47)+
     *MI(49)+MI(60)+MI(64)+MI(72)+MI(73)+MI(74)+MI(75)+MI(98)+
     *MI(99)+MI(353)+2*MI(354)+MI(355)+2*MI(356)+3*MI(357)+MI(374)+
     *MI(376)))
      C1 = MI(44) * GAMMA(44)
      ALFA(44) = C1
C
      DO 110 J = 1 , 21
      I = LISTE4(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  110 CONTINUE
C
C**** MASS BALANCE ON CHLORIDE */
C
  120 IF (CLTOT .LE. 0.0) GOTO 140
      MI(15)  = KT(5)    * ALFA(8)   / GAMMA(15)
      MI(27)  = KT(6)    * ALFA(8)   * ALFA(4)    / GAMMA(27)
      MI(32)  = KT(7)    * ALFA(8)   * ALFA(4)**2 / GAMMA(32)
      MI(111) = KT(170)  * ALFA(109) / GAMMA(111)
      MI(112) = KT(171)  * ALFA(109) * ALFA(4)    / GAMMA(112)
      MI(113) = KT(172)  * ALFA(109) * ALFA(4)**2 / GAMMA(113)
      MI(128) = (KT(206) / KT(208))  * ALFA(127) * ALFA(4) / GAMMA(128)
      MI(129) = (KT(207) / KT(208))  * ALFA(127)*ALFA(4)**2 /GAMMA(129)
      MI(133) = KT(211)  * ALFA(130) / GAMMA(133)
      MI(134) = KT(212)  * ALFA(130) * ALFA(4)    / GAMMA(134)
      MI(135) = KT(213)  * ALFA(130) * ALFA(4)**2 / GAMMA(135)
      MI(136) = KT(214)  * ALFA(130) * ALFA(4)**3 / GAMMA(136)
      MI(146) = KT(251)  * ALFA(145) / GAMMA(146)
      MI(147) = KT(252)  * ALFA(145) * ALFA(4)    / GAMMA(147)
      MI(148) = KT(253)  * ALFA(145) * ALFA(4)**2 / GAMMA(148)
      MI(149) = KT(254)  * ALFA(145) * ALFA(4)**3 / GAMMA(149)
      MI(155) = KT(260)  * ALFA(145) * AH2O*TENPH / GAMMA(155)
      MI(161) = KT(294)  * ALFA(160) / GAMMA(161)
      MI(162) = KT(295)  * ALFA(160) * ALFA(4)    / GAMMA(162)
      MI(163) = KT(296)  * ALFA(160) * ALFA(4)**2 / GAMMA(163)
      MI(172) = KT(305)  * ALFA(160) * AH2O*TENPH / GAMMA(172)
      MI(183) = KT(341)  * ALFA(182) / GAMMA(183)
      MI(184) = KT(342)  * ALFA(182) * ALFA(4)    / GAMMA(184)
      MI(185) = KT(343)  * ALFA(182) * ALFA(4)**2 / GAMMA(185)
      MI(186) = KT(344)  * ALFA(182) * ALFA(4)**3 / GAMMA(186)
      MI(206) = KT(404)  * ALFA(204) / GAMMA(206)
      MI(215) = KT(423)  * ALFA(212) / GAMMA(215)
```

```
      MI(216) = KT(424)  * ALFA(212) * ALFA(4)    / GAMMA(216)
      MI(217) = KT(425)  * ALFA(212) * ALFA(4)**2 / GAMMA(217)
      MI(218) = KT(426)  * ALFA(212) * ALFA(4)**3 / GAMMA(218)
      MI(279) = KT(518)  * ALFA(204) * ALFA(4)    / GAMMA(279)
      MI(315) = KT(542)  * ALFA(7)   / GAMMA(315)
      MI(332) = KT(586)  * ALFA(317) / GAMMA(332)
      MI(350) = KT(611)  * ALFA(318) / GAMMA(350)
      MI(371) = KT(644)  * ALFA(318) * ALFA(4)    / GAMMA(371)
C
      MI(4) = CLTOT/(1.0 + GAMMA(4) * (MI(15) +2.*MI(27) +3.*MI(32)
     *+MI(111) +2.*MI(112) +3.*MI(113) +2.*MI(128) +3.*MI(129)+
     *MI(133) +2.*MI(134) +3.*MI(135) +4.*MI(136) +MI(146) +2.*MI(147)+
     *3.*MI(148) +4.*MI(149) +MI(155) +MI(161) +2.*MI(162) +3.*MI(163)+
     *MI(172) +MI(183) +2.*MI(184) +3.*MI(185) +4.*MI(186) +MI(206)+
     *MI(215) +2.*MI(216) +3.*MI(217) +4.*MI(218) +2.*MI(279) +MI(315)+
     *MI(332) +MI(350) +2.*MI(371)))
C
      C1 = MI(4) * GAMMA(4)
      ALFA(4) = C1
      DO 130 J = 1 , 35
      I = LISTE5(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  130 CONTINUE
C
C**** MASS BALANCE ON SULFIDE */
C
  140 IF (H2STOT .LE. 0.0) GOTO 160
      MI(13)=1/(KT(91)*TENPH*GAMMA(13))
      MI(67)=KT(92)*TENPH/GAMMA(67)
      MI(247)=KT(476)*ALFA(7)*ALFA(66)/GAMMA(247)
      MI(248)=KT(477)*ALFA(7)*ALFA(66)**2/GAMMA(248)
      MI(144)=KT(222)*ALFA(130)*ALFA(66)**2/GAMMA(144)
      MI(156)=KT(261)*ALFA(145)*ALFA(66)/GAMMA(156)
      MI(157)=KT(262)*ALFA(145)*ALFA(66)**2/GAMMA(157)
      MI(175)=KT(308)*ALFA(160)/GAMMA(175)
      MI(176)=KT(309)*ALFA(160)*ALFA(66)/GAMMA(176)
      MI(177)=KT(310)*ALFA(160)*ALFA(66)**2/GAMMA(177)
      MI(178)=KT(311)*ALFA(160)*ALFA(66)**3/GAMMA(178)
      MI(198)=KT(356)*ALFA(182)*ALFA(66)/GAMMA(198)
      MI(199)=KT(357)*ALFA(182)*ALFA(66)**2/GAMMA(199)
      MI(220)=KT(428)*ALFA(212)/GAMMA(220)
      MI(221)=KT(429)*ALFA(212)*ALFA(66)/GAMMA(221)
      MI(259)=KT(485)*ALFA(127)*ALFA(66)*TENPH**2/GAMMA(259)/KT(208)
      MI(260)=KT(486)*ALFA(127)*ALFA(66)*TENPH**2/GAMMA(260)/KT(208)
      MI(263)=KT(502)*TENPH/GAMMA(263)
      MI(264)=KT(503)*TENPH/GAMMA(264)
      MI(265)=KT(504)*TENPH/GAMMA(265)
      MI(266)=KT(505)*TENPH/GAMMA(266)
      MI(267)=KT(506)*TENPH/GAMMA(267)
      MI(268)=KT(507)*ALFA(212)*ALFA(66)*TENPH**2/GAMMA(268)
      MI(269)=KT(508)*ALFA(212)*ALFA(66)*TENPH**2/GAMMA(269)
      MI(270)=KT(509)*ALFA(212)*ALFA(66)*TENPH/GAMMA(270)
      MI(66)=H2STOT/(1.+GAMMA(66)*(MI(13)+MI(67)+2.*MI(247)+3.*MI(248)+
     *3.*MI(144)+2.*MI(156)+3.*MI(157)+MI(175)+2.*MI(176)+3.*MI(177)+
     *4.*MI(178)+2.*MI(198)+3.*MI(199)+MI(220)+2.*MI(221)+2.*MI(259)+
     *2.*MI(260)+MI(263)+MI(264)+MI(265)+MI(266)+MI(267)+
     *2.*MI(268)+2.*MI(269)+2*MI(270)))
      C1 = MI(66) * GAMMA(66)
      ALFA(66) = C1
      DO 150 J = 1 , 25
      I = LISTE6(J)
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  150 CONTINUE
```

```
      IF (ALFA(5)*ALFA(13) .LE. 0.0) GOTO 155
      PE(5) = 0.125 * LOGKT(90)+0.125 * DLOG10(ALFA(5))-1.25*PH
     *-0.125 * DLOG10(ALFA(13))-0.5*LH2O
      EH(5) = PE(5)* C*R*T / F
  155 IF (ALFA(13) .LE. 0.0) GOTO 160
      PE(7) = (LOGKT(538)-DLOG10(ALFA(13)))/2E0-PH
      EH(7) = PE(7) * C*R*T/F
C
C**** MASS BALANCE ON FULVATE */
C
  160 IF (FULVTT .LE. 0.0) GOTO 180
      MI(286)=KT(523)/(TENPH*GAMMA(286))
      MI(288)=KT(525)*ALFA(8)/GAMMA(288)
      MI(290)=KT(527)*ALFA(130)/GAMMA(290)
      MI(292)=KT(529)*ALFA(160)/GAMMA(292)
      MI(294)=KT(531)*ALFA(212)/GAMMA(294)
      MI(284)=FULVTT/(1.+ GAMMA(284)*(MI(286)+MI(288)+MI(290)+MI(292)+
     *MI(294)))
      C1 = MI(284) * GAMMA(284)
      ALFA(284) = C1
      DO 170 I=286 , 294 , 2
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  170 CONTINUE
C
C**** MASS BALANCE ON HUMATE */
C
  180 IF (HUMTOT .LE. 0.0) GOTO 200
      MI(287)=KT(524)/(TENPH*GAMMA(287))
      MI(289)=KT(526)*ALFA(8)/GAMMA(289)
      MI(291)=KT(528)*ALFA(130)/GAMMA(291)
      MI(293)=KT(530)*ALFA(160)/GAMMA(293)
      MI(295)=KT(532)*ALFA(212)/GAMMA(295)
      MI(285)=HUMTOT/(1.+ GAMMA(285)*(MI(287)+MI(289)+MI(291)+MI(293)+
     *MI(295)))
      C1 = MI(285) * GAMMA(285)
      ALFA(285) =C1
      DO 190 I = 287 , 295 , 2
      MI(I) = C1 * MI(I)
      ALFA(I) = MI(I) * GAMMA(I)
  190 CONTINUE
C
C**** ITERATIVE TESTS */
C
  200 RBIT = 0
      IF (ABS(S1 + M1 - ANLCO3) .GT. 1E-3  * ANLCO3) RBIT = 1
      IF (ABS(S2 + M2 - SO4TOT) .GT. 1E-3  * SO4TOT) RBIT = 1
      IF (ABS(S3 + M3 - FTOT) .GT. 1E-3  * FTOT) RBIT = 1
      IF (ABS(S4 + M4 - PTOT) .GT. 1E-3  * PTOT) RBIT = 1
      IF (ABS(S5 + M5 - CLTOT) .GT. 1E-3  * CLTOT) RBIT = 1
      IF (ABS(S6 + M6 - H2STOT) .GT. 1E-3  * H2STOT) RBIT = 1
      IF (ABS(S7 + M7 - FULVTT) .GT. 1E-3 * FULVTT) RBIT = 1
      IF (ABS(S8 + M8 - HUMTOT) .GT. 1E-3 * HUMTOT) RBIT = 1
C
      S1 = S1 + M1 - ANLCO3
      S2 = S2 + M2 - SO4TOT
      S3 = S3 + M3 - FTOT
      S4 = S4 + M4 - PTOT
      S5 = S5 + M5 - CLTOT
      S6 = S6 + M6 - H2STOT
      S7 = S7 + M7 - FULVTT
      S8 = S8 + M8 - HUMTOT
C
      WRITE(K,1000)ITER,S1,S2,S3,S4,S5,S6,S7,S8
 1000 FORMAT(I4,1PE14.6,7E15.6)
```

```
C
C**** ITERATION MONITOR */
C
      IF (ITER .LT. 200) GOTO 210
      RBIT = 0
      WRITE(K,1010)
 1010 FORMAT(/,'**********************************************************
     **********************************************')
      WRITE(K,1020)
 1020 FORMAT(/,' CONVERGENCE NOT REACHED IN 200 ITERATIONS.  CALCULATION
     * TERMINATED.',/,' PRINT OF CALCULATIONS FOLLOWS FOR CHECKING ONLY.
     *')
      WRITE(K,1010)
      WRITE(*,1030)
 1030 FORMAT(/' CONVERGENCE NOT REACHED IN 200 ITERATIONS.  CALCULATION
     *TERMINATED.'/' RESULTS PRINTED OUT FOR CHECKING ONLY.')
  210 IF (ITER .LT. 3) RBIT = 1
      RETURN
      END
      SUBROUTINE SOLUTS(ANAL,Z,PAGE1,ALFA,ANALMI,CUNITS,GAMMA,GFW,
     *MI,LOGKT,SIGMA,ERR)
C
      REAL*8 ALFA(0:377),ANALMI(0:377),CUNITS(0:377),ERR(0:653),
     *GAMMA(0:377),GFW(0:377),MI(0:377),LOGKT(0:653),
     *SIGMA(0:377),RSD(0:377),LZERO(10),X(10),CONV(10)
      REAL*8 PCT,S1,S2,S3,S4,S5,S6,S7,S8
      INTEGER ANAL(0:377),Z(0:377),LISTE(14),LISTE1(71),LISTE2(13)
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*2 STARS
C
      INTEGER*2 IDAY,IMONTH,IYEAR,IHOUR,IMIN,ISEC,IHSEC
C
      LOGICAL PRFLAG
$INCLUDE:'COMMON_BLK'
C
      DATA LISTE/5,7,8,13,38,84,202,261,262,299,300,301,317,318/
      DATA LISTE1/0,1,2,3,4,5,6,7,8,9,10,13,16,17,23,25,26,34,35,38,39,
     *44,46,48,50,51,53,61,66,67,80,84,86,87,89,94,96,97,101,106,108,
     *109,110,114,127,130,138,145,151,160,167,182,192,202,204,208,212,
     *224,249,250,255,257,258,261,262,298,302,305,316,317,318/
      DATA LISTE2/4,26,48,63,84,94,96,97,202,284,285,286,287/
      DATA LZERO /59.5,53,50.1,73.5,76.35,80,44.5,71.46,349.8,198.3/
      DATA X /115.1,109.2,41.8,47.1,47.8,133.9,40.5,46.7,110.42,75.73/
      DATA CONV /4.99E-5,8.226E-5,4.35E-5,2.557E-5,2.821E-5,2.082E-5,
     *1.639E-5,1.613E-5,99.209E-5,5.88E-5/
C
      C2 = 0
      DO 10 N = 0 , D
      C2 = C2 + ANALMI(N) * GFW(N) * 1E3
   10 CONTINUE
      C2 = C2 * 1E6 / (C2 + 1E6)
C
C       CONDUCTANCE-TEST
C
      CUNITS(26) = MI(26) * 1E3 * GFW(26) * (1 - 1E-6 * C2)
      CUNITS(63) = MI(63) * 1E3 * GFW(63) * (1 - 1E-6 * C2)
      C1 = 0.0
      N = 0
      DO 15 I = 0 , 6
      N = N + 1
      LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)
      NORM = CUNITS(I) * CONV(N)
      C1 = C1 + LAMBDA * NORM
   15 CONTINUE
      N = N + 1
```

```
      LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)
      NORM = CUNITS(84) * CONV(N)
      C1 = C1 + LAMBDA * NORM
      N = N + 1
      LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)
      NORM = CUNITS(63) * CONV(N)
      C1 = C1 + LAMBDA * NORM
      N = N + 1
      LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)
      NORM = CUNITS(26) * CONV(N)
      C1 = C1 + LAMBDA * NORM
      CONCLC = 1E3 * C1
      CUNITS(26) = 0.0
      CUNITS(63) = 0.0
C
C      END CONDUCTANCE-TEST
C
C**** AUXILIARY PE CALCULATIONS */
C
      SIGMPE = SIGMEH * F / (C*R*T)
      IF (ALFA(5)*ALFA(13) .LE. 0.0) GOTO 20
      PE(5) = 0.125 * LOGKT(90)+0.125 * DLOG10(ALFA(5))-1.25*PH
     *-0.125 * DLOG10(ALFA(13))-0.5*LH2O
      EH(5) = PE(5)* C*R*T / F
C      END
   20 IF (ALFA(38)*ALFA(84) .LE. 0.0) GOTO 30
      PE(4)=(-LOGKT(127)+DLOG10(ALFA(84))- 10.0 * PH - DLOG10(ALFA(38))
     *-3E0*LH2O)/8E0
      EH(4) = PE(4)* C*R*T / F
C      END
   30 IF (ALFA(202)*ALFA(84) .LE. 0.0) GOTO 40
      PE(6) = (LOGKT(400) + DLOG10(ALFA(84))-DLOG10(ALFA(202))
     *-LH2O-2*PH)/2E0
      EH(6) = PE(6) * C*R*T/F
C      END
   40 IF (ALFA(250)*ALFA(255) .LE. 0.0) GOTO 42
      PE(8) = (DLOG10(ALFA(255)/ALFA(250)) - LOGKT(487)-LH2O)/2E0-PH
      EH(8) = PE(8) * C*R*T/F
C      END
   42 IF (ALFA(250) .LE. 0.0) GOTO 50
      PE(9) = (LOGKT(557) + DLOG10(ALFA(250)))/3E0-LH2O-PH
      EH(9) = PE(9) * C*R*T/F
C      END
   50 IF (ALFA(305)*ALFA(307) .LE. 0.0) GOTO 52
      PE(10) = (DLOG10(ALFA(307)/ALFA(305)) - LOGKT(548)-LH2O)/2E0-PH
      EH(10) = PE(10) * C*R*T/F
C      END
   52 IF (ALFA(305) .LE. 0.0) GOTO 54
      PE(11) = (DLOG10(ALFA(305)) + LOGKT(551)-3*LH2O-6*PH)/4E0
      EH(11) = PE(11) * C*R*T/F
C      END
   54 IF (ALFA(302) .LE. 0.0) GOTO 56
      PE(12) = (LOGKT(550)- DLOG10(ALFA(302)) - PH)/2E0
      EH(12) = PE(12) * C*R*T/F
C      END
   56 IF (ALFA(13) .LE. 0.0) GOTO 58
      PE(7) = (LOGKT(538)-DLOG10(ALFA(13)))/2E0-PH
      EH(7) = PE(7) * C*R*T/F
   58 IF (ALFA(317).GT.1D-78 .AND. ALFA(318).GT.1D-78) THEN
        PE(13) =-0.5*(-LOGKT(565)+LOG10(ALFA(317))+2*LH2O-
     *  LOG10(ALFA(318))+4*PH)
        EH(13)=PE(13)*C*R*T/F
      END IF
C
C     EHERR
```

```
C
      DO 45 I = 0, 307
      RSD (I) = 2.0E7
   45 CONTINUE
C
      DO 55 J = 1 , 14
      I = LISTE(J)
      IF (CUNITS(I)*SIGMA(I) .GT. 0.0) RSD(I)=SIGMA(I)/CUNITS(I)/C
   55 CONTINUE
      IF (SIGMDO * DOX .GT. 0.0) RSDDO = SIGMDO / DOX / C
      IF (SIGMDO * DOX .LE. 0.0) RSDDO = 2E7
      ERR(0)=SQRT(RSD(7)**2 + RSD(8)**2)
      ERR(1)=SQRT(SIGMPH**2+(.5*RSD(84))**2+(.5*RSD(202))**2)
      ERR(2)=SQRT((1.25*SIGMPH)**2+(.125*RSD(84))**2+
     *(.125*RSD(38))**2)
      ERR(3)=SQRT((1.25*SIGMPH)**2+(.125*RSD(5))**2+(.125*RSD(13))**2)
      ERR(4)=SQRT(0.5*RSD(13)**2*SIGMPH**2)
      ERR(5)=SQRT(SIGMPH**2 + RSDDO**2)
      ERR(6)=ERR(5)
      ERR(7)=SQRT(0.5*(RSD(261))**2+0.5*(RSD(262))**2+SIGMPH**2)
      ERR(8)=SQRT(0.5*(RSD(300))**2+0.5*(RSD(301))**2+SIGMPH**2)
      ERR(9)=SQRT(0.25*(RSD(300))**2+(1.5*SIGMPH)**2)
      ERR(10)=SQRT((RSD(299)/6.)**2+(RSD(300)/6.)**2+
     *       ((7.*SIGMPH)/6.)**2)
      DO 60 I = 0 , 11
      IF (ERR(I).GT.1E2) ERR(I) = 0.0
      ERR(I+12) = ERR(I) * C*R*T/F
   60 CONTINUE
      IF (ALFA(5) .LE. 0.0) GOTO 65
      S4 = LOGKT(90) - 4.0 * LH2O + DLOG10(ALFA(5)) - 10.0 * PH
     *     - 8.0 * PE(EHOPT(8))
      IF(ABS(S4) .LE. 78) THEN
        ALFA(65) = 10.**(S4)
        MI(65) = ALFA(65) / GAMMA(65)
      END IF
C
C**** PRINT OF INPUT */
C
   65 CALL GETDAT(IYEAR,IMONTH,IDAY)
      CALL GETTIM(IHOUR,IMIN,ISEC,IHSEC)
      WRITE(K,1003)CARD1,IMONTH,IDAY,IYEAR-1900,IHOUR,IMIN
 1003 FORMAT(1H1,1X,A80:,9X,'Date = ',I2,2('/',I2.2),2X,I2,':',I2.2)
      WRITE(K,1005) CARD2
 1005 FORMAT(1H ,A80)
      WRITE(K,1010)DOX,DOC,ITDS
 1010 FORMAT('       DOX =  ',F11.4,'          DOC =  ',F8.1,
     *'       INPUT TDS = ',F8.1)
      WRITE(K,1040)COND,CONCLC,ALFA(65)
 1040 FORMAT(' Anal Cond = ',F8.1,'       Calc Cond = ',F8.1,
     *'       Activity H2S calc from SO4 and pe = ',1PE9.2)
      INADD=0
   70 DIFF1 = 200. * (EPMCAT-EPMAN)/(EPMAN+EPMCAT)
      EPCAT1 = EPMCAT * 1000.
      EPMAN1 = EPMAN  * 1000.
      WRITE(K,1080)EPCAT1,EPMAN1,DIFF1
 1080 FORMAT(' Anal EPMCAT =',F12.4,'   Anal EPMAN =',F12.4,
     *'   Percent difference in input cation/anion balance = ',F9.4)
C
C**** RECALCULATION OF CATION-ANION BALANCE */
C
      EPMAN  = 0.0
      EPMCAT = 0.0
      DO 100 I = 0 , D
      IF(I.EQ.16 .OR. I.EQ.34 .OR. I.EQ.69 .OR. I.EQ.70 .OR.I.EQ.71
     *.OR. I.EQ.83 .OR. I.EQ.86) GOTO 100
```

```
      IF (Z(I) .GT. 0) EPMCAT = EPMCAT + Z(I) * MI(I)
      IF (Z(I) .LE. 0) EPMAN  = EPMAN  - Z(I) * MI(I)
  100 CONTINUE
      EPCAT1 = EPMCAT * 1000.
      EPMAN1 = EPMAN  * 1000.
      DIFF1 = 200. * (EPMCAT-EPMAN)/(EPMAN+EPMCAT)
      IF (ABS(DIFF1) .LE. 30.) GOTO 320
      INADD=INADD+2
      WRITE(*,1000)
      WRITE(K,1000)
 1000 FORMAT(' DIFFERENCE IN CALCULATED CHARGE BALANCE GREATER THAN 30
     *PERCENT.  CHECK INPUT DATA.'/)
      WRITE(*,1100)EPCAT1,EPMAN1,DIFF1
C
C****  Calculation of total ionic strength (from speciation)
C
  320 WRITE(K,1100)EPCAT1,EPMAN1,DIFF1
 1100 FORMAT(' Calc EPMCAT =',F12.4,'   Calc EPMAN =',F12.4,
     *'   Percent difference in calc  cation/anion balance = ',F9.4)
C
      WRITE(K,1102) XMUSAV
 1102 FORMAT(' Total  Ionic  Strength   (T.I.S.) from input data = ',
     *F10.5)
      WRITE(K,1104) XMU
 1104 FORMAT(' Effective Ionic Strength (E.I.S.) from speciation = ',
     *F10.5)
C
C**** CALC. OF PO2 */
C
      IF (ABS(PE(EHOPT(7))) .GE. 19.0) GOTO 110
      C1 = LOGKT(93) + PH + PE(EHOPT(7)) + 0.5 * LH2O
      ALFA(69) = 10.  ** (4E0 * C1)
C
  110 PCO2=0.0
      IF (ALFA(85) .LE. 0.0) GOTO 120
      PCO2=10.**(DLOG10(ALFA(85))-2385.73E0/T-1.5264E-2*T+14.0184E0+
     *XMU * (0.119 - 8.33E-4 * TEMP + 6.66E-6 * TEMP**2))
  120 NONCRB=MI(24)+2*MI(25)+MI(26)+MI(36)+2*MI(44)+MI(46)
     *+MI(53)+MI(66)+2*MI(67)
      CARBON = MI(6) + 2 * MI(17)
      S6 = MI(6) + MI(17) + MI(20) + MI(21) + MI(29) + MI(30) + MI(41)
     *+ MI(42) + MI(68) + MI(85) + MI(95) + MI(119) + MI(131)
     *+ 2*MI(132) + 2*MI(166) + 2*MI(187) + MI(241) + MI(271) + MI(272)
     *+ MI(273) + 2*MI(274) + MI(275) + MI(276) + MI(278) + MI(280)
     *+ MI(281) + 2*MI(282) + MI(309) + MI(310) + MI(311) + MI(312)
     *+ MI(313) + 4*MI(335) + 5*MI(336) + MI(343) + 2*MI(344)
     *+ 3*MI(345) + 6*MI(375) + 3*MI(377)
      TDS = 0.0
      DO 130 I = 0 , D
      TDS = TDS + ANALMI(I) * GFW(I) * 1E3 * (1-1E-6*C2)
  130 CONTINUE
C     IF (ABS(PE(0)) .GT. 19.0) PE(0) = 99.9999
C
C**** PRINT OF SOLUTE DATA */
C
C     Eh, pe CALCULATIONS
C
      WRITE(K,1110)
 1110 FORMAT(' ',98X,'Sato')
      WRITE(K,1120)
 1120 FORMAT('    Input  Sigma   Fe3/Fe2 Sigma   NO3/NO2 Sigma   NO3/NH4
     *Sigma   SO4/S=  Sigma     S/S=  Sigma   H2O2/O2 Sigma    H2O/O2 Si
     *gma'/'   - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     * - Eh - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     *-')
```

```
C
  110 PCO2=0.0
      IF (ALFA(85) .LE. 0.0) GOTO 120
      PCO2=10.**(DLOG10(ALFA(85))-2385.73E0/T-1.5264E-2*T+14.0184E0+
     *XMU * (0.119 - 8.33E-4 * TEMP + 6.66E-6 * TEMP**2))
  120 NONCRB=MI(24)+2*MI(25)+MI(26)+MI(36)+2*MI(44)+MI(46)
     *+MI(53)+MI(66)+2*MI(67)
      CARBON = MI(6) + 2 * MI(17)
      S6 = MI(6) + MI(17) + MI(20) + MI(21) + MI(29) + MI(30) + MI(41)
     *+ MI(42) + MI(68) + MI(85) + MI(95) + MI(119) + MI(131)
     *+ 2*MI(132) + 2*MI(166) + 2*MI(187) + MI(241) + MI(271) + MI(272)
     *+ MI(273) + 2*MI(274) + MI(275) + MI(276) + MI(278) + MI(280)
     *+ MI(281) + 2*MI(282) + MI(309) + MI(310) + MI(311) + MI(312)
     *+ MI(313) + 4*MI(335) + 5*MI(336) + MI(343) + 2*MI(344)
     *+ 3*MI(345) + 6*MI(375) + 3*MI(377)
      TDS = 0.0
      DO 130 I = 0 , D
      TDS = TDS + ANALMI(I) * GFW(I) * 1E3 * (1-1E-6*C2)
  130 CONTINUE
C     IF (ABS(PE(0)) .GT. 19.0) PE(0) = 99.9999
C
C**** PRINT OF SOLUTE DATA */
C
C     Eh, pe CALCULATIONS
C
      WRITE(K,1110)
 1110 FORMAT(' ',98X,'Sato')
      WRITE(K,1120)
 1120 FORMAT('   Input  Sigma   Fe3/Fe2 Sigma   NO3/NO2 Sigma   NO3/NH4
     *Sigma   SO4/S=  Sigma     S/S=  Sigma   H2O2/O2 Sigma    H2O/O2 Si
     *gma'/'   - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     * - Eh - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     *-')
      WRITE(K,1130)EH(0),SIGMEH,EH(1),ERR(12),EH(6),ERR(13),EH(4),
     *ERR(14),EH(5),ERR(15),EH(7),ERR(16),EH(2),ERR(17),EH(3),ERR(18)
 1130 FORMAT(1H ,2F7.3,7(F9.3,F7.3))
      WRITE(K,1150)
 1150 FORMAT(/'   - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     *- - - pe - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     * - -')
      WRITE(K,1130)PE(0),SIGMPE,PE(1),ERR(0),PE(6),ERR(1),PE(4),ERR(2),
     *PE(5),ERR(3),PE(7),ERR(4),PE(2),ERR(5),PE(3),ERR(6)
      WRITE(K,1160)
 1160 FORMAT(/,'  As5/As3 Sigma    As3/As Sigma   Se6/Se4 Sigma   Se4/Se
     *  Sigma    Se/Se= Sigma    U6/U4  Sigma          Sigma
     *Sigma'/'   - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     * - - Eh - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     *- -')
      WRITE(K,1130)EH(8),ERR(19),EH(9),ERR(20),EH(10),ERR(21),EH(11),
     *ERR(22),EH(12),ERR(23),EH(13)
      WRITE(K,1150)
      WRITE(K,1130)PE(8),ERR(7),PE(9),ERR(8),PE(10),ERR(9),PE(11),
     *ERR(10),PE(12),ERR(11),PE(13)
C
      WRITE(K,1178)
 1178 FORMAT(/'                                Effective')
      WRITE(K,1180)
      S2 = 4.4E4*PCO2
      S3 = 3.2E4*ALFA(69)
      S5=0
      IF(PCO2 .GT. 0.) S5=ALOG10(PCO2)
 1180 FORMAT( '     T      pH     TDS ppm  Ionic Str  pO2 Atm  ppm O2 Atm
     *  pCO2 Atm  ppm CO2 Atm  log pCO2   CO2 Tot              Ncrb Alk
     * aH2O')
      WRITE(K,1190)TEMP,PH,TDS,XMU,ALFA(69),S3,PCO2,S2,S5,S6,NONCRB,AH2O
```

```
  155 CONTINUE
C
      C1 = 0.0
      STARS = '  '
      IF (ALFA(I) .GT. 0.0) C1 = -DLOG10 (ALFA(I))
      IF (FULFLG .NE. 1) GOTO 170
      DO 160 J = 284 , 294 , 2
      IF (I .EQ. J) STARS = '**'
  160 CONTINUE
  170 IF (HUMFLG .NE. 1) GOTO 185
      DO 180 J = 285 , 295 , 2
      IF (I .EQ. J) STARS= '**'
  180 CONTINUE
  185 S1 = CUNITS(I)
      S2 = MI(I) * GFW(I) * 1E3 * (1. - 1E-6 * C2)
      IF(S1.GT.0.0 .AND. MI(I).GT.0.0) THEN
        IF(S2.LT.1E-2) THEN
          WRITE(K,1300)I,STARS,PAGE1(I),Z(I),S1,S2,ANALMI(I),MI(I),
     *    PCT,ALFA(I),GAMMA(I),C1
        ELSE
          WRITE(K,1301)I,STARS,PAGE1(I),Z(I),S1,S2,ANALMI(I),MI(I),
     *    PCT,ALFA(I),GAMMA(I),C1
        END IF
      ELSE
        IF(S1.LT.1D-78 .AND. MI(I).GT.0E0) THEN
          IF(S2.LT.1E-2) THEN
            WRITE(K,1302)I,STARS,PAGE1(I),Z(I),S2,MI(I),PCT,ALFA(I),
     *      GAMMA(I),C1
          ELSE
            WRITE(K,1303)I,STARS,PAGE1(I),Z(I),S2,MI(I),PCT,ALFA(I),
     *      GAMMA(I),C1
          END IF
        ELSE
          IF(ANAL(I).EQ.0) THEN
            IF(S1.LT.1E-2) THEN
              WRITE(K,1304)I,STARS,PAGE1(I),Z(I),S1,ANALMI(I)
            ELSE
              WRITE(K,1305)I,STARS,PAGE1(I),Z(I),S1,ANALMI(I)
            END IF
          ELSE
            WRITE(K,1305)I,STARS,PAGE1(I),Z(I),S1
          END IF
        END IF
      END IF
      IN = IN + 1
      IF (IN .LT.57) GOTO 145
      IN = 0
      WRITE(K,1003) CARD1
      WRITE(K,1400)
      GOTO 145
  150 CLOSE(15)
C
      IF (EH(0) .GT. 9.0) PE(0) = 999
      IF (CUNITS(7)*CUNITS(8) .LE. 0.0) PE(1) = 999
      IF (PE(0) .GT. 9E1) PE(0) = 2E1
C
C**** RECONSTITUTE TOTAL CONCENTRATIONS OF Fe, As, Se & U FOR RATIO CALCS
C
      CUNITS(16)=CUNITS(16)+CUNITS(7)+CUNITS(8)
      CUNITS(249)=CUNITS(249)+CUNITS(261)+CUNITS(262)
      CUNITS(298)=CUNITS(298)+CUNITS(299)+CUNITS(300)+CUNITS(301)
      CUNITS(316)=CUNITS(316)+CUNITS(317)+CUNITS(359)
C
C**** CONVERSION OF ALFA AND CUNITS TO LOG FORM FOR AP CALCS & PUNCHING
C
```

```
      DO 190 I = 0 ,D
      IF ( ALFA(I) .LE. 0.0) ALFA(I) = -2E4
      IF ( ALFA(I) .GT. 0.0) ALFA(I) = DLOG10(ALFA(I))
      IF (CUNITS(I) .LE. 0.0) CUNITS(I) = -2E4
      IF (CUNITS(I) .GT. 0.0) CUNITS(I) = DLOG10(CUNITS(I))
  190 CONTINUE
      RETURN
 1300 FORMAT(' ',I3,A2,A8,I3,F16.6,F16.6,1X,2(1PE12.3),0PF10.2,1PE14.3,
     *0PF12.4,F12.3)
 1301 FORMAT(' ',I3,A2,A8,I3,F13.3,3X,F13.3,4X,2(1PE12.3),0PF10.2,
     *1PE14.3,0PF12.4,F12.3)
 1302 FORMAT(' ',I3,A2,A8,I3,16X,F16.6,13X,1PE12.3,0PF10.2,1PE14.3,
     *0PF12.4,F12.3)
 1303 FORMAT(' ',I3,A2,A8,I3,16X,F13.3,16X,1PE12.3,0PF10.2,1PE14.3,
     *0PF12.4,F12.3)
 1304 FORMAT(' ',I3,A2,A8,I3,F16.6,17X,1PE12.3)
 1305 FORMAT(' ',I3,A2,A8,I3,F13.3,20X,1PE12.3)
      END
      SUBROUTINE PCTEST(I,ANALMI,MI,S1,PCT,PRFLAG)
      DIMENSION LISTE(56,27),LIST22(27),NPOLY(0:377)
      REAL*8 AMI,ANALMI(0:377),MI(0:377),PCT,S1
      LOGICAL PRFLAG
$INCLUDE:'COMMON.BLK'
      DATA LISTE/0,28,31,81,29,30,100,75,73,74,46*-1,
     *           1,18,22,21,20,19,40,72,39,47*-1,
     *           2,43,42,41,49,297,50*-1,
     *           3,45,60,53*-1,
     *           7,10,79,11,315,247,248,33,122,309,310,308,99,64,8,9,76,
     *77,78,179,180,14,108,123,15,27,32,105,106,107,12,98,288,289,22*-1,
     *           50,51,52,53,54,55,56,57,58,59,181,203,44*-1,
     *           23,24,25,124,52*-1,
     *           35,36,101,102,103,104,50*-1,
     *           37,38,91,53*-1,
     *           87,68,88,95,314,51*-1,
     *           89,90,201,312,313,51*-1,
     *           80,82,54*-1,
     *           109,110,111,112,113,114,115,116,117,118,119,120,121,
     *311,42*-1,
     *           130,127,128,129,131,132,133,134,135,136,137,138,139,
     *140,141,142,143,144,259,260,271,290,291,33*-1,
     *           145,146,147,148,149,150,151,152,153,154,155,156,157,
     *158,159,229,230,231,232,272,273,274,34*-1,
     *           160,161,162,163,164,165,166,167,168,169,170,171,172,
     *173,174,175,176,177,178,233,234,235,236,275,276,277,292,293,28*-1,
     *           182,183,184,185,186,187,188,189,190,191,192,193,194,
     *195,196,197,198,199,200,237,238,239,240,241,242,243,278,29*-1,
     *           204,205,206,207,208,209,210,211,279,280,281,282,283,
     *43*-1,
     *           212,213,214,215,216,217,218,219,220,221,222,223,224,
     *225,226,227,228,244,245,246,268,269,270,294,295,31*-1,
     *           250,251,252,253,254,255,256,257,258,47*-1,
     *           299,302,303,304,305,306,307,49*-1,
     *           13,65,66,67,263,264,265,266,267,47*-1,
     *           6,17,85,53*-1,
     *           61,125,126,296,52*-1,
     *           44,46,47,53*-1,
     *           5,62,54*-1,
     *           317,318,319,320,321,322,323,325,326,327,328,
     *329,330,331,332,333,334,335,336,339,340,341,342,343,344,
     *345,346,347,348,349,350,351,352,353,354,355,356,357,360,361,
     *362,363,365,366,367,368,369,370,371,372,373,374,375,376,377,-1/
      DATA LIST22/0,1,2,3,7,50,34,86,38,87,89,80,109,130,145,160,182,
     *204,212,249,298,13,6,61,44,5,316/
      DATA NPOLY/126*1,2,15*1,2,28*1,2,7*1,2,3,14*1,2,4*1,3,62*1,2,3,4,
     *5,6,28*1,2,28*1,6,15*1,2,3,24*1,2,3,3,4,4*1,3,1,1/
```

```
C
      PCT=0.0
      DO 20 L=1,27
        AMI=ANALMI(LIST22(L))
        IF(L.EQ.5)  AMI=ANALMI(7)+ANALMI(8)+ANALMI(16)
        IF(L.EQ.20) AMI=ANALMI(249)+ANALMI(261)+ANALMI(262)
        IF(L.EQ.21) AMI=ANALMI(298)+ANALMI(299)+ANALMI(300)+ANALMI(301)
        IF(L.EQ.23) AMI=S1
        IF(L.EQ.27) AMI=ANALMI(316)+ANALMI(317)+ANALMI(359)
        IF(AMI.EQ.0.0) GOTO 20
        DO 10 J=1,56
          IF(LISTE(J,L).EQ.-1) GOTO 10
          IF(I.EQ.LISTE(J,L)) THEN
            PCT=100.0*MI(I)*NPOLY(I)/AMI
            IF(PCT .LT. 1.0) THEN
              PRFLAG=.FALSE.
              RETURN
            END IF
          END IF
   10   CONTINUE
   20 CONTINUE
      PRFLAG=.TRUE.
      RETURN
      END
      SUBROUTINE RATIO(PAGE1,ANALMI,CUNITS)
C
      INTEGER LISTE(23),LISTE2(10),LISTE3(6)
      REAL*8 ANALMI(0:377),CUNITS(0:377)
      CHARACTER*8 PAGE1(0:377)
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE/0,1,2,3,50,16,109,87,89,80,48,94,130,145,160,182,204,
     *249,298,86,61,97,96/
      DATA LISTE2/109,130,145,160,182,204,212,249,298,316/
      DATA LISTE3/0,1,2,3,61,87/
C
C**** CALCULATION OF WEIGHT AND MOLAR CONCENTRATION RATIOS*
C
      WRITE(K,990)CARD1
  990 FORMAT(1H1,1X,A80)
      WRITE(K,1000)
 1000 FORMAT(/,1X,'   Weight ratios from analytical ppm   -   ',
     *'Mole ratios from analytical molality',/)
C
C  Ratios to Cl and SO4
C
      DO 20 J = 1,23
      I = LISTE(J)
      IF (ANALMI(I) .LE. 0.0) GOTO 20
      C1 = 0.0
      IF (CUNITS(I).GT.-2E4.AND.CUNITS(4).GT.-2E4)
     * C1=10.**(CUNITS(I)-CUNITS(4))
      C2 = 0.0
      IF (ANALMI(I) .GT. 0.0 .AND. CLTOT .GT. 0.0) C2 = ANALMI(I)/CLTOT
      C3 = 0.0
      IF (CUNITS(I).GT.-2E4.AND.CUNITS(5).GT.-2E4)
     * C3=10.**(CUNITS(I)-CUNITS(5))
      C4 = 0.0
      IF (ANALMI(I) .GT. 0.0 .AND. SO4TOT .GT. 0.0)C4 = ANALMI(I)/SO4TOT
      IF (C1.GT.0. .AND. C2.GT.0.)
     * WRITE(K,1010) PAGE1(I)(1:2),C1,PAGE1(I)(1:2),C2
 1010 FORMAT(10X,A2,'/C1  = ',1PE11.4,20X,A2,'/C1  = ',1PE11.4)
      IF (C3.GT.0. .AND. C4.GT.0.)
     * WRITE(K,1020) PAGE1(I)(1:2),C3,PAGE1(I)(1:2),C4
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 1020 FORMAT(10X,A2,'/SO4 = ',1PE11.4,20X,A2,'/SO4 = ',1PE11.4)
   20 CONTINUE
      WRITE(K,*)
C
C  Ratios to HCO3
C
      C1=0
      IF (CUNITS(6).GT.-78.) C1=10.**CUNITS(6)
      C2=0
      IF (CUNITS(17).GT.-78.) C1=10.**CUNITS(17)
      IF (C1+C2.GT.1D-78) THEN
        C3=DLOG10(C1+C2)
        C4=CO2TIT
        DO 30 J = 1, 6
        I = LISTE3(J)
        C1 = 0.0
        IF (CUNITS(I).GT.-2E4 .AND. C3.GT.-2E4) C1=10.**(CUNITS(I)-C3)
        C2 = 0.0
        IF (ANALMI(I) .GT. 0.0 .AND. C4 .GT. 0.0) C2 = ANALMI(I)/C4
        IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1030) PAGE1(I)(1:2),C1,
     *   PAGE1(I)(1:2),C2
 1030 FORMAT(10X,A2,'/HCO3= ',1PE11.4,20X,A2,'/HCO3= ',1PE11.4)
   30   CONTINUE
      END IF
C
C  Ca/Mg, Na/K, Fe2/Fe3, Zn/Cd
C
      C1 = 0.0
      IF (CUNITS(0).GT.-2E4.AND.CUNITS(1).GT.-2E4)
     * C1=10.**(CUNITS(0)-CUNITS(1))
      C2 = 0.0
      IF (ANALMI(0).GT.0.0.AND.ANALMI(1).GT.0.0) C2=ANALMI(0)/ANALMI(1)
      C3 = 0.0
      IF (CUNITS(2).GT.-2E4.AND.CUNITS(3).GT.-2E4)
     * C3=10.**(CUNITS(2)-CUNITS(3))
      C4 = 0.0
      IF (ANALMI(2).GT.0.0.AND.ANALMI(3).GT.0.0) C4=ANALMI(2)/ANALMI(3)
      IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1040) C1,C2
 1040 FORMAT(/,10X,'Ca/Mg  = ',1PE11.4,20X,'Ca/Mg  = ',1PE11.4)
      IF (C3.GT.0. .AND. C4.GT.0.) WRITE(K,1050) C3,C4
 1050 FORMAT(10X,'Na/K   = ',1PE11.4,20X,'Na/K   = ',1PE11.4)
      C1 = 0.0
      IF (CUNITS(7).GT.-2E4.AND.CUNITS(8).GT.-2E4)
     * C1=10.**(CUNITS(7)-CUNITS(8))
      C2 = 0.0
      IF (ANALMI(7).GT.0.0.AND.ANALMI(8).GT.0.0) C2=ANALMI(7)/ANALMI(8)
      C3 = 0.0
      IF (CUNITS(145).GT.-2E4.AND.CUNITS(160).GT.-2E4)
     * C3=10.**(CUNITS(145)-CUNITS(160))
      C4 = 0.0
      IF (ANALMI(145).GT.0.0.AND.ANALMI(160).GT.0.0)
     * C4=ANALMI(145)/ANALMI(160)
      IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1060) C1,C2
 1060 FORMAT(10X,'Fe2/Fe3= ',1PE11.4,20X,'Fe2/Fe3= ',1PE11.4)
      IF (C3.GT.0. .AND. C4.GT.0.) WRITE(K,1070) C3,C4
 1070 FORMAT(10X,'Zn/Cd  = ',1PE11.4,20X,'Zn/Cd  = ',1PE11.4)
C
C  Na/Ca, Sr/Ca, B/F, B/As
C
      C1 = 0.0
      IF (CUNITS(2).GT.-2E4.AND.CUNITS(0).GT.-2E4)
     * C1=10.**(CUNITS(2)-CUNITS(0))
      C2 = 0.0
      IF (ANALMI(2).GT.0.0.AND.ANALMI(0).GT.0.0) C2=ANALMI(2)/ANALMI(0)
      C3 = 0.0
```

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      IF (CUNITS(87).GT.-2E4.AND.CUNITS(0).GT.-2E4)
     * C3=10.**(CUNITS(87)-CUNITS(0))
      C4 = 0.0
      IF(ANALMI(87).GT.0.0.AND.ANALMI(0).GT.0.0) C4=ANALMI(87)/ANALMI(0)
      IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1080) C1,C2
 1080 FORMAT(10X,'Na/Ca  = ',1PE11.4,20X,'Na/Ca  = ',1PE11.4)
      IF (C3.GT.0. .AND. C4.GT.0.) WRITE(K,1090) C3,C4
 1090 FORMAT(10X,'Sr/Ca  = ',1PE11.4,20X,'Sr/Ca  = ',1PE11.4)
      C1 = 0.0
      IF (CUNITS(86).GT.-2E4.AND.CUNITS(61).GT.-2E4)
     * C1=10.**(CUNITS(86)-CUNITS(61))
      C2 = 0.0
      IF (ANALMI(86).GT.0.0.AND.ANALMI(61).GT.0.0)
     * C2=ANALMI(86)/ANALMI(61)
      C3 = 0.0
      IF (CUNITS(86).GT.-2E4.AND.CUNITS(249).GT.-2E4)
     * C3=10.**(CUNITS(86)-CUNITS(249))
      C4 = 0.0
      IF (ANALMI(86).GT.0.0.AND.ANALMI(249).GT.0.0)
     * C4=ANALMI(86)/ANALMI(249)
      IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1100) C1,C2
 1100 FORMAT(10X,'  B/F  = ',1PE11.4,20X,'  B/F  = ',1PE11.4)
      IF (C3.GT.0. .AND. C4.GT.0.) WRITE(K,1110) C3,C4
 1110 FORMAT(10X,' B/As  = ',1PE11.4,20X,' B/As  = ',1PE11.4,/)
C
C  Trace metals/Fe total
C
      IF(FE2TOT.EQ.0. .AND. FE2TOT.EQ.0. .AND. FETOTL.EQ.0.) GOTO 50
      C3=DLOG10(10.**CUNITS(7)+10.**CUNITS(8)+10.**CUNITS(16))
      C4=FE2TOT+FE3TOT+FETOTL
      DO 40 J = 1,10
      I = LISTE2(J)
      C1 = 0.0
      IF (CUNITS(I).GT.-2E4 .AND. C3.GT.-2E4) C1=10.**(CUNITS(I)-C3)
      C2 = 0.0
      IF (ANALMI(I) .GT. 0.0 .AND. C4 .GT. 0.0) C2 = ANALMI(I)/C4
      IF (C1.GT.0. .AND. C2.GT.0.) WRITE(K,1120) PAGE1(I)(1:2),C1,
     * PAGE1(I)(1:2),C2
 1120 FORMAT(10X,A2,'/Fe  = ',1PE11.4,20X,A2,'/Fe  = ',1PE11.4)
   40 CONTINUE
   50 RETURN
      END
      SUBROUTINE APCALC(AP,ALFA,GAMMA,MI)
C
      REAL*8 AP(0:653),ALFA(0:377),GAMMA(0:377),MI(0:377)
      INTEGER LISTE(41)
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE/114,134,183,184,185,186,187,189,195,196,197,198,199,
     *200,223,224,225,226,227,228,229,265,312,313,360,386,387,388,402,
     *437,459,460,533,534,535,536,550,551,552,575,576/
C
C**** CALC. OF ION ACTIVITY PRODUCTS (IN TERMS OF LOGS) */
C
      AP(9)=ALFA(7)+ALFA(17)
      AP(10)=ALFA(1)+ALFA(17)
      AP(11)=ALFA(0)+AP(10)+ALFA(17)
      AP(12)=ALFA(0)+ALFA(17)
      AP(21)=ALFA(0)+ALFA(17)
      AP(17)=ALFA(0)+ALFA(5)
      AP(18)=ALFA(0)+ALFA(5)+2E0*LH2O
      AP(19)=ALFA(1)+2E0*(LH2O+PH)
      AP(20)=3E0*ALFA(1)+2E0*ALFA(23)+LH2O+6E0*PH
      AP(27)=2E0*ALFA(1)+ALFA(23)+4E0*PH
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 AP(28)=ALFA(0)+ALFA(1)+2E0*ALFA(23)+4E0*PH-2E0*LH2O
 AP(29)=ALFA(1)+ALFA(23)+2E0*PH-LH2O
 AP(31)=2E0*ALFA(0)+5E0*ALFA(1)+8E0*ALFA(23)+14E0*PH-8E0*LH2O
 AP(36)=2*ALFA(1)+3*ALFA(23)+4*PH-0.5*LH2O
 AP(37)=3*ALFA(1)+4*ALFA(23)+6*PH-4*LH2O
 AP(38)=5E0*ALFA(1)+4E0*ALFA(17)+2E0*PH+6E0*LH2O
 AP(39)=ALFA(3)+ALFA(53)+3E0*ALFA(23)-8E0*LH2O
 AP(40)=ALFA(2)+ALFA(53)+3E0*ALFA(23)-8E0*LH2O
 AP(41)=ALFA(0)+2E0*(ALFA(53)+ALFA(23))-8E0*LH2O
 AP(42)=ALFA(2)+ALFA(53)+2E0*ALFA(23)-5E0*LH2O
 AP(43)=ALFA(3)+3*(ALFA(50)+ALFA(23))+10*PH
 AP(44)=ALFA(3)+ALFA(53)+3E0*(ALFA(1)+ALFA(23))+6E0*PH
*       -4E0*LH2O
 AP(45)=.6E0*ALFA(3)+.25E0*ALFA(1)+2.3E0*ALFA(53)+3.5E0*ALFA(23)-
*       1.2E0*PH-11.2E0*LH2O
 AP(46)=2E0*(ALFA(50)+ALFA(23))+LH2O+6E0*PH
 AP(47)=2E0*(ALFA(50)+ALFA(23))+LH2O+6E0*PH
 IF ((MI(1)+MI(2)+MI(3)).LT.1D-78) THEN
   C1=2E4
 ELSE
   C1=DLOG10(SQRT(MI(1)*GAMMA(1))+MI(2)*GAMMA(2)+MI(3)*GAMMA(3))
 END IF
 AP(48)=.33E0*C1+2.33E0*ALFA(53)+3.67E0*ALFA(23)-2E0*PH-12E0*LH2O
 AP(49)=5*ALFA(1)+2*ALFA(50)+3*ALFA(23)+16*PH+6*LH2O
 AP(50)=ALFA(3)+3E0*ALFA(50)+6E0*(LH2O+PH)+2E0*ALFA(5)
 AP(51)=ALFA(50)+3E0*(LH2O+PH)
 AP(52)=ALFA(50)+3E0*PH+2E0*LH2O
 AP(53)=2E0*ALFA(53)+4E0*ALFA(23)-2E0*PH-12.0*LH2O
 AP(54)=.5E0*(ALFA(2)+ALFA(3))+ALFA(53)+3E0*ALFA(23)-7E0*LH2O
 AP(55) = ALFA(2)+ALFA(53)+3.5E0*ALFA(23)-6E0*LH2O
 IF ((MI(2)+MI(3)).GT.1D-78) THEN
   AP(56)=.5E0*DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3))+ALFA(53)
*    +5E0*ALFA(23)-8.5E0*LH2O
   AP(57)=.5E0*DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3))+ALFA(53)
*    +4.5E0*ALFA(23)-8E0*LH2O
 END IF
 AP(58)=ALFA(2)+ALFA(6)
 AP(59)=3E0*ALFA(2)+ALFA(6)+ALFA(17)+2E0*LH2O
 AP(60)=2E0*ALFA(2)+ALFA(17)+1E1*LH2O
 AP(61)=2E0*ALFA(2)+ALFA(17)+LH2O
 AP(62)=ALFA(0)+2E0*ALFA(61)
 AP(63) = .167E0*ALFA(0)+2.33E0*ALFA(53)+3.67E0*ALFA(23)
*         -2E0*PH-12E0*LH2O
 AP(64)=ALFA(2)+ALFA(4)
 AP(65)=2E0*ALFA(2)+ALFA(5)
 AP(66)=2E0*ALFA(2)+ALFA(5)+1E1*LH2O
 AP(67)=ALFA(7)+ALFA(66)+PH
 AP(94)=ALFA(7)+ALFA(17)
 AP(95)=5E0*ALFA(0)+3E0*ALFA(46)+4E0*PH+LH2O
 AP(96)=5E0*ALFA(0)+3E0*ALFA(46)+3E0*PH+ALFA(61)
 AP(98)=ALFA(3)+7E0*ALFA(23)+PH       -9E0*LH2O
 AP(97)=ALFA(23)-2E0*LH2O
 AP(99)=ALFA(23)-2E0*LH2O
 AP(100)=ALFA(23)-2E0*LH2O
 AP(101)=ALFA(23)-2E0*LH2O
 AP(106)=3E0*ALFA(7)+2E0*ALFA(44)+8E0*LH2O
 AP(107)=2E0*ALFA(8)+ALFA(7)+4E0*LH2O+8E0*PH
 AP(108)=2E0*ALFA(8)+3E0*LH2O+6E0*PH
 AP(109)=2E0*ALFA(8)+3E0*LH2O+6E0*PH
 AP(110)=ALFA(8)+3E0*PH+2E0*LH2O
 AP(111)=3E0*ALFA(7)+2E0*ALFA(23)+6E0*PH+LH2O
 AP(112)=ALFA(8)+3E0*(LH2O+PH)
 AP(113)=ALFA(3)+3*ALFA(7)+ALFA(53)+3*ALFA(23)-10*LH2O
 AP(114)=ALFA(7)+2E0*(ALFA(66)+PE(EHOPT(6))+PH)
 C1=DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3)+MI(63)*GAMMA(63))
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 AP(115)=0.83E0*C1+0.29E0*ALFA(1)+.23E0*ALFA(8)+1.58E0*ALFA(53)
*         +3.93E0*ALFA(23)-1E1*LH2O
 AP(116)=0.83E0*C1+.45E0*ALFA(1)+.34E0*ALFA(8)+1.47E0*ALFA(53)+
*         3.82E0*ALFA(23)-9.2*LH2O+.76E0*PH
 AP(117)=3E0*ALFA(1)+ALFA(0)+4E0*ALFA(17)
 AP(118)=2E0*ALFA(8)+ALFA(7)+4E0*(ALFA(66)+PH)
 AP(119)=ALFA(7)+ALFA(66)+PH
 AP(125)=5*ALFA(1)+2*ALFA(50)+3*ALFA(23)+16*PH+6*LH2O
 AP(128)=ALFA(0)+2E0*ALFA(53)+4E0*ALFA(23)-8E0*LH2O
 AP(133)=ALFA(2)*.02+ALFA(3)*.75+ALFA(8)*3.+ALFA(5)*2.+PH*5.77
*         +LH2O*6.23
 AP(134)=2E0*ALFA(110)+3E0*ALFA(5)
 AP(140)=ALFA(50)+3E0*(LH2O+PH)
 AP(141)=2E0*(ALFA(0)+ALFA(53)+PH       )+3E0*ALFA(23)-8E0*LH2O
 AP(142)=ALFA(87)+ALFA(17)
 AP(143)=ALFA(87)+ALFA(5)
 AP(144)=ALFA(89)+ALFA(5)
 AP(145)=ALFA(89)+ALFA(17)
 AP(146)=ALFA(8)+ALFA(44)+2E0*LH2O
 AP(147)=2E0*ALFA(0)+4E0*ALFA(53)+8E0*ALFA(23)-17E0*LH2O
 AP(149)=ALFA(1)+ALFA(17)+3E0*LH2O
 AP(150)=2E0*ALFA(0)+ALFA(17)+2E0*PH+5E0*LH2O
 AP(153)=2*ALFA(1)+3*ALFA(23)+4*PH-0.5*LH2O
 AP(154)=ALFA(50)+3E0*PH+2E0*LH2O
 AP(155)=ALFA(0)+2E0*ALFA(53)+4E0*ALFA(23)-1E1*LH2O
 C1=1.24E0-0.135E0*PH
 AP(157)=(1E0-C1)*ALFA(50)+C1*ALFA(23)+(3E0-3E0*C1)*PH
 AP(158)=(1E0-C1)*ALFA(50)+C1*ALFA(23)+(3E0-3E0*C1)*PH
 AP(181)=ALFA(8)+0.3*ALFA(4)+2.7*(LH2O+PH)
 AP(182)=ALFA(109)+ALFA(5)
 AP(183)=ALFA(109)+2*LH2O+4*PH+2*PE(EHOPT(6))
 AP(184)=ALFA(109)+2*LH2O+4*PH+2*PE(EHOPT(6))
 AP(185)=ALFA(109)+2*LH2O+4*PH+2*PE(EHOPT(6))
 AP(186)=2*ALFA(110)+3*LH2O+6*PH
 AP(187)=3*ALFA(109)+4*LH2O+8*PH+2*PE(EHOPT(6))
 AP(188)=ALFA(109)+2*(LH2O+PH)
 AP(189)=ALFA(109)+2*LH2O+3*PH+PE(EHOPT(6))
 AP(190)=ALFA(109)+ALFA(17)
 AP(191)=ALFA(109)+2*ALFA(4)+4*LH2O
 AP(192)=ALFA(109)+ALFA(66)+PH
 AP(193)=3*ALFA(109)+2*ALFA(44)
 AP(194)=ALFA(109)+ALFA(46)
 AP(195)=16*ALFA(110)+.8*ALFA(3)+17*LH2O+34*PH-7.4*ALFA(109)
 AP(196)=14*ALFA(110)+.57*ALFA(7)+.82*ALFA(89)+16*LH2O+32*PH
*         -6.41*ALFA(109)
 AP(197)=14*ALFA(110)+.78*ALFA(89)+.19*ALFA(0)+.03*ALFA(3)
*         +18.485*LH2O+31.97*PH-6*ALFA(109)
 AP(198)=10*ALFA(110)+.393*ALFA(0)+.473*ALFA(1)+14*LH2O+24*PH
*         -3.866*ALFA(109)
 AP(199)=20*ALFA(110)+2*ALFA(80)+8*ALFA(50)+49*LH2O+70*PH
*         -8*ALFA(109)
 AP(200)=8*ALFA(110)+.44*ALFA(0)+12*LH2O+18*PH-3.44*ALFA(109)
 AP(204)=3*ALFA(8)+2*ALFA(5)+ALFA(2)+6*(LH2O+PH)
 AP(205)=3*ALFA(8)+2*ALFA(5)+ALFA(3)+6*(LH2O+PH)
 AP(223)=ALFA(127)-PE(EHOPT(6))
 AP(224)=ALFA(127)+ALFA(4)
 AP(225)=ALFA(127)+ALFA(61)
 AP(226)=2*ALFA(127)+LH2O+2*PH
 AP(227)=2*ALFA(127)+ALFA(66)+PH
 AP(228)=2*ALFA(127)+ALFA(5)
 AP(229)=ALFA(127)+ALFA(8)+2*LH2O+4*PH
 AP(230)=ALFA(130)+2*ALFA(4)
 AP(231)=ALFA(130)+ALFA(17)
 AP(232)=ALFA(130)+2*ALFA(61)
 AP(233)=ALFA(130)+2*ALFA(61)+2*LH2O
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AP(234)=ALFA(130)+2*LH2O+2*PH
AP(235)=2*ALFA(130)+2*LH2O+ALFA(6)+3*PH
AP(236)=3*ALFA(130)+2*LH2O+2*ALFA(6)+4*PH
AP(237)=2*ALFA(130)+3*LH2O+ALFA(4)+3*PH
AP(238)=2*ALFA(130)+3*LH2O+ALFA(84)+3*PH
AP(239)=3*ALFA(130)+4*LH2O+ALFA(5)+4*PH
AP(240)=4*ALFA(130)+6*LH2O+ALFA(5)+6*PH
AP(241)=4*ALFA(130)+7*LH2O+ALFA(5)+6*PH
AP(242)=ALFA(130)+LH2O+2*PH
AP(243)=2*ALFA(130)+LH2O+ALFA(5)
AP(244)=3*ALFA(130)+2*ALFA(44)
AP(245)=3*ALFA(130)+2*ALFA(44)+3*LH2O
AP(246)=ALFA(130)+ALFA(66)+PH
AP(247)=ALFA(130)+ALFA(5)
AP(248)=ALFA(130)+ALFA(5)+5*LH2O
AP(249)=ALFA(130)+2*ALFA(8)+4*LH2O+8*PH
AP(250)=ALFA(130)+ALFA(7)+2*(ALFA(66)+PH)
AP(265)=ALFA(145)-2*PE(EHOPT(6))
AP(266)=ALFA(145)+2*ALFA(35)+2*PH-2*LH2O
AP(267)=ALFA(145)+2*ALFA(4)
AP(268)=ALFA(145)+ALFA(17)
AP(269)=ALFA(145)+ALFA(17)+LH2O
AP(270)=ALFA(145)+2*ALFA(61)
AP(271)=ALFA(145)+2*(LH2O+PH)
AP(272)=ALFA(145)+2*(LH2O+PH)
AP(273)=ALFA(145)+2*(LH2O+PH)
AP(274)=ALFA(145)+2*(LH2O+PH)
AP(275)=ALFA(145)+2*(LH2O+PH)
AP(276)=2*ALFA(145)+3*(LH2O+PH)+ALFA(4)
AP(277)=5*ALFA(145)+8*(LH2O+PH)+2*ALFA(4)
AP(278)=2*ALFA(145)+2*(LH2O+PH)+ALFA(5)
AP(279)=4*ALFA(145)+6*(LH2O+PH)+ALFA(5)
AP(280)=ALFA(145)+2*ALFA(84)+6*LH2O
AP(281)=ALFA(145)+LH2O+2*PH
AP(282)=ALFA(145)+LH2O+2*PH
AP(283)=3*ALFA(145)+2*ALFA(5)+LH2O+2*PH
AP(284)=3*ALFA(145)+2*ALFA(44)+4*LH2O
AP(285)=ALFA(145)+ALFA(66)+PH
AP(286)=ALFA(145)+ALFA(66)+PH
AP(287)=ALFA(145)+ALFA(66)+PH
AP(288)=ALFA(145)+ALFA(23)+2*PH-LH2O
AP(289)=2*ALFA(145)+ALFA(23)+4*PH
AP(290)=ALFA(145)+ALFA(5)
AP(291)=ALFA(145)+ALFA(5)+LH2O
AP(292)=ALFA(145)+ALFA(5)+6*LH2O
AP(293)=ALFA(145)+ALFA(5)+7*LH2O
AP(312)=ALFA(160)-2*PE(EHOPT(6))
AP(313)=ALFA(160)-2*PE(EHOPT(6))
AP(314)=ALFA(160)+2*ALFA(35)+2*PH-2*LH2O
AP(315)=ALFA(160)+ALFA(17)
AP(316)=ALFA(160)+2*ALFA(4)
AP(317)=ALFA(160)+2*ALFA(4)+LH2O
AP(318)=ALFA(160)+2*ALFA(4)+2.5*LH2O
AP(319)=ALFA(160)+2*ALFA(61)
AP(320)=ALFA(160)+2*(LH2O+PH)
AP(321)=ALFA(160)+2*(LH2O+PH)
AP(322)=ALFA(160)+LH2O+PH+ALFA(4)
AP(323)=3*ALFA(160)+4*(LH2O+PH)+ALFA(5)
AP(324)=3*ALFA(160)+2*(LH2O+PH)+2*ALFA(5)
AP(325)=4*ALFA(160)+6*(LH2O+PH)+ALFA(5)
AP(326)=ALFA(160)+LH2O+2*PH
AP(327)=3*ALFA(160)+2*ALFA(44)
AP(328)=ALFA(160)+ALFA(23)+2*PH-LH2O
AP(329)=ALFA(160)+ALFA(5)
AP(330)=ALFA(160)+ALFA(5)+LH2O
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      AP(331)=ALFA(160)+ALFA(5)+LH2O*8/3
      AP(332)=ALFA(160)+ALFA(66)+PH
      AP(337)=ALFA(8)*3+ALFA(5)*2+PH*5+LH2O*7
      AP(338)=ALFA(3)+ALFA(50)+ALFA(5)*2+LH2O*12
      AP(339)=ALFA(7)+ALFA(5)+LH2O*7
      AP(340)=ALFA(1)+ALFA(5)+LH2O*7
      AP(360)=ALFA(182)-2*PE(EHOPT(6))
      AP(361)=ALFA(182)+2*ALFA(35)+2*PH-2*LH2O
      AP(362)=ALFA(182)+2*ALFA(4)
      AP(363)=ALFA(182)+ALFA(4)+ALFA(61)
      AP(364)=ALFA(182)*2+ALFA(4)*2+ALFA(17)
      AP(365)=ALFA(182)+ALFA(17)
      AP(366)=ALFA(182)+ALFA(61)*2
      AP(367)=ALFA(182)+LH2O+2*PH
      AP(368)=ALFA(182)+LH2O+2*PH
      AP(369)=ALFA(182)+LH2O*4/3+2*PH
      AP(370)=ALFA(182)*2+LH2O+ALFA(17)+2*PH
      AP(371)=ALFA(182)*2+LH2O+ALFA(5)+2*PH
      AP(372)=ALFA(182)*3+LH2O*2+ALFA(5)+4*PH
      AP(373)=ALFA(182)*4+LH2O*3+ALFA(5)+6*PH
      AP(374)=ALFA(182)+ALFA(46)
      AP(375)=ALFA(182)*3+ALFA(46)*2+2*PH
      AP(376)=ALFA(182)*5+ALFA(44)*3+ALFA(4)
      AP(377)=ALFA(182)*5+ALFA(44)*3+LH2O+PH
      AP(378)=ALFA(182)*3+2*LH2O+ALFA(17)+4*PH
      AP(379)=ALFA(182)+3*ALFA(50)+2*ALFA(44)+5*PH+6*LH2O
      AP(380)=ALFA(182)+3*ALFA(50)+ALFA(44)+6*(LH2O+PH)+ALFA(5)
      AP(381)=ALFA(182)*2+ALFA(130)+ALFA(44)+3*PH+6*LH2O
      AP(382)=ALFA(182)+ALFA(23)-LH2O+2*PH
      AP(383)=ALFA(182)*2+ALFA(23)+4*PH
      AP(384)=ALFA(182)+ALFA(5)
      AP(385)=ALFA(182)+ALFA(66)+PH
      AP(386)=ALFA(182)+2*LH2O+4*PH+2*PE(EHOPT(6))
      AP(387)=ALFA(182)*2+LH2O*3+6*PH+2*PE(EHOPT(6))
      AP(388)=ALFA(182)*3+LH2O*4+8*PH+2*PE(EHOPT(6))
      AP(389)=ALFA(182)+(LH2O+PH)*2
      AP(390)=ALFA(182)+LH2O+PH+ALFA(4)
      AP(391)=ALFA(182)*2+(LH2O+PH)*3+ALFA(4)
      AP(392)=ALFA(182)*3+(LH2O+PH)*2+ALFA(17)*2
      AP(393)=ALFA(182)*2+LH2O*3+4*PH
      AP(394)=ALFA(182)*4+LH2O*6+6*PH+ALFA(5)
      AP(395)=ALFA(23)-2E0*LH2O
      AP(396)=9.496*ALFA(0)+0.36*ALFA(2)+0.144*ALFA(1)+4.8*ALFA(44)
     *       +1.2*ALFA(17)+2.48*ALFA(61)
      AP(398)=ALFA(89)+2*ALFA(61)
      AP(399)=ALFA(87)+2*ALFA(61)
      AP(401)=ALFA(0)+AP(10)+ALFA(17)
      AP(402)=ALFA(67)+2*PE(EHOPT(6))
      AP(410)=ALFA(204)+ALFA(17)
      AP(411)=ALFA(204)+2*(LH2O+PH)
      AP(412)=4*ALFA(204)+6*(LH2O+PH)+ALFA(5)
      AP(413)=ALFA(204)+LH2O+2*PH
      AP(414)=3*ALFA(204)+2*ALFA(44)
      AP(415)=ALFA(204)+ALFA(66)+PH
      AP(416)=ALFA(204)+ALFA(5)+6*LH2O
      AP(417)=ALFA(204)+ALFA(5)+7*LH2O
      AP(418)=2*ALFA(204)+ALFA(23)+4*PH
      AP(419)=2*ALFA(8)+ALFA(7)+8*(LH2O+PH)
      AP(420)=ALFA(130)+ALFA(23)+2*PH
      AP(437)=ALFA(212)-PE(EHOPT(6))
      AP(438)=ALFA(212)+ALFA(97)
      AP(439)=ALFA(212)+ALFA(4)
      AP(440)=2*ALFA(212)+ALFA(17)
      AP(441)=ALFA(212)+ALFA(61)+4*LH2O
      AP(442)=ALFA(212)+ALFA(96)
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AP(443)=2*ALFA(212)+LH2O+2*PH
AP(444)=3*ALFA(212)+ALFA(44)
AP(445)=2*ALFA(212)+ALFA(66)+PH
AP(446)=2*ALFA(212)+ALFA(5)
AP(459)=ALFA(127)+ALFA(97)
AP(460)=ALFA(127)+ALFA(96)
AP(461)=ALFA(145)+2*ALFA(97)+2*LH2O
AP(462)=ALFA(145)+2*ALFA(96)
AP(463)=ALFA(160)+2*ALFA(97)+4*LH2O
AP(464)=ALFA(160)+2*ALFA(96)
AP(465)=ALFA(182)+2*ALFA(97)
AP(466)=ALFA(182)+ALFA(97)+ALFA(61)
AP(467)=ALFA(182)+2*ALFA(96)
AP(471)=ALFA(50)+ALFA(5)+LH2O+PH
AP(472)=4*ALFA(50)+ALFA(5)+10*(LH2O+PH)
AP(488)=2*ALFA(255)-3*LH2O
AP(489)=ALFA(50)+ALFA(258)+2*LH2O
AP(541)=3*ALFA(89)+2*ALFA(258)
AP(490)=3*ALFA(0)+2*ALFA(258)+4*LH2O
AP(491)=3*ALFA(130)+2*ALFA(258)+6*LH2O
AP(492)=ALFA(8)+ALFA(258)+2*LH2O
AP(493)=3*ALFA(109)+2*ALFA(258)+8*LH2O
AP(494)=3*ALFA(204)+2*ALFA(258)+8*LH2O
AP(495)=3*ALFA(182)+2*ALFA(258)
AP(496)=3*ALFA(145)+2*ALFA(258)+2.5*LH2O
AP(497)=4*ALFA(250)-6*LH2O
AP(498)=4*ALFA(250)-6*LH2O
AP(499)=ALFA(250)+3*ALFA(96)-3*(LH2O+PH)
AP(500)=2*ALFA(250)+3*ALFA(66)-3*PH-6*LH2O
AP(501)=ALFA(250)+ALFA(66)-3*LH2O-2*PH-PE(EHOPT(6))
AP(533)=0.9*ALFA(130)+0.2*ALFA(127)+ALFA(66)+PH
AP(534)=0.6*ALFA(130)+0.8*ALFA(127)+ALFA(66)+PH
AP(535)=.25*ALFA(130)+1.5*ALFA(127)+ALFA(66)+PH
AP(536)=.066*ALFA(130)+1.868*ALFA(127)+ALFA(66)+PH
AP(539)=ALFA(0)+2E0*(LH2O+PH)
AP(550)=ALFA(302)+PH+2*PE(EHOPT(6))
AP(551)=ALFA(305)-3*LH2O-6*PH-4*PE(EHOPT(6))
AP(552)=ALFA(7)+2*ALFA(302)+2*PH+2*PE(EHOPT(6))
AP(553)=ALFA(305)-LH2O-2*PH
AP(554)=ALFA(0)+ALFA(305)
AP(555)=ALFA(89)+ALFA(305)
AP(556)=2*ALFA(8)+3*ALFA(305)
AP(564)=ALFA(109)+ALFA(17)
AP(571)=ALFA(318)+4*ALFA(2)+3*ALFA(17)
AP(573)=ALFA(317)+2*LH2O+4*PH
AP(574)=ALFA(317)+2*LH2O+4*PH
AP(575)=4*ALFA(317)+9*LH2O+18*PH+2*PE(EHOPT(6))
AP(576)=3*ALFA(317)+8*LH2O+16*PH+4*PE(EHOPT(6))
AP(577)=ALFA(317)+4*PH+ALFA(23)
AP(584)=ALFA(317)+4*ALFA(61)
AP(585)=ALFA(317)+4*ALFA(61)+2.5*LH2O
AP(591)=ALFA(317)+ALFA(5)+2*(LH2O+PH)
AP(592)=ALFA(318)+ALFA(46)+4*LH2O
AP(593)=ALFA(317)+2*ALFA(44)+4*LH2O-2*PH
AP(594)=ALFA(317)+2*ALFA(44)+2*LH2O+ALFA(0)
AP(599)=ALFA(318)+LH2O+2*PH
AP(600)=ALFA(318)+LH2O+2*PH
AP(601)=ALFA(318)+2*LH2O+2*PH
AP(602)=ALFA(318)+3*LH2O+2*PH
AP(606)=ALFA(318)+ALFA(17)
AP(619)=3*ALFA(318)+2*ALFA(44)+4*LH2O
AP(620)=2*ALFA(318)+2*ALFA(44)-2*PH
AP(621)=2*ALFA(318)+2*ALFA(44)+2*ALFA(2)
AP(622)=2*ALFA(318)+2*ALFA(44)+2*ALFA(3)
AP(623)=2*ALFA(318)+2*ALFA(44)+2*ALFA(38)
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      AP(624)=2*ALFA(318)+2*ALFA(44)+ALFA(1)
      AP(625)=2*ALFA(318)+2*ALFA(44)+ALFA(0)
      AP(626)=2*ALFA(318)+2*ALFA(44)+ALFA(87)
      AP(627)=2*ALFA(318)+2*ALFA(44)+ALFA(89)
      AP(628)=2*ALFA(318)+2*ALFA(44)+ALFA(7)
      AP(629)=2*ALFA(318)+2*ALFA(44)+ALFA(130)
      AP(630)=2*ALFA(318)+2*ALFA(44)+ALFA(182)
      AP(632)=2*ALFA(318)+ALFA(0)+2*ALFA(23)+6*PH
      AP(651)=3*ALFA(317)+4*ALFA(44)
      AP(652)=ALFA(318)+ALFA(257)+4*LH2O
      AP(653)=2*ALFA(318)+ALFA(130)+2*ALFA(258)+8*LH2O
C
C     LISTE
C
      IF (ABS(PE(EHOPT(6))) .LE. 19E0) GOTO 40
      DO 30 J = 1,41
      I = LISTE(J)
      AP(I)=2E4
   30 CONTINUE
   40 CONTINUE
      RETURN
      END
      SUBROUTINE OUTPCH(ALFA,AP,CUNITS,LOGKT)
C
      REAL*8 ALFA(0:377),AP(0:653),CUNITS(0:377),LOGKT(0:653),LP(600)
      INTEGER LISTE(50),LISTE1(79),LISTE2(27)
      CHARACTER*80 LINE
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE/0,1,2,3,4,5,6,7,8,9,10,17,23,26,35,38,44,46,48,50,51,
     *61,67,80,84,87,89,94,96,97,101,106,108,109,114,130,138,145,151,
     *160,167,182,192,204,208,212,224,250,255,258/
      DATA LISTE1/10,11,12,17,18,36,40,43,45,46,48,49,51,54,62,63,95,96,
     *97,99,100,106,110,111,112,114,119,128,140,155,157,158,159,47,50,
     *52,65,66,107,108,109,113,115,184,185,190,193,194,195,198,199,204,
     *205,239,240,242,248,288,289,292,293,330,331,337,338,339,340,365,
     *376,389,396,401,411,419,437,445,472,500,501/
      DATA LISTE2/0,1,2,3,4,5,6,7,8,13,16,17,34,38,44,48,50,61,80,84,86,
     *87,89,94,96,97,202/
C
C     **  CONVERT VALUES OF ALPHA AND CUNITS TO LOG FORM FOR EQPLOT  **
C     **  PUNCHOUT BY INSERTING PAGE1 REFERENCE NUMBERS INTO RECORDS **
C     **  20070 TO 20100 AT BEGINNING OF PROCEDURE SOLUTS. ARRAY     **
C     **  BOUND ALSO MUST BE MODIFIED ON RECORDS 19840 AND 22370.    **
C
C**** DUPLICATE DESCRIPTOR CARDS */
C
      OPEN (UNIT=7,FILE='CARDS.EQP')
    4 READ(7,1000,END=7)LINE
      GOTO 4
    7 BACKSPACE(UNIT=7)
      WRITE(7,1000) CARD1
      WRITE(7,1000) CARD2
 1000 FORMAT(A80)
C
C**** LOG ACTIVITY VALUES FOR SOLUTE CONSTITUENTS */
C
      N=0
C
      DO 10 J = 1, 50
      I = LISTE(J)
      N=N+1
      LP(N)=999.
      IF (ALFA(I).GT. -1D2 .AND. ALFA(I) .LT. 1D3) LP(N) = ALFA(I)
```

```
   10 CONTINUE
C
C**** LOG(AP) AND LOG(AP/K) FOR MINERAL PHASES */
C
      DO 20 J = 1, 79
      I = LISTE1(J)
      N = N + 1
      LP(N) = 999.
      IF (AP(I).GT.-1D3 .AND. AP(I).LT.1D3) LP(N) = AP(I)
      N=N+1
      C3 = AP(I) - LOGKT(I)
      LP(N) = 999.
      IF (C3.GT.-1D2 .AND. C3.LT.1D3) LP(N) = C3
   20 CONTINUE
C
C**** LOG CONCENTRATION OF MAJOR CONSTITUENTS */
C
      DO 25 J = 1, 27
      I = LISTE2(J)
      N=N+1
      LP(N) = 999.
      IF (CUNITS(I).GT.-1D2 .AND. CUNITS(I).LT.1D3) LP(N) = CUNITS(I)
   25 CONTINUE
C
C**** LOG CONCENTRATION(UG/L)OF TRACE ELEMENTS */
C
      N=N+1
      LP(N) = 999.
      IF (CUNITS(212).GT.-1D2 .AND. CUNITS(212).LT.1D3)
     *LP(N)=CUNITS(212)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(249).GT.-1D2 .AND. CUNITS(249).LT.1D3)
     *LP(N)=CUNITS(249)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(261).GT.-1D2 .AND. CUNITS(261).LT.1D3)
     *LP(N)=CUNITS(261)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(262).GT.-1D2 .AND. CUNITS(262).LT.1D3)
     *LP(N)=CUNITS(262)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(160).GT.-1D2 .AND. CUNITS(160).LT.1D3)
     *LP(N)=CUNITS(160)+3.
      N=N+1
      LP(N)=999.
      IF (CO .GT. 0.0) LP(N)=DLOG10(CO*1D3)
      N=N+1
      LP(N) = 999.
      IF (CR .GT. 0.0) LP(N) =DLOG10(CR*1D3)
      N=N+1
      LP(N) = 999.
      IF (CUNITS(130).GT.-1D2 .AND. CUNITS(130).LT.1D3)
     *LP(N)=CUNITS(130)+3
      N=N+1
      LP(N) = 999.
      IF (HG.GT.0.0) LP(N) = DLOG10(HG*1D3)
      N=N+1
      LP(N) = 999.
      IF (CUNITS(109).GT.-1D2 .AND. CUNITS(109).LT.1D3)
     *LP(N)=CUNITS(109)+3
      N=N+1
      LP(N) = 999.
```

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      IF (MO.GT.0.0) LP(N) = DLOG10(MO*1D3)
      N=N+1
      LP(N) = 999.
      IF (CUNITS(204).GT.-1D2 .AND. CUNITS(204).LT.1D3)
     *LP(N)=CUNITS(204)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(182).GT.-1D2 .AND. CUNITS(182).LT.1D3)
     *LP(N)=CUNITS(182)+3.
      N=N+1
      LP(N) = 999.
      IF (CUNITS(145).GT.-1D2 .AND. CUNITS(145).LT.1D3)
     *LP(N)=CUNITS(145)+3.
C
      IF (PE(0).GT.19.) PE(0) = 999.
      IF (PE(1).GT.19.) PE(1) = 999.
      IF (PE(6).GT.19.) PE(6) = 999.
C
C**** PLACE THE SPECIATED CHARGE BALANCE IN THE CARDS.EQP FILE
C
      N=N+1
      LP(N) = 100. * (EPMCAT-EPMAN)/(EPMAN+EPMCAT)
C
C**** PUNCH OUT THE ARRAY LP WITH ALL SELECTED VALUES IN SEQUENCE */
C
      WRITE(7,1010)TEMP,PH,PE(0),PE(1),PE(6),AH2O,(LP(I), I = 1, N)
 1010 FORMAT(10F8.3)
C
C**** BLANK DATASET SEPARATOR CARD */
C
      WRITE(7,1020)
 1020 FORMAT(1H ,1X)
      CLOSE(7)
      RETURN
      END
      SUBROUTINE ERRCLC(CUNITS,SIGMA,ERR)
C
      REAL*8 CUNITS(0:377),SIGMA(0:377),ERR(0:653),RSD(0:377)
      INTEGER LISTE(40)
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE/0,1,2,3,4,5,6,7,8,13,16,17,26,34,38,44,48,50,61,63,
     *71,80,84,86,87,89,94,96,97,109,130,145,160,182,202,204,212,249,
     *261,262/
      DO 10 I = 0, D
      RSD(I) = 2E7
   10 CONTINUE
      DO 20 J = 1, 40
      I = LISTE(J)
      C1 = 10.**CUNITS(I)
      IF (C1 * SIGMA(I) .GT. 0.0) RSD(I) = SIGMA(I)/C1/C
   20 CONTINUE
      IF (RSD(17).GT. 1E7) RSD(17) = RSD(6)
      IF (RSD(8) .GT. 1E7) RSD(8) = RSD(7) * 2
      ERR(9)=SQRT((RSD(7))**2+(RSD(17))**2)
      ERR(10)=SQRT((RSD(1))**2+(RSD(17))**2)
      ERR(11)=SQRT((RSD(0))**2+(RSD(1))**2+(2*RSD(17))**2)
      ERR(21) = SQRT((RSD(0))**2 + (RSD(17))**2)
      ERR(12) = ERR(21)
      ERR(18) = SQRT((RSD(0))**2 + (RSD(5))**2)
      ERR(17) = ERR(18)
      ERR(153)=SQRT((2*RSD(1))**2 + (3*RSD(34))**2 + (4*SIGMPH)**2)
      ERR(36) = ERR(153)
      ERR(40)=SQRT(RSD(2)**2+RSD(50)**2+(3*RSD(34))**2)
```

```
      ERR(41) = SQRT(RSD(0)**2 + (2*RSD(50))**2 + (2*RSD(34))**2)
      ERR(45) = SQRT((.6*RSD(3))**2 +(.25*RSD(1))**2 +(2.3*RSD(50))**2
     *+(3.5*RSD(34))**2+(1.2*SIGMPH)**2)
      ERR(46)  = SQRT((2*RSD(50))**2 + (2*RSD(34))**2 + (2*SIGMPH)**2)
      ERR(47)  = ERR(46)
      ERR(168) = SQRT((RSD(50))**2+(3*SIGMPH)**2)
      ERR(51)  = ERR(168)
      ERR(140)= ERR(168)
      ERR(54) =SQRT( (.5*(RSD(2)+RSD(3)))**2 + (RSD(50))**2+
     *(3*RSD(34))**2)
      ERR(62) = SQRT((RSD(0))**2 + (2*RSD(61))**2)
      ERR(63) = SQRT((.167*RSD(0))**2 + (2.33*RSD(50))**2
     *+(3.67*RSD(34))**2 + (2*SIGMPH)**2)
      ERR(67) = SQRT((RSD(7))**2+(RSD(13))**2)
      ERR(119) = ERR(67)
      ERR(95) = SQRT((5*RSD(0))**2 +(3*RSD(44))**2 +(4*SIGMPH)**2)
C
C**** SIO2
C
      ERR(97)  = RSD(34)
      ERR(99)  = RSD(34)
      ERR(100) = RSD(34)
      ERR(101) = RSD(34)
      ERR(395) = RSD(34)
C
      ERR(106) = SQRT((3*RSD(7))**2 + (2*RSD(44))**2)
      ERR(112) = SQRT((RSD(8))**2 + (3*SIGMPH)**2)
      ERR(115) = SQRT((.277*RSD(2))**2 + (.277*RSD(3))**2
     *+(.277*SIGMPH)**2 + (.29*RSD(1))**2 + (.23*RSD(8))**2
     *+(1.58*RSD(50))**2 + (3.93*RSD(34))**2)
      ERR(116) = SQRT((.277*RSD(2))**2 + (.277*RSD(3))**2
     *+(.277*SIGMPH)**2 + (.45*RSD(1))**2 + (.34*RSD(8))**2
     *+(1.47*RSD(50))**2 + (3.82*RSD(34))**2 + (.76*SIGMPH)**2)
      ERR(117) = SQRT((3*RSD(1))**2 + (RSD(0))**2 + (4*RSD(17))**2)
      ERR(142) = SQRT(RSD(87)**2 + RSD(17)**2)
      ERR(143) = SQRT(RSD(87)**2 + RSD(5)**2)
      ERR(144) = SQRT(RSD(89)**2 + RSD(5)**2)
      ERR(145) = SQRT(RSD(89)**2 + RSD(17)**2)
      ERR(147) = SQRT((2*RSD(0))**2 + (4*RSD(50))**2 + (8*RSD(34))**2)
      C1 = 1.24 - .135*PH
      ERR(157) = SQRT(((1-C1)*RSD(50))**2 + (C1*RSD(34))**2
     *+((3-3*C1)*SIGMPH)**2)
      ERR(158) = ERR(157)
      ERR(204) = SQRT((RSD(2))**2 + (2*RSD(5))**2 + (3*RSD(8))**2
     *+(6*SIGMPH)**2)
      ERR(205) = SQRT((RSD(3))**2 + (2*RSD(5))**2 + (3*RSD(8))**2
     *+(6*SIGMPH)**2)
      ERR(230) = SQRT((RSD(130))**2 + (2*RSD(4))**2)
      ERR(235) = SQRT((2*RSD(130))**2 + (RSD(6))**2 + (3*SIGMPH)**2)
      ERR(236) = SQRT((3*RSD(130))**2 +(2*RSD(6))**2 +(4*SIGMPH)**2)
      ERR(242) = SQRT((RSD(130))**2 + (2*SIGMPH)**2)
      ERR(268) = SQRT((RSD(145))**2 + (RSD(17))**2)
      ERR(269) = ERR(268)
      ERR(288) = SQRT((RSD(145))**2 + (RSD(34))**2 + (2*SIGMPH)**2)
      ERR(315) = SQRT((RSD(160))**2 + (RSD(17))**2)
      ERR(339) = SQRT((RSD(7))**2 + (RSD(5))**2)
      ERR(365) = SQRT((RSD(182))**2 + (RSD(17))**2)
      ERR(374) = SQRT((RSD(182))**2 + (RSD(44))**2)
      ERR(376) = SQRT((5*RSD(182))**2 + (3*RSD(44))**2 + RSD(4)**2)
      ERR(379) = SQRT((RSD(182))**2 + (3*RSD(50))**2 + (2*RSD(44))**2+
     *(5*SIGMPH)**2)
      ERR(419) = SQRT((2*RSD(8))**2 + (RSD(7))**2 +2*(2*RSD(8))*(RSD(7)
     *)+(8*SIGMPH)**2)
      ERR(471) = SQRT((RSD(50))**2 + (RSD(5))**2+SIGMPH**2)
      ERR(472) = SQRT((4*RSD(50))**2 + (RSD(5))**2 + (10*SIGMPH)**2)
```

```
      RETURN
      END
      SUBROUTINE PHASES(PAGE2,AP,LOGKT,ERR,ERRT)
C
      REAL*8 AP(0:653),LOGKT(0:653),ERR(0:653),ERRT(0:653)
      CHARACTER*12 PAGE2(0:653)
      CHARACTER*11 SC(5)
      CHARACTER*6 IXFILE
      DIMENSION S(5)
C
$INCLUDE:'COMMON.BLK'
C
      OPEN(UNIT=12,STATUS='NEW')
      WRITE(K,1000) CARD1
 1000 FORMAT(1H1,1X,A80/)
      WRITE(K,1010)
 1010 FORMAT('      Phase          Log IAP/KT    Log IAP     Sigma(A)
     *Log KT     Sigma(T)')
      IN = 0
C
      IXFILE='TABLE3'
      IF(PRNT.EQ.0) IXFILE='TABL3A'
      OPEN(UNIT=14,FILE=IXFILE,STATUS='OLD')
   10 READ(14,*) I
      IF(I.GE.900) GOTO 20
      S(2) = AP(I)
      IF (ABS(S(2)) .GE. 5E2) GOTO 10
      S(4) = LOGKT(I)
      S(1) = 0.0
      IF (ABS(LOGKT(I)) .GT. 1D-78) S(1) = S(2) - LOGKT(I)
      S(3) = 0.0
      S(5) = 0.0
      IF (ERR(I) .LT. 5E2) S(3) = ERR(I)
      IF (ERRT(I) .GT. 0.0) S(5) = ERRT(I)
      REWIND 12
      DO 40 J = 1, 5
        IF(ABS(S(J)) .GT. 1D-78) THEN
          WRITE(12,1120) S(J)
        ELSE
          WRITE(12,1130)
        END IF
   40 CONTINUE
      REWIND 12
      DO 50 J=1,5
        READ(12,1140)SC(J)
   50 CONTINUE
      WRITE(K,1100)I,PAGE2(I),(SC(J), J=1,5)
      IN = IN + 1
      IF (IN .LT.57) GOTO 10
      IN = 0
      WRITE(K,1000) CARD1
      WRITE(K,1010)
      GOTO 10
   20 CLOSE(14)
      RETURN
 1100 FORMAT(' ',I3,1X,10A12)
 1120 FORMAT(F11.3)
 1130 FORMAT('           ')
 1140 FORMAT(A11)
      END
      SUBROUTINE INPUT(PAGE1,CUNITS,SIGMA,LOGKTO)
C
      REAL*8 XIN(17),CUNITS(0:377),SIGMA(0:377),LOGKTO(0:653)
      INTEGER LISTE(17),VAL(4)
      CHARACTER*90 EHFMT
```

```
      CHARACTER*24 SPCALC(9)
      CHARACTER*16 EHMODE(0:13)
      CHARACTER*8 PAGE1(0:377)
      CHARACTER*4 CARD(4),CONZ(5),WORD,FLG
      CHARACTER*2 EHMDFM(0:13)
C
$INCLUDE:'COMMON.BLK'
C
      DATA LISTE/0,1,2,3,4,5,6,16,13,17,34,38,86,44,50,61,84/
      DATA CARD/'CUN ','SIGM','LOKT','    '/
      DATA CONZ/'MQ/L','MG/L','PPM ','MMOL','MOL '/
      DATA SPCALC/'Fe species distribution','Mn species other than +2',
     *'Cu +1 species','As species distribution','Se species distribution
     *','Ion Activity Products','atmospheric pO2','H2S from SO4','U spec
     *ies distribution'/
      DATA EHMODE/'measured','Fe +2/+3','H2O2/O2 Sato','H2O/O2 classical
     *','NH4/NO3','S-/SO4','NO2/NO3','S-/S(s)','As +3/+5','As(s)/As +3',
     *'Se +4/+6','Se(s)/Se +4','Se-/Se(s)','U +4/+6'/
      DATA EHFMT/'('' EHOPT('',I1,'') - '',I8,
     *2X,''Use '',A16,'' Eh to calculate '',A24)'/
      DATA EHMDFM/'8','8','12','16','7','6','7','7','8','11','8','11',
     *'9','7'/
C
      READ(5,560)CARD1
      READ(5,560)CARD2
  560 FORMAT(A80)
      WRITE(*,1111)CARD1
 1011 FORMAT(1H1,1X,A80)
 1111 FORMAT(1H ,A80)
      IF (K.NE.1) THEN
         WRITE(K,1011)CARD1
         WRITE(K,1111)CARD2
      END IF
      READ(5,570)
      READ(5,570) TEMP, PH, EH(0), DOC, DOX, CORALK
  570 FORMAT (5(F8.2,1X),I8)
      WRITE(K,1112)TEMP , PH ,EH(0) ,DOC ,DOX ,CORALK
 1112 FORMAT (1X,'                    TEMP      = ',F16.6,/,
     *'                      PH        = ',F16.6,/,
     *'                      EH(0)     = ',F16.6,/,
     *'                      DOC       = ',F16.6,/,
     *'                      DOX       = ',F16.6,/,
     *'                      CORALK    = ',I9)
      READ(5,575)
      READ(5,575) FLG,DENS,PRNT,PUNCH,(EHOPT(I), I=1,9)
  575 FORMAT (A4,F11.5,2I6,6X,9I3)
      IF (DENS .LT. 1D-78) DENS = 1.0
      IF (FLG .EQ. CONZ(1)) FLAG = 1
      IF (FLG .EQ. CONZ(2)) FLAG = 2
      IF (FLG .EQ. CONZ(3)) FLAG = 3
      IF (FLG .EQ. CONZ(4)) FLAG = 4
      IF (FLG .EQ. CONZ(5)) FLAG = 5
      WRITE(K,1113)FLG,DENS,PRNT,PUNCH
 1113 FORMAT('                      FLG       =       ',A4,/,
     *'                      DENS      = ',F16.6,/,
     *'                      PRNT      =  ',I8,/,
     *'                      PUNCH     =  ',I8)
      DO 580 I=1,9
        EHFMT(62:63)=EHMDFM(EHOPT(I))
        WRITE(K,EHFMT)I,EHOPT(I),EHMODE(EHOPT(I)),SPCALC(I)
  580 CONTINUE
      READ(5,570)
      READ(5,585) EMPOX, ITDS, COND, SIGMDO, SIGMEH, SIGMPH
  585 FORMAT(I8,1X,2(F8.2,1X),3F12.4)
      WRITE(K,1114)EMPOX,ITDS,COND,SIGMDO,SIGMEH,SIGMPH
```

```
 1114 FORMAT('                    EMPOX     =   ',I8,/,
     *'                    ITDS      =  ',F16.6,/,
     *'                    COND      =  ',F16.6,/,
     *'                    SIGMDO    =  ',F16.6,/,
     *'                    SIGMEH    =  ',F16.6,/,
     *'                    SIGMPH    =  ',F16.6,//,
     *'      Species    Index No      Input Concentration'/,
     *'      ----------------------------------------')
      READ(5,620)
      READ(5,620)(XIN(I),I=1,6)
      READ(5,620)
      READ(5,620)(XIN(I),I=7,12)
      READ(5,620)
      READ(5,620)(XIN(I),I=13,17)
  620 FORMAT(6F12.4)
      DO 90 I=1,17
      J = LISTE(I)
      CUNITS(J) = XIN(I)
      WRITE(K,1116)PAGE1(J),J,CUNITS(J)
 1116 FORMAT('      ',A8,'  :   ',I3,'   :  ',F16.8)
   90 CONTINUE
      READ(5,620)
C
   80 READ(5,630) WORD,(VAL(I),XIN(I),I=1,4)
  630 FORMAT(A4,4(1X,I3,1X,F12.5))
C
      IF(WORD .NE. CARD(1)) GOTO 100
      DO 95 I = 1 ,4
      IF (XIN(I) .LT. 1D-78) GOTO 95
      J = VAL(I)
      CUNITS(J) = XIN(I)
      WRITE(K,1116)PAGE1(J),J,CUNITS(J)
   95 CONTINUE
      GOTO 80
C
  100 IF(WORD .NE. CARD(2)) GOTO 120
      DO 110 I = 1 ,4
      IF (XIN(I) .LT. 1D-78) GOTO 110
      J = VAL(I)
      SIGMA(J) = XIN(I)
  110 CONTINUE
      GOTO 80
C
  120 IF(WORD .NE. CARD(3)) GOTO 140
      DO 130 I = 1 ,4
      IF (XIN(I) .LT. 1D-78) GOTO 130
      J = VAL(I)
      LOGKTO(J) = XIN(I)
  130 CONTINUE
      GOTO 80
  140 CONTINUE
      RETURN
      END
C
C   FOLLOWING IS THE 'INCLUDE' FILE COMMON.BLK:
C
      REAL*8 EH(0:13),PE(0:13),ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,
     *FULVTT,HUMTOT,ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,
     *EPMCAT,NATOT,NEQU,NH4TOT,NITOT,NONCRB,NORM,NO2TOT,C1,C2,C3,C4
      INTEGER EHOPT(9),CORALK,D,E,G,H,PRNT,EMPOX,FULFLG,HUMFLG,ISDATA,
     *ITER,NMBR,PUNCH,RBIT,FLAG,ENDE
      CHARACTER*80 CARD1,CARD2
C
      COMMON EH,PE,EHOPT,A,AGTOT,AH2O,ALTOT,ANLCO3,ASTOTL,AS3TOT,AS5TOT,
     *B,BATOT,BTOT,C,CARBON,CATOT,CDTOT,CLTOT,CONCLC,COND,CORALK,CO2TIT,
```

```
*CO3ALC,CSTOT,CUTOT,C1,C2,C3,C4,D,DENS,DIFF,DISCHG,DOC,DOX,E,
*EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,FULVTT,
*G,H,HCO3TT,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,ITDS,ITER,K,
*KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,XMU,XMUHL,NEQU,NH4TOT,NITOT,
*NMBR,NONCRB,NORM,NO2TOT,PBTOT,PCO2,PH,PRNT,PTOT,PUNCH,R,RBIT,
*RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,T,TDS,TEMP,TENMPE,
*TENPH,XMI120,XMI121,XMI178,ZNTOT,SETOTL,H2SETT,SEO3TT,SEO4TT,
*UTOTAL,U4TOT,U6TOT
 COMMON/CHRDAT/CARD1,CARD2
```

Attachment D. Program Listing of BASIC version of WQ4FINPT

```
10 '"WQ4FINPT",A
20    '  ************************************************************************
30    '  ****                                                                ****
40    '  ****                    IBM PC WQ4FINPT                             ****
50    '  ****                                                                ****
60    '  ****        An IBM BASICA program to assist in                      ****
70    '  ****       preparing input data files to WATEQ4F.                   ****
80    '  ****                                                                ****
90    '  ****                    by J. W. Ball                               ****
100   '  ****                                                                ****
110   '  ****             U. S. Geological Survey                            ****
120   '  ****                                                                ****
130   '  ****  This version features reading of data from MASTER disk        ****
140   '  ****  files prepared by MEGACRUNCH from Plasma-Spec output,         ****
150   '  ****  with non-plasma data manually added by the user, and the      ****
160   '  ****  input and formatting of Se, Cr, Co, Mo and V data.            ****
170   '  ****                                                                ****
180   '  ****  This version will not do sigmas.  Cr, Co, Mo and V data       ****
190   '  ****  are placed at the end of record number 2.                     ****
200   '  ****                                                                ****
210   '  ****  12/19/89:                                                     ****
220   '  ****  Modified to write to a batch file READNAME.BAT, to run        ****
230   '  ****  under direction of batch program WQ4F.BAT.  Allows WQ4F       ****
240   '  ****  to "know" name of input file supplied to WQ4FINPT.            ****
250   '  ****                                                                ****
260   '  ****  3/22/90:                                                      ****
270   '  ****  Modified to accept and format input for the revised Eh        ****
280   '  ****  and print options, and for uranium.  NOTE: Data sets          ****
290   '  ****  made with earlier versions of WQ4FINPT ARE compatible         ****
300   '  ****  with Version 2.0 of WATEQ4F.                                  ****
310   '  ****                                                                ****
320   '  ****  This version operational:  8/15/90                            ****
330   '  ****                                                                ****
340   '  ************************************************************************
350   DEFDBL A
360   DIM L2(80),REC$(30),IMAGE$(6),EHPHRASE$(9)
370   BELL$=CHR$(7)
380   RESTORE 400: FOR I=1 TO 80: READ L2(I): NEXT I
390   '     Ca   Mg  Na   K  Si  Al  Fe   Mn   B   Sr    Ba    Cu   Zn
400   DATA 0.05,0.50,0.2,0.3,0.5,0.5,0.1,0.02,0.2,0.002,0.005,0.05,0.01
410    '    Cd    Co    Cr   Mo   Ni   Pb    V   As   Be    Ti   P
420   DATA 0.005,0.002,0.01,0.05,0.003,0.2,0.075,0.3,0.001,0.01,0.5
430    '    Se  W  LiRbTlU  (Note:  U is element number 30)
440   DATA 0.3,0.2,0,0,0,0
450   REM
460   REM  Old Limits, from Tektronix version of WQ4FINPT:
470   REM
480   REM  #31   #32   #33   #34   #35  #36   #37  #38   #39 #40
490   DATA 0.002,0.003,0.005,0.002,0.02,0.005,0.04,0.004,0.1,0.02
500   DATA 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
510   DATA 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
520   FOR I=1 TO 6: READ IMAGE$(I): NEXT
530   DATA "#####.##","######.##","#####.###","######.##","######.##","#########
"
540   FOR I=1 TO 9: READ EHPHRASE$(I): NEXT
550   DATA "Fe species distribution","Mn species other than +2"
560   DATA "Cu +1 species","As species distribution","Se species distribution"
570   DATA "Ion Activity Product calculations","pO2 calculation"
580   DATA "H2S from SO4, pH and Eh","U species distribution"
590   CLS:INPUT "Do you want color? ",Q$:IF Q$<>"N" OR Q$<>"n" THEN COLOR 15,1
600   CLS:PRINT "WELCOME!  WELCOME!":BEEP
610   PRINT: PRINT "Defaulting to parallel printer port 1('LPT1')":PRINT
620   PRINT "This version reads data from disk, but does not accept sigmas."
630   PRINT:PRINT "Pressing the Enter key always selects the stated default.  In
 the "
```

```
640   PRINT "case of numerical input, the default is always zero unless otherwis
e stated"
650   PRINT:INPUT "All data from Keyboard (K [the default]), or some data from D
isk (D)? ",V$
660   IF LEN(V$)=0 THEN V$="K"
670   IF V$="K" OR V$="k" GOTO 840
680   PRINT:PRINT "Insert data diskette in drive A and strike a key when ready."
690   KB$=INKEY$: IF KB$="" GOTO 690
700   SHELL "DIR A:*.>DIR.TMP"
710   OPEN "DIR.TMP" FOR INPUT AS #1
720   INPUT #1,A$: IF EOF(1) GOTO 760
730   IF INSTR(A$,"Volume in drive")>0 THEN VOLID$=MID$(A$,23,11):PRINT A$:PRINT
:PRINT "Available directories:":PRINT
740   IF INSTR(A$,"<DIR>")>0 THEN A$=MID$(A$,1,10):PRINT "   "+A$
750   GOTO 720
760   CLOSE 1:KILL"DIR.TMP"
770   PRINT:INPUT "Enter directory name you want: ",LIB$
780   OPEN "A:\"+LIB$+"\DESCRIPT.DAT" FOR INPUT AS #1
790   INPUT #1,SMPSTR$
800   CLOSE 1
810   GOSUB 6600
820   N2=80:OPEN "A:\"+LIB$+"\MASTER" AS #2 LEN=4
830   FIELD #2, 4 AS VV$
840   FILNAM$="WATEQ4F.DAT"
850   PRINT:PRINT"Hit <Enter> to append data to file ";FILNAM$;".  Otherwise, "
860   INPUT "enter the name of a different file: ",Z$
870   IF LEN(Z$)>0 THEN FILNAM$=Z$: GOSUB 7430
880   IF ERRCODE>0 GOTO 840
890   PRINT: PRINT "Data will be appended to file ";FILNAM$
900   Z$="N": REC$(0)="****"
910   IF V$="K" OR V$="k" THEN J3=1:J4=100
920   REM        J3 IS STARTING SEQUENCE # IN RANDOM-ACCESS DISK FILE
930   REM        J4 IS ENDING SEQUENCE # IN THE RANDOM-ACCESS FILE
940   N=J3-1
950   REC$(1)=""
960   ' [START OF **GIANT** LOOP]
970   N=N+1
980   IF N>J4 GOTO 6400
990   IF V$="K" OR V$="k" GOTO 1040
1000  U$=MID$(SMPSTR$,10*N-9,10)
1010  PRINT "Sample # ";N;": ";U$
1020  N4=(N-1)*N2
1030  ' [RECORD 1]
1040  PRINT:PRINT " Enter descriptor (72 chars maximum, <Enter> to QUIT):"
1050  LINE INPUT "",REC$(1)
1060  IF LEN(REC$(1))=0 THEN 6400
1070  IF LEN(REC$(1))>72 THEN BEEP:GOTO 1040
1080  WHILE LEN(REC$(1))<72: REC$(1)=REC$(1)+" ": WEND
1090  INPUT "Enter dataset number (5 digit maximum): ",REC$(2)
1100  IF LEN(REC$(2))>5 THEN BEEP:GOTO 1090
1110  WHILE LEN(REC$(2))<5: REC$(2)=" "+REC$(2): WEND
1120  REC$(1)=REC$(1)+REC$(2)+" "
1130  INPUT "Enter plot symbol (1 char only): ",REC$(2)
1140  IF LEN(REC$(2))<>1 THEN BEEP:GOTO 1130
1150  REC$(1)=REC$(1)+REC$(2)+"5"
1160  PRINT: PRINT "RECORD 1:"
1170  PRINT REC$(0)
1180  PRINT REC$(1): PRINT
1190  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 1040
1200  ' [RECORD 2]
1210  IF V$="K" OR V$="k" GOTO 1250
1220  N3=N4+49
1230  GET #2,N3:A=CVS(VV$)
1240  GOTO 1260
1250  INPUT "Enter conductivity(uS): ",A
```

```
1260  COND=A
1270  IF A>99999! THEN PRINT BELL$;"CONDUCTIVITY TOO LARGE.  REENTER. . .":GOTO
 1250
1280  REC$(2)=STR$(A):REC$(2)=RIGHT$(REC$(2),LEN(REC$(2))-1)
1290  WHILE LEN(REC$(2))<5: REC$(2)=" "+REC$(2): WEND
1300  IF V$="K" OR V$="k" GOTO 1350
1310  N3=N4+50
1320  GET #2,N3:A=CVS(VV$)
1330  A=A*.001
1340  GOTO 1360
1350  INPUT "Enter total dissolved solids(mg/L): ",A
1360  ITDS=A
1370  IF A>999999! THEN PRINT BELL$;"TDS VALUE TOO LARGE.  REENTER. . .":GOTO 13
50
1380  C$=STR$(A):C$=RIGHT$(C$,LEN(C$)-1)
1390  WHILE LEN(C$)<6: C$=" "+C$: WEND
1400  REC$(2)=REC$(2)+C$
1410  IF V$="K" OR V$="k" GOTO 1460
1420  N3=N4+64
1430  GET #2,N3:A=CVS(VV$)
1440  C$=STR$(A):C$=RIGHT$(C$,LEN(C$)-1)
1450  GOTO 1470
1460  INPUT "Enter date(6 chars max): ",C$
1470  IF LEN(C$)>6 THEN PRINT BELL$;:PRINT"TOO MANY CHARACTERS FOR DATE.  REENTE
R.  .  .":GOTO 1460
1480  WHILE LEN(C$)<6: C$="0"+C$: WEND
1490  REC$(2)=REC$(2)+" "+C$
1500  IF V$="K" OR V$="k" GOTO 1550
1510  N3=N4+67
1520  GET #2,N3:A=CVS(VV$)
1530  GOSUB 6520
1540  GOTO 1570
1550  PRINT "Enter discharge(cfs): ";
1560  GOSUB 6510
1570  IF V$="K" OR V$="k" GOTO 1630
1580  N3=N4+66
1590  GET #2,N3:A=CVS(VV$)
1600  A=A*.001
1610  GOSUB 6520
1620  GOTO 1650
1630  PRINT "Enter dissolved organic carbon(mg/L): ";
1640  GOSUB 6510
1650  DOC=A
1660  IF V$="K" OR V$="k" GOTO 1710
1670  N3=N4+65
1680  GET #2,N3:A=CVS(VV$)
1690  GOSUB 6520
1700  GOTO 1730
1710  PRINT "Enter salinity(o/oo): ";
1720  GOSUB 6510
1730  IF V$="K" OR V$="k" GOTO 1790
1740  N3=N4+68
1750  GET #2,N3:A=CVS(VV$)
1760  C$=STR$(A)
1770  GOSUB 6520
1780  GOTO 1870
1790  PRINT "Enter Cr: ";
1800  GOSUB 6510
1810  PRINT "Enter Co: ";
1820  GOSUB 6510
1830  PRINT "Enter Mo: ";
1840  GOSUB 6510
1850  PRINT "Enter V: ";
1860  GOSUB 6510
1870  PRINT: PRINT "RECORDS 1 AND 2:"
```

```
1880  PRINT REC$(0)
1890  PRINT REC$(1)
1900  PRINT REC$(2): PRINT
1910  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 1210
1920  ' [RECORDS 3/4]
1930  Y$="temperature pH Eh dox coralk "
1940  ON ERROR GOTO 6870
1950  ERASE Y,Y1,Y2
1960  ON ERROR GOTO 0
1970  DIM Y(7),Y1(6),Y2(6)
1980  RESTORE 2000
1990  READ Y1(1),Y1(2),Y1(3),Y1(4),Y1(5),Y1(6)
2000  DATA 25,7,9.9,0,0,0
2010  REC$(3)="TEMP-.-- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--"
2020  REC$(4)=""
2030  J1=1
2040  FOR F=1 TO 6
2050  IF V$="K" OR V$="k" GOTO 2090
2060  IF F=1 THEN N3=N4+69 ELSE N3=N4+39+F
2070  GET #2,N3:A=CVS(VV$)
2080  GOTO 2110
2090  IF F=6 THEN GOSUB 2190:GOTO 2140
2100  IF F<>4 THEN J=INSTR(J1,Y$," "): X$=MID$(Y$,J1,J-J1): J1=J+1:PRINT USING
"&& &##.#&";"Enter ";X$;"(default=";Y1(F);"): ";: INPUT "",A ELSE A=DOC
2110  IF A=0 THEN A=Y1(F)
2120  IF F=3 THEN EHM=A
2130  IF F=5 THEN DOX=A
2140  OPEN "O",#3,"JUNK":PRINT#3,USING IMAGE$(F);A:CLOSE 3:OPEN "I",#3,"JUNK"
2150  LINE INPUT#3,REC$(5): CLOSE 3
2160  REC$(4)=REC$(4)+REC$(5)
2170  NEXT F
2180  GOTO 2260
2190  PRINT: PRINT "CORALK options:"
2200  PRINT "0.  Alkalinity input has not been corrected for noncarbonate":PRINT
"    species (the default)"
2210  PRINT "1.  Alkalinity input has been corrected for noncarbonate species"
2220  PRINT "2.  Alkalinity input is total carbon"
2230  INPUT "Enter option number: ",F$: IF F$="" THEN A=0 ELSE A=VAL(F$)
2240  IF A<0 OR A>2 THEN PRINT BELL$;: GOTO 2190
2250  RETURN
2260  S$=""
2270  IF Z$="N" GOTO 2300
2280  INPUT "Enter sigma value for pH: ",SIGPH
2290  INPUT "Enter sigma value for Eh: ",SIGEH
2300  PRINT: PRINT "RECORDS 1 TO 4:"
2310  FOR I=0 TO 4:PRINT REC$(I):NEXT:PRINT
2320  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 2020
2330  '  [RECORDS 5/6]
2340  REC$(5)="FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8--9"
2350  REC$(6)="MG/L    1.0         0     1         0  0  0  0  0  0  0  0  0"
2360  F=1:IF V$<>"K" AND V$<>"k" GOTO 2470
2370  PRINT: PRINT "Flag options:"
2380  PRINT "1.  mg/l  (the default)"
2390  PRINT "2.  ppm"
2400  PRINT "3.  meq/l"
2405  PRINT "4.  mmol/l"
2410  PRINT "5.  mol"
2420  INPUT "Enter option number: ",F$:IF F$=""THEN F=1 ELSE F=VAL(F$)
2430  IF F<1 OR F>5 THEN PRINT BELL$;: GOTO 2370
2440  Y$="MG/LPPM MQ/LMMOLMOL  "
2450  REC$(7)=MID$(Y$,4*F-3,4)
2460  MID$(REC$(6),1,4)=REC$(7)
2470  PRINT:INPUT "Enter density (default=1.00): ",REC$(7)
2480  A=VAL(REC$(7))
2490  IF A=0 THEN A=1
```

```
2500  REC$(7)=STR$(A)
2510  P=INSTR(1,REC$(7),".")
2520  IF P=0 THEN REC$(7)=REC$(7)+".0": GOTO 2510
2530  P2=INSTR(5,REC$(6),".")
2540  MID$(REC$(6),P2-P+1,LEN(REC$(7)))=REC$(7)
2550  PRINT: PRINT "Print options:"
2560  PRINT "0.  Print minimum output (the default)"
2570  PRINT "1.  Print complete aqueous speciation and mineral solubility
listing"
2580  PRINT "2.  Print minimum output plus weight and molar ratios page"
2590  PRINT "3.  Print complete output (1 plus 2)"
2600  PRINT "4.  0 plus generate the thermodynamic data table"
2610  PRINT "5.  1 plus generate the thermodynamic data table"
2620  PRINT "6.  2 plus generate the thermodynamic data table"
2630  PRINT "7.  3 plus generate the thermodynamic data table"
2640  INPUT "Enter option number: ",F$:IF F$=""THEN A=0 ELSE A=VAL(F$)
2650  IF A<0 OR A>7 THEN PRINT BELL$;: GOTO 2550
2660  IF A<>0 THEN REC$(7)=STR$(A): MID$(REC$(6),20,2)=REC$(7)
2670  PRINT: PRINT "Punch options:"
2680  PRINT "0.  Generate an input dataset for EQPRPLOT"
2690  PRINT "1.  Omit the EQPRPLOT dataset (the default)"
2700  INPUT "Enter option number: ",F$:IF F$=""THEN A=1 ELSE A=VAL(F$)
2710  IF A<0 OR A>1 THEN PRINT BELL$;: GOTO 2670
2720  IF A<>1 THEN REC$(7)=STR$(A): MID$(REC$(6),26,2)=REC$(7)
2730  CLS: LOCATE 1,54:PRINT "Eh options:"
2740  LOCATE  2,42: PRINT "-----------------------------------";
2750  LOCATE  3,42: PRINT " 0.  Use measured Eh (the default)";
2760  LOCATE  4,42: PRINT " 1.  Use Fe 2/3 Eh";
2770  LOCATE  5,42: PRINT " 2.  Use H2O/O2 Eh with Sato relation";
2780  LOCATE  6,42: PRINT " 3.  Use H2O/O2 Eh w/classical relation";
2790  LOCATE  7,42: PRINT " 4.  Use NH4/NO3 Eh";
2800  LOCATE  8,42: PRINT " 5.  Use S -2/SO4 Eh";
2810  LOCATE  9,42: PRINT " 6.  Use NO2/NO3 Eh";
2820  LOCATE 10,42: PRINT " 7.  Use S -2/S(s) Eh";
2830  LOCATE 11,42: PRINT " 8.  Use As 3/5 Eh";
2840  LOCATE 12,42: PRINT " 9.  Use As(s)/As +3 Eh";
2850  LOCATE 13,42: PRINT "10.  Use Se 4/6 Eh";
2860  LOCATE 14,42: PRINT "11.  Use Se(s)/Se +4 Eh";
2870  LOCATE 15,42: PRINT "12.  Use Se -2/Se(s) Eh";
2880  LOCATE 16,42: PRINT "13.  Use U 4/6 Eh";
2890  LOCATE 18,40: PRINT "NOTE:  Use these options with caution!"
2900  LOCATE 19,47: PRINT "To use an option you must have"
2910  LOCATE 20,47: PRINT "input data for the redox specie"
2920  LOCATE 21,47: PRINT "or species referred to."
2930  LOCATE 3,1
2940  FOR I=1 TO 9
2950    PRINT USING "#. &";I,"Enter number of Eh to use for"
2960    PRINT "   ";EHPHRASE$(I);": ";
2970    INPUT "",F$:IF F$=""THEN A=0 ELSE A=VAL(F$)
2980    IF A<0 OR A>13 THEN PRINT BELL$;:LOCATE CSRLIN-2,1:GOTO 2950
2990    IF A=0 GOTO 3040
3000    REC$(7)=STR$(A)
3010    IF LEN(REC$(7))=2 THEN REC$(7)=" "+REC$(7)
3020    MID$(REC$(6),31+I*3,3)=REC$(7)
3030    EHOPT(I)=A
3040  NEXT
3050  ' [RECORDS 7/8]
3060  REC$(7)="EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.----SIGMPH-.----"
3070  REC$(8)="       0     0.0      0.0         0.0          0.0          0.0   "
3080  I$=STR$(ITDS)
3090  P=INSTR(I$,".")
3100  IF P=0 THEN I$=I$+".0": GOTO 3090
3110  P2=INSTR(1,REC$(8),".")
3120  MID$(REC$(8),P2-P+1,LEN(I$))=I$
3130  P1=P2+1
```

```
3140  I$=STR$(COND)
3150  P=INSTR(I$,".")
3160  IF P=0 THEN I$=I$+".0": GOTO 3150
3170  P2=INSTR(P1,REC$(8),".")
3180  MID$(REC$(8),P2-P+1,LEN(I$))=I$
3190  PRINT: PRINT "RECORDS 1 THROUGH 8:"
3200  FOR I=0 TO 8
3210  PRINT REC$(I)
3220  NEXT I
3230  PRINT
3240  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 2350
3250  ' [RECORDS 9/10]
3260  Y$="CaMgNaKClSO4"
3270  ON ERROR GOTO 6870
3280  ERASE Y,Y1,Y2
3290  ON ERROR GOTO 0
3300  DIM Y(7),Y1(6),Y2(6)
3310  RESTORE 3330
3320  READ Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7)
3330  DATA 1,3,5,7,8,10,13
3340  RESTORE 3360
3350  READ Y1(1),Y1(2),Y1(3),Y1(4),Y1(5),Y1(6)
3360  DATA 0,1,2,3,4,5
3370  RESTORE 3390
3380  READ Y2(1),Y2(2),Y2(3),Y2(4),Y2(5),Y2(6)
3390  DATA 1,2,3,4,52,51
3400  REC$(9)="CA-----.----MG-----.----NA-----.----K------.----CL-----.----"
3410  REC$(9)=REC$(9)+"SO4----.----"
3420  REC$(10)=""
3430  IF V$="S" OR Z$="N" THEN 3460
3440  INPUT "Any sigma values for Ca through SO4? ",ZZ$
3450  ON INSTR("YN",ZZ$)+1 GOTO 3440,3460,3460
3460  P1=1
3470  FOR F=1 TO 6
3480  YY$=MID$(Y$,Y(F),Y(F+1)-Y(F))
3490  IF V$="K" OR V$="k" GOTO 3580
3500  N3=N4+Y2(F)
3510  GET #2,N3:A=CVS(VV$)
3520  IF A>=L2(Y2(F)) OR A=0 GOTO 3550
3530  A=-1
3540  GOTO 3600
3550  A=A*.001
3560  GOSUB 6710  '  ROUNDOFF GOSUB
3570  GOTO 3600
3580  PRINT "ENTER ";YY$;" VALUE: ";
3590  INPUT "",A
3600  HH$=STR$(A): IF F=6 THEN SO4=A
3610  IF INSTR(HH$,".")=0 THEN HH$=HH$+".0"
3620  NUM.LENGTH=LEN(HH$)
3630  FOR I=NUM.LENGTH TO 11: HH$=" "+HH$: NEXT
3640  REC$(10)=REC$(10)+HH$
3650  IF Z$="N" THEN 3770
3660  IF V$="S" AND N=1 THEN 3680
3670  ON INSTR("YN",ZZ$) GOTO 3700,3770
3680  A=L2(Y2(F))
3690  IF A>0 THEN 3760
3700  PRINT "ENTER SIGMA VALUE FOR ";YY$;": ";
3710  INPUT "",A
3720  IF A=0 THEN 3770
3730  IF A>0 THEN 3760
3740  PRINT BELL$;"NEGATIVE SIGMA VALUES NOT ALLOWED.  ABSOLUTE VALUE TAKEN."
3750  A=ABS(A)
3760  GOSUB 6750  '  CONSTRUCT "SIGM" RECORDS
3770  NEXT F
3780  IF V$="S" THEN 3850
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3790  PRINT: PRINT "RECORDS 1 TO 10:"
3800  FOR I=0 TO 10
3810  PRINT REC$(I)
3820  NEXT I
3830  PRINT
3840   ' PRINT S$: PRINT
3850  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 3420
3860  ' [RECORDS 11/12]
3870  Y$="HCO3Fe(tot)H2SCO3SiO2NH4"
3880  ERASE Y,Y1,Y2
3890  DIM Y(7),Y1(6),Y2(6)
3900  RESTORE 3920
3910  READ Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7)
3920  DATA 1,5,12,15,18,22,25
3930  RESTORE 3960
3940  READ Y1(1),Y1(2),Y1(3),Y1(4),Y1(5),Y1(6)
3950  DATA 17,34,38,86,44,50,61,84
3960  DATA 6,16,13,17,34,38
3970  RESTORE 3990
3980  READ Y2(1),Y2(2),Y2(3),Y2(4),Y2(5),Y2(6)
3990  DATA 48,40,37,54,5,55
4000  REC$(11)="HCO3---.----FE TOT-.----H2S AQ-.----CO3----.----SIO2TOT.----"
4010  REC$(11)=REC$(11)+"NH4----.----"
4020  REC$(12)=""
4030  IF V$="S" OR Z$="N" THEN 4060
4040  INPUT "Any sigma values for HCO3 through NH4? ",ZZ$
4050  ON INSTR("YN",ZZ$)+1 GOTO 4040,4060,4060
4060  P1=1
4070  FOR F=1 TO 6
4080  YY$=MID$(Y$,Y(F),Y(F+1)-Y(F))
4090  IF V$="K" OR V$="k" GOTO 4260
4100  N3=N4+Y2(F)
4110  GET #2,N3:A=CVS(VV$)
4120  IF A>=L2(Y2(F)) OR A=0 THEN 4150
4130  A=-1
4140  GOTO 4280
4150  ON F GOTO 4230,4190,4170,4230,4220,4230
4160  ' [CONVERT S= TO H2S]
4170  A=A*34.07994/32.064
4180  GOTO 4230
4190  PRINT BELL$: PRINT "COLORIMETRIC ";YY$;" USED AS INPUT DATA"
4200  GOTO 4230
4210  ' [CONVERT Si TO SiO2]
4220  A=A*60.0848/28.086
4230  A=A*.001
4240  GOSUB 6710
4250  GOTO 4280
4260  PRINT "ENTER ";YY$;" VALUE: ";
4270  INPUT "",A
4280  HH$=STR$(A)
4290  IF F=2 THEN FET=A
4300  IF F=3 THEN H2S=A
4310  IF F=6 THEN NH4=A
4320  P=INSTR(REC$(13),".")
4330  IF INSTR(HH$,".")=0 THEN HH$=HH$+".0"
4340  NUM.LENGTH=LEN(HH$)
4350  FOR I=NUM.LENGTH TO 11: HH$=" "+HH$: NEXT
4360  REC$(12)=REC$(12)+HH$
4370  IF Z$="N" THEN 4550
4380  IF V$="S" AND N=1 THEN 4400
4390  ON INSTR("YN",ZZ$) GOTO 4420,4550
4400  A=L2(Y2(F))
4410  IF A>0 THEN 4480
4420  PRINT "ENTER SIGMA VALUE FOR ";REC$(6);": ";
4430  INPUT A
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4440  IF A=0 THEN 4550
4450  IF A>0 THEN 4480
4460  PRINT BELL$;"NEGATIVE SIGMA VALUES NOT ALLOWED.  ABSOLUTE VALUE TAKEN."
4470  A=ABS(A)
4480  ON F GOTO 4550,4550,4550,4550,4490,4550
4490  A=A*60.0848/28.086  '  Si/SiO2
4500  GOTO 4540
4510  A=A*94.9714/30.9738  '  P/PO4
4520  GOTO 4540
4530  A=A*62.0049/14.0067  '  N/NO3
4540  GOSUB 6710
4550  NEXT F
4560  IF V$="S" THEN 4620
4570  PRINT: PRINT "RECORDS 1 TO 12:"
4580  FOR I=0 TO 12
4590  PRINT REC$(I)
4600  NEXT I
4610   ' PRINT S$: PRINT
4620  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 4020
4630  ' [RECORDS 13/14]
4640  Y$="B(tot)PO4AlFNO3"
4650  ERASE Y,Y1,Y2
4660  DIM Y(6),Y1(5),Y2(5)
4670  RESTORE 4690
4680  READ Y(1),Y(2),Y(3),Y(4),Y(5),Y(6)
4690  DATA 1,7,10,12,13,16
4700  RESTORE 4720
4710  READ Y1(1),Y1(2),Y1(3),Y1(4),Y1(5)
4720  DATA 86,44,50,61,84
4730  RESTORE 4750
4740  READ Y2(1),Y2(2),Y2(3),Y2(4),Y2(5)
4750  DATA 9,24,6,53,56
4760  REC$(13)="B TOT--.----PO4----.----AL-----.----F------.----NO3----.----"
4770  REC$(14)=""
4780  IF V$="S" OR Z$="N" THEN 4810
4790  INPUT "Any sigma values for B tot through NO3? ",ZZ$
4800  ON INSTR("YN",ZZ$)+1 GOTO 4790,4810,4810
4810  P1=1
4820  FOR F=1 TO 5
4830  YY$=MID$(Y$,Y(F),Y(F+1)-Y(F))
4840  IF V$="K" OR V$="k" GOTO 4990
4850  N3=N4+Y2(F)
4860  GET #2,N3:A=CVS(VV$)
4870  IF A>=L2(Y2(F)) OR A=0 THEN 4900
4880  A=-1
4890  GOTO 5010
4900  ON F GOTO 4960,4920,4960,4960,4950
4910  ' [CONVERT P TO PO4]
4920  A=A*94.9714/30.9738
4930  GOTO 4960
4940  ' [CONVERT N TO NO3]
4950  A=A*62.0049/14.0067
4960  A=A*.001
4970  GOSUB 6710
4980  GOTO 5010
4990  PRINT "ENTER ";YY$;" VALUE: ";
5000  INPUT "",A
5010  HH$=STR$(A): IF F=5 THEN NO3=A
5020  IF INSTR(HH$,".")=0 THEN HH$=HH$+".0"
5030  NUM.LENGTH=LEN(HH$)
5040  FOR I=NUM.LENGTH TO 11: HH$=" "+HH$: NEXT
5050  REC$(14)=REC$(14)+HH$
5060  P1=P2+1
5070  IF Z$="N" THEN 5230
5080  IF V$="S" AND N=1 THEN 5100
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5090  ON INSTR("YN",Z$) GOTO 5120,5230
5100  A=L2(Y2(F))
5110  IF A>0 THEN 5180
5120  PRINT "ENTER SIGMA VALUE FOR ";REC$(6);": ";
5130  INPUT "",A
5140  IF A=0 THEN 5230
5150  IF A>0 THEN 5180
5160  PRINT BELL$;"NEGATIVE SIGMA VALUES NOT ALLOWED.  ABSOLUTE VALUE TAKEN."
5170  A=ABS(A)
5180  ON F GOTO 5220,5190,5220,5220,5210
5190  A=A*94.9714/30.9738  '  CONVERT P TO PO4
5200  GOTO 5220
5210  A=A*62.0049/14.0067  '  CONVERT N TO NO3
5220  GOSUB 6710
5230  NEXT F
5240  PRINT: PRINT "RECORDS 1 TO 14:"
5250  FOR I=0 TO 14: PRINT REC$(I): NEXT: PRINT
5260   ' PRINT S$: PRINT
5270  GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 4770
5280  ' [INPUT OF OPTIONAL CONCENTRATION DATA AND SIGMAS]
5290  Y$="Fe+2Fe+3CsLiSrBaRbIBrMnCuZnCdPbNO2NiAgAs(total)As+3As+5Fulvate"
5300  Y$=Y$+"HumateSe(total)H2SeSe+4Se+6U(total)U+4U+6"
5310  ERASE Y,Y1,Y2
5320  DIM Y(30),Y1(29),Y2(29)
5330  RESTORE 5350
5340  FOR I=1 TO 30:READ Y(I):NEXT
5350  DATA 1,5,9,11,13,15,17,19,20,22,24,26,28,30,32,35,37,39,48,52,56,63,69
5360  DATA 78,82,86,90,98,101,104
5370  RESTORE 5390
5380  FOR I=1 TO 29:READ Y1(I):NEXT
5390  DATA 7,8,48,80,87,89,94,96,97,109,130,145,160,182,202,204,212
5400  DATA 249,261,262,284,285,298,299,300,301,316,317,359
5410  RESTORE 5430
5420  FOR I=1 TO 29:READ Y2(I):NEXT
5430  DATA 38,39,59,27,10,11,28,58,61,8,12,13,14,19,57,18,36,46,44,45,62,63
5440  DATA 0,0,0,0,0,0,0
5450  REC$(15)="$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ --- "
5460  REC$(15)=REC$(15)+"++++++.+++++"
5470  REC$(21)="CUN                                                          "
5480  REC$(21)=REC$(21)+"             "
5490  I$=REC$(21)
5500  FOR I=16 TO 20:REC$(I)="":NEXT
5510  IF V$="S" OR Z$="N" THEN 5530
5520  INPUT "Any sigma values for optional data? ",ZZ$
5530  P1=1
5540  P4=1
5550  NVAL=0
5560  FOR F=1 TO 29
5570  YY$=MID$(Y$,Y(F),Y(F+1)-Y(F))
5580  IF V$="K" OR V$="k" OR Y2(F)=0 GOTO 5720
5590  N3=N4+Y2(F)
5600  ON F GOTO 5630,5630,5640,5640,5640,5640,5640,5640,5640,5640
5610  ON F-10 GOTO 5640,5640,5640,5640,5640,5640,5640,5630,5630,5630
5620  GOTO 5640
5630  PRINT BELL$;"Colorimetric ";YY$;" used as input data"
5640  GET #2,N3:A=CVS(VV$)
5650  IF A>=L2(Y2(F)) OR A=0 THEN 5680
5660  A=-1
5670  GOTO 5870
5680  A=A*.001
5690  IF F=15 THEN A=A*46.0055/14.0067  '  CONVERT N TO NO2
5700  GOSUB 6710
5710  GOTO 5740
5720  PRINT "Enter ";YY$;
5730  INPUT " value(<Enter> for no data): ",A
```

```
5740  IF F=1 THEN FE2=A
5750  IF F=2 THEN FE3=A
5760  IF F=15 THEN NO2=A
5770  IF F=18 THEN AST=A
5780  IF F=19 THEN AS3=A
5790  IF F=20 THEN AS5=A
5800  IF F=23 THEN SET=A
5810  IF F=25 THEN SE4=A
5820  IF F=26 THEN SE6=A
5830  IF F=27 THEN UT=A
5840  IF F=28 THEN U4=A
5850  IF F=29 THEN U6=A
5860  IF A=0 THEN 6090
5870  NVAL=NVAL+1
5880  IF (NVAL-1)/4 <> INT((NVAL-1)/4) GOTO 5920
5890  ON (NVAL-1)/4 GOSUB 6780,6790,6800,6810,6820
5900  REC$(21)=I$
5910  P1=22: P3=8
5920  HH$=STR$(A)
5930  II$=STR$(Y1(F))
5940  P=INSTR(HH$,"."): IF P=0 AND INSTR(HH$,"E")=0 THEN HH$=HH$+".0": GOTO 5940
5950  MID$(REC$(21),P1-LEN(HH$),LEN(HH$))=HH$
5960  MID$(REC$(21),P3-LEN(II$)+1,LEN(II$))=II$
5970  P3=P3+17: P1=P1+17
5980  IF Z$="N" GOTO 6090
5990  IF V$="S" AND N=1 GOTO 6010
6000  ON INSTR("YN",ZZ$) GOTO 6030,6090
6010  A=L2(Y2(F))
6020  IF A>0 GOTO 6070
6030  PRINT "Enter sigma value for ";YY$;": ";
6040  INPUT "",A
6050  IF A=0 GOTO 6090
6060  IF A<0 THEN PRINT BELL$;"Negative sigma values not allowed.  Absolute
value taken.":A=ABS(A)
6070  IF F=15 THEN A=A*46.0055/14.0067: GOSUB 6710
6080  HH$=STR$(A)
6090  NEXT F
6100  FOR I=16 TO 21: IF REC$(I)=I$ THEN REC$(I)=""
6110  NEXT
6120  GOSUB 6950
6130  PRINT: PRINT "Final data:"
6140  FOR I=0 TO 15: PRINT REC$(I): NEXT
6150  FOR I=16 TO 21: IF REC$(I)<>"" THEN PRINT REC$(I)
6160  NEXT
6170  PRINT: GOSUB 6890:IF ANSW$="N" OR ANSW$="n" GOTO 5450
6180  PRINT: INPUT "Printed copy of dataset? ",W$
6190  ON INSTR("YyNn",W$)+1 GOTO 6180,6200,6200,6270,6270
6200  INPUT "Press <Enter> when printer is ready.",W$
6210  PRINT "Data set #";N;"is now being printed . . ."
6220  LPRINT: LPRINT: LPRINT "Dataset #";N;":": LPRINT
6230  FOR I=0 TO 15: LPRINT REC$(I): NEXT
6240  FOR I=16 TO 21: IF REC$(I)<>"" THEN LPRINT REC$(I)
6250  NEXT
6260  LPRINT
6270  INPUT "Store this dataset on disk? ",W$
6280  ON INSTR("YyNn",W$)+1 GOTO 6270,6290,6290,6360,6360
6290  PRINT "Data set #";N;"now being appended to file ";FILNAM$;" . . ."
6300  OPEN FILNAM$ FOR APPEND AS #1
6310  FOR I=0 TO 15: PRINT#1,REC$(I): NEXT
6320  FOR I=16 TO 21: IF REC$(I)<>"" THEN PRINT#1,REC$(I)
6330  NEXT
6340  PRINT #1,"    "
6350  CLOSE 1
6360  IF W$="N" OR W$="n" THEN PRINT "Data set #";N;"has been discarded."
6370  FOR I=1 TO 30:REC$(I)="":NEXT
```

```
6380  GOTO 970
6390  ' [END OF **GIANT** LOOP]
6400  N=N-1
6410  OPEN "READNAME.BAT" FOR OUTPUT AS #2
6420  PRINT #2, "SET FILNAM=";FILNAM$
6430  PRINT #2, "%PGMNAM% %FILNAM% %PRTOPT%"
6440  CLOSE 2
6450  PRINT "Exiting this program.  Your data file name is ";FILNAM$;"."
6460  REM  PRINT "Remember to copy or rename it to WATEQ4F.DAT before running
WATEQ4F."
6470  KILL "JUNK"
6480  SYSTEM
6490  ' [SERVICE SUBROUTINES]
6500  ' [SUBROUTINE TO INPUT SECOND DESCRIPTOR VALUES]
6510  INPUT "",A
6520  C$=STR$(A):C$=RIGHT$(C$,LEN(C$)-1)
6530  IF LEN(C$)>=8 THEN PRINT "Value too large.  Start over.  .  .":GOTO 6510
6540  WHILE LEN(C$)<8
6550  C$=" "+C$
6560  WEND
6570  REC$(2)=REC$(2)+C$
6580  RETURN
6590  ' [SUBROUTINE TO SELECT SAMPLES TO GET FROM DISK]
6600  PRINT "Index"
6610  PRINT "Number        Sample ID"
6620  PRINT "----------------------"
6630  FOR I=1 TO LEN(SMPSTR$)/10
6640  ID$=MID$(SMPSTR$,10*I-9,10)
6650  PRINT I,ID$
6660  NEXT I
6670  PRINT: INPUT "Enter starting Index Number: ",J3
6680  PRINT: INPUT "Enter  ending  Index Number: ",J4
6690  RETURN
6700  ' [SUBROUTINE FOR ROUNDING OFF TO 3 SIG FIGS]
6710  IF A=0 THEN RETURN
6720  L1=10*10^-(INT(LOG(ABS(A))/LOG(10))-1)
6730  A=INT(A*L1+.5)/L1
6740  RETURN
6750  '  [DUMMY GOSUB TO CONSTRUCT "SIGM" RECORDS]
6760  RETURN
6770  '  [GOSUBS TO INDEX OPTIONAL DATA RECORDS AND SET DEFAULT TEMP, pH, Eh]
6780  REC$(16)=REC$(21): RETURN
6790  REC$(17)=REC$(21): RETURN
6800  REC$(18)=REC$(21): RETURN
6810  REC$(19)=REC$(21): RETURN
6820  REC$(20)=REC$(21): RETURN
6830  A=25: RETURN
6840  A=7: RETURN
6850  A=9.899999: RETURN
6860  '  [GOSUB TO IGNORE ERROR TRAP ON 'ERASE' STATEMENT]
6870  RESUME NEXT
6880  '  [GOSUB TO ASK IF DATA JUST CONSTRUCTED IS ACCEPTABLE]
6890  INPUT "Are these data OK (<Enter>=Yes)? ",ANSW$
6900  ANSW$=LEFT$(ANSW$,1)
6910  ON INSTR("YyNn",ANSW$) +1 GOTO 6890,6930,6930,6930,6930
6920  GOTO 6890
6930  RETURN
6940  '  [GOSUB TO CHECK FOR ERRONEOUS EHOPT SETTINGS]
6950  IF FET>0 AND FE2>0 AND FE3<=0 THEN FE3=FET-FE2
6960  IF FET>0 AND FE3>0 AND FE2<=0 THEN FE2=FET-FE3
6970  IF AST>0 AND AS3>0 AND AS5<=0 THEN AS5=AST-AS3
6980  IF AST>0 AND AS5>0 AND AS3<=0 THEN AS3=AST-AS5
6990  IF SET>0 AND SE4>0 AND SE6<=0 THEN SE6=SET-SE4
7000  IF SET>0 AND SE6>0 AND SE4<=0 THEN SE4=SET-SE6
7010  IF UT>0 AND U4>0 AND U6<=0 THEN U6=UT-U4
```

```
7020  IF UT>0 AND U6>0 AND U4<=0 THEN U4=UT-U6
7030  CLS
7040  IF EHOPT(1)=1 THEN PRINT "It is invalid to use Eh calculated FROM
";EHPHRASE$(1);" to calculate ";EHPHRASE$(1)
7050  IF EHOPT(4)=8 THEN PRINT "It is invalid to use Eh calculated FROM
";EHPHRASE$(4);" to calculate ";EHPHRASE$(4)
7060  IF EHOPT(5)=10 THEN PRINT "It is invalid to use Eh calculated FROM
";EHPHRASE$(5);" to calculate ";EHPHRASE$(5)
7070  IF EHOPT(8)=5 THEN PRINT "It is invalid to use Eh calculated FROM H2S and
SO4 to calculate ";EHPHRASE$(8)
7080  IF EHOPT(9)=13 THEN PRINT "It is invalid to use Eh calculated FROM
";EHPHRASE$(9);" to calculate ";EHPHRASE$(9)
7090  FOR I=1 TO 9
7100  IF (EHOPT(I)=2 OR EHOPT(I)=3) AND DOX<=0 THEN PRINT "You must have D.O.
input to use the Eh calculated from D.O.":I=9
7110  NEXT I
7120  FOR I=1 TO 9
7130  IF EHOPT(I)=4 AND (NH4<=0 OR NO3<=0) THEN PRINT "You must have NH4 and NO3
input to use the Eh calculated from NH4 and NO3.":I=9
7140  NEXT I
7150  FOR I=1 TO 9
7160  IF EHOPT(I)=5 AND (H2S<=0 OR SO4<=0) THEN PRINT "You must have H2S and SO4
input to use the Eh calculated from H2S and SO4.":I=9
7170  NEXT I
7180  FOR I=1 TO 9
7190  IF EHOPT(I)=6 AND (NO2<=0 OR NO3<=0) THEN PRINT "You must have NO2 and NO3
input to use the Eh calculated from NO2 and NO3.":I=9
7200  NEXT I
7210  FOR I=1 TO 9
7220  IF EHOPT(I)=1 AND (FE2<=0 OR FE3<=0) THEN PRINT "You must have FE2 and FE3
input to use the Eh calculated from FE2 and FE3.":I=9
7230  NEXT I
7240  FOR I=1 TO 9
7250  IF EHOPT(I)=8 AND (AS3<=0 OR AS5<=0) THEN PRINT "You must have AS3 and AS5
input to use the Eh calculated from AS3 and AS5.":I=9
7260  NEXT I
7270  FOR I=1 TO 9
7280  IF EHOPT(I)=10 AND (SE4<=0 OR SE6<=0) THEN PRINT "You must have SE4 and
SE6 input to use the Eh calculated from SE4 and SE6.":I=9
7290  NEXT I
7300  FOR I=1 TO 9
7310  IF EHOPT(I)=13 AND (U4<=0 OR U6<=0) THEN PRINT "You must have U4 and U6
input to use the Eh calculated from U4 and U6.":I=9
7320  NEXT I
7330  FOR I=1 TO 9
7340  IF EHOPT(I)=7 AND H2S<=0 THEN PRINT "You must have H2S input to use the Eh
calculated from S= and S(s).":I=9
7350  NEXT I
7360  FOR I=1 TO 9
7370  IF EHOPT(I)=0 AND EHM=9.899999 THEN PRINT "**WARNING**  No input Eh was
supplied.  Use of any EHOPT=0 will result in those calculations being
skipped.":I=9
7380  NEXT I
7390  PRINT: PRINT "Eh inconsistency tests completed.": PRINT: PRINT "Press any
key to continue . . . ";
7400  K$=INKEY$:IF LEN(K$)=0 GOTO 7400
7410  RETURN
7420  '   [GOSUB TO CHECK INPUT TO SEE IF IT IS A VALID DOS FILENAME]
7430  REFSTR$="!^&*_+=[]:;<>/\":REFSTR$=REFSTR$+CHR$(63)+CHR$(34)
7440  ERRCODE=0
7450  FOR N=1 TO LEN(REFSTR$)
7460    IF INSTR(FILNAM$,MID$(REFSTR$,N,1))>0 GOTO 7530
7470  NEXT N
7480  PER=INSTR(FILNAM$,".")
7490  IF PER>9 GOTO 7530
```

```
7500  IF PER=0 AND LEN(FILNAM$)<9 THEN RETURN
7510  IF LEN(FILNAM$)-PER > 3 GOTO 7530
7520  RETURN
7530  PRINT "The filename you entered is not a valid DOS file name."
7540  ERRCODE=1
7550  RETURN
7560  '  *******  END OF CODE - WQ4FINPT  *******
```

Attachment E. Program Listing of FORTRAN version of WQ4FINPT

```
      PROGRAM WQ4FINPT
C     ******************************************************************
C     ****                                                          ****
C     ****                  FORTRAN WQ4FINPT                        ****
C     ****                                                          ****
C     ****     A PC FORTRAN program to assist the user in           ****
C     ****     preparing input data files to WATEQ4F.               ****
C     ****                                                          ****
C     ****                  by James W. Ball                        ****
C     ****                                                          ****
C     ****              U. S. Geological Survey                     ****
C     ****                                                          ****
C     ****  This version will not do sigmas.  This version features ****
C     ****  the input and formatting of Se, Cr, Co, Mo and V data.   ****
C     ****  Cr, Co, Mo and V data are placed at the end of record   ****
C     ****  number 2.                                               ****
C     ****                                                          ****
C     ****  12/19/89:                                               ****
C     ****  Modified to write to a batch file READNAME.BAT, to run  ****
C     ****  under direction of batch program WQ4F.BAT.  Allows WQ4F ****
C     ****  to "know" name of input file supplied to WQ4FINPT.      ****
C     ****                                                          ****
C     ****  3/22/90:                                                ****
C     ****  Modified to accept and format input for the revised Eh  ****
C     ****  and print options, and for uranium.  NOTE: Data sets    ****
C     ****  made with earlier versions of WQ4FINPT ARE compatible   ****
C     ****  with Version 2.0 of WATEQ4F.                            ****
C     ****                                                          ****
C     ****  This version operational:  8/25/90                      ****
C     ****                                                          ****
C     ******************************************************************
      COMMON/IONS/EHM,DOX,SO4,FET,H2S,NH4,NO3,FE2,FE3,NO2,AST,AS3,AS5,
     *SET,SE4,SE6,UT,U4,U6
      DIMENSION A(11),IA(11),XIN(4)
      INTEGER EHOPT(9),ERCODE,VAL(4),TBVAL(29)
      REAL ITDS,NH4,NO2,NO3
      CHARACTER*80 REC(0:30)
      CHARACTER*36 EHPHRA(9)
      CHARACTER*20 FILNAM,TMPFIL,VNAME(67)
      CHARACTER*8 C
      CHARACTER*4 IMAGE(6),CONZ(5)
      CHARACTER*5 FMT
      CHARACTER*1 ANSW,Z,ZZ
      DATA CONZ/'MG/L','PPM ','MQ/L','MMOL','MOL '/
      DATA EHPHRA/'Fe species distribution','Mn species other than +2',
     *'Cu +1 species','As species distribution','Se species distribution
     *','Ion Activity Product calculations','pO2 calculation',
     *'H2S from SO4, pH and Eh','U species distribution'/
      DATA VNAME/'Conductivity(uS)','Total Diss Solids',
     *'Date(6 chars max)','Discharge(cfs)','Diss Org Carbon',
     *'Salinity(o/oo)','Cr','Co','Mo','V','Temperature(deg C)','pH',
     *'Eh','DOC','Dissolved Oxygen','CORALK','Flag Option','Density',
     *'Print Option','PO','Eh Option','Ca','Mg','Na','K','Cl','SO4',
     *'HCO3','Fe(total)','H2S','CO3','SiO2','NH4','B','PO4','Al','F',
     *'NO3','Fe(+2)','Fe(+3)','Cs','Li','Sr','Ba','Rb','I','Br','Mn',
     *'Cu','Zn','Cd','Pb','NO2','Ni','Ag','As(total)','As(+3)','As(+5)',
     *'Fulvate','Humate','Se(total)','H2Se','Se(+4)','Se(+6)',
     *'U(total)','U(+4)','U(+6)'/
      DATA TBVAL/7,8,48,80,87,89,94,96,97,109,130,145,160,182,202,204,
     *212,249,261,262,284,285,298,299,300,301,316,317,359/
      DATA IMAGE/'F8.2','F9.2','F9.3','F9.2','F9.2','I9'/
      PRINT*, '
     *                    '
      PRINT*, '
     *                    '
```

```
      PRINT*, '
     *                    '
      PRINT*, '                              WELCOME TO WQ4FINPT!
     *                    '
      PRINT*, '                    NOTE:  This version does not accept si
     *gmas.               '
      PRINT*, '
     *                    '
      PRINT*, '            Hitting <Enter> always selects the indicated
     *default value.      '
      PRINT*, '                 If no default is indicated, it is zero.
     *                    '
      PRINT*, '
     *                    '
   95 FILNAM='WATEQ4F.DAT'
      ERCODE=0
      PRINT*, '
     *                    '
      PRINT*, '                                 OUTPUT FILE SELECTION
     *                    '
      PRINT*, '                Hit <Enter> to append data to file ',
     *FILNAM,'       '
      PRINT*, '                Otherwise, enter the name of a different
     *file:               '
  100 FORMAT(1X,A51,A20,A9)
      READ(5,120) TMPFIL
  120 FORMAT(A20)
      IF(TMPFIL(1:1) .EQ. ' ') GOTO 125
      CALL FILCHK(TMPFIL,ERCODE)
      IF (ERCODE .EQ. 1) GOTO 95
      FILNAM=TMPFIL
  125 Z='N'
      REC(0)='****'
      J3=1
      J4=100
      N=J3-1
      REC(1)=' '
C       [START OF **GIANT** LOOP]
  770 N=N+1
      IF (N.GT.J4) GOTO 5710
C       [RECORD 1]
  840 PRINT*, ' '
      PRINT*, 'Enter descriptor (72 chars maximum, <Enter> to QUIT):'
      READ(5,130) REC(1)(:72)
  130 FORMAT(A72)
      IF (REC(1)(1:1).EQ.' ') GOTO 5710
      PRINT*, 'Enter dataset number (5 character maximum): '
      READ(5,140) REC(1)(73:77)
  140 FORMAT(A5)
      PRINT*, 'Enter plot symbol (1 char only): '
      READ(5,150) REC(1)(79:79)
  150 FORMAT(A1)
      REC(1)(80:80)='5'
      PRINT*,' '
      PRINT*, 'RECORD 1:'
      WRITE(6,160) REC(0)
  160 FORMAT(1X,A79)
      WRITE(6,160) REC(1)
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 840
C       [RECORD 2]
 1050 DO 1 I=1,10
        CALL READV (VNAME(I),I,A(I))
    1 CONTINUE
```

```
      IF (A(1).GT.99999) THEN
        PRINT*,'CONDUCTIVITY TOO LARGE.  REENTER. . .'
        CALL READV(VNAME(1),1,A(1))
        GOTO 1050
      END IF
   10 L=LEN(REC(2))
      IF(L.LT.5) THEN
        REC(2)=' '//REC(2)
        GOTO 10
      END IF
 1150 IF (A(2).GT.999999) THEN
        PRINT*, 'TDS VALUE TOO LARGE.  REENTER. . .'
        CALL READV(VNAME(2),2,A(2))
        GOTO 1150
      END IF
      COND=A(1)
      ITDS=A(2)
      DOC=A(5)
      IA(1)=INT(A(3))
      WRITE(REC(2),170)(A(I), I=1,2),IA(1),(A(I), I=4,10)
  170 FORMAT(F5.0,F6.0,1X,I6,7F8.4)
C     REC(2)(19:19)=' '
      PRINT*,' '
      PRINT*, 'RECORDS 1 AND 2:'
      WRITE(6,160) REC(0)
      WRITE(6,160) REC(1)
      WRITE(6,160) REC(2)
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 1050
C       [RECORDS 3/4]
      REC(3)='TEMP-.-- PH---.-- EHM-.--- DOC--.-- DOX--.-- CORALK--'
      REC(4)=' '
 1820 DO 2 I=1,6
        J=I+10
        IF (I.EQ.4) THEN
          A(I)=DOC
        ELSE
          IF(I.EQ.6) THEN
            PRINT*,' '
            PRINT*, 'CORALK options:'
            PRINT*, '0.  Alkalinity input has not been corrected for'
            PRINT*, '    noncarbonate species (the default)'
            PRINT*, '1.  Alkalinity input has been corrected for noncarb
     *onate species'
            PRINT*, '2.  Alkalinity input is total carbon'
          END IF
          CALL READV (VNAME(J),J,A(I))
        END IF
    2 CONTINUE
      IA(1)=INT(A(6))
      EHM=A(3)
      DOX=A(5)
      WRITE(REC(4),180) (A(I), I=1,5),IA(1)
  180 FORMAT(2(F8.2,1X),F8.3,1X,2(F8.2,1X),I8)
      PRINT*,' '
      PRINT*, 'RECORDS 0 THROUGH 4:'
      WRITE(6,160) REC(0)
      WRITE(6,160) REC(1)
      WRITE(6,160) REC(2)
      WRITE(6,160) REC(3)
      WRITE(6,160) REC(4)
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 1820
```

```
C       [RECORDS 5/6]
      REC(5)='FLAG---DE.NS---- PRNT PUNCH EHOPT:-1--2--3--4--5--6--7--8-
     *-9'
 2130 REC(6)='MG/L    1.0         0     1        0  0  0  0  0  0  0  0
     * 0'
      DO 3 I=1,13
        J=I+16
        IF (I.EQ.4) THEN
          A(I)=1.0
        ELSE
          IF(I.EQ.1) THEN
            PRINT*, ' '
            PRINT*, 'Flag options:'
            PRINT*, '1.  mg/L  (the default)'
            PRINT*, '2.  ppm'
            PRINT*, '3.  meq/L'
            PRINT*, '4.  mmol/L'
            PRINT*, '5.  mol/kg'
          END IF
          IF(I.EQ.3) THEN
            PRINT*, ' '
            PRINT*, 'Print options:'
            PRINT*, '0.  Print minimum output (the default)'
            PRINT*, '1.  Print complete aqueous speciation and mineral s
     *olubility listing'
            PRINT*, '2.  Print minimum output plus weight and molar rati
     *os page'
            PRINT*, '3.  Print complete output (1 plus 2)'
            PRINT*, '4.  0 plus generate the thermodynamic data table'
            PRINT*, '5.  1 plus generate the thermodynamic data table'
            PRINT*, '6.  2 plus generate the thermodynamic data table'
            PRINT*, '7.  3 plus generate the thermodynamic data table'
          END IF
          IF(I.GE.5) THEN
            PRINT*,' '
            PRINT*, 'Eh options:'
            PRINT*,'-----------------------------------'
            PRINT*,' 0.  Use measured Eh (the default)'
            PRINT*,' 1.  Use Fe 2/3 Eh'
            PRINT*,' 2.  Use H2O/O2 Eh with Sato relation'
            PRINT*,' 3.  Use H2O/O2 Eh w/classical relation'
            PRINT*,' 4.  Use NH4/NO3 Eh'
            PRINT*,' 5.  Use S -2/SO4 Eh'
            PRINT*,' 6.  Use NO2/NO3 Eh'
            PRINT*,' 7.  Use S -2/S(s) Eh'
            PRINT*,' 8.  Use As 3/5 Eh'
            PRINT*,' 9.  Use As(s)/As +3 Eh'
            PRINT*,'10.  Use Se 4/6 Eh'
            PRINT*,'11.  Use Se(s)/Se +4 Eh'
            PRINT*,'12.  Use Se -2/Se(s) Eh'
            PRINT*,'13.  Use U 4/6 Eh'
            PRINT*,' '
            PRINT*,'NOTE:  Use these options with caution!  To use'
            PRINT*,'an option you must have input data for the'
            PRINT*,'redox specie or species referred to.'
            PRINT*,' '
            K=I-4
            WRITE(6,185)K,EHPHRA(K)
          END IF
          IF(I.GE.5) THEN
            CALL READEH (VNAME(J),J,A(I))
          ELSE
            CALL READV (VNAME(J),J,A(I))
          END IF
          IF(I.GE.5) EHOPT(I-4)=INT(A(I))
```

```
        END IF
    3 CONTINUE
  185 FORMAT(I2,'.  Enter number of Eh to use for ',A36)
      DO 11 I=3,13
        IA(I)=INT(A(I))
   11 CONTINUE
      WRITE(REC(6),190) CONZ(A(1)),A(2),(IA(I), I=3,13)
  190 FORMAT(A4,F11.6,2I6,6X,9I3)

C       [RECORDS 7/8]
      REC(7)='EMPOX--- ITDS-.-- COND-.-- SIGMDO-.----SIGMEH-.----SIGMPH-
     *.----'
      REC(8)='       0     0.0      0.0        0.0         0.0          0
     *.0   '
      WRITE(REC(8)(10:27),200)ITDS,COND
  200 FORMAT(2(F8.2,1X))
      PRINT*,' '
      PRINT*, 'RECORDS 0 THROUGH 8:'
      DO 30 I=0,8
        WRITE(6,160) REC(I)
   30 CONTINUE
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 2130

C       [RECORDS 9/10]
      REC(9)='CA-----.----MG-----.----NA-----.----K------.----CL------.--
     *--SO4----.----'
 2910 DO 4 I=1,6
        J=I+21
        CALL READV (VNAME(J),J,A(I))
    4 CONTINUE
      SO4=A(6)
      WRITE(REC(10),210) (A(I), I=1,6)
  210 FORMAT(6F12.4)
      PRINT*,' '
      PRINT*, 'RECORDS 0 THROUGH 10:'
      DO 40 I=0,10
        WRITE(6,160) REC(I)
   40 CONTINUE
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 2910

C       [RECORDS 11/12]
      REC(11)='HCO3---.----FE TOT-.----H2S AQ-.----CO3----.----SIO2TOT.-
     *---NH4----.----'
 3560 DO 5 I=1,6
        J=I+27
        CALL READV (VNAME(J),J,A(I))
    5 CONTINUE
      FET=A(2)
      H2S=A(3)
      NH4=A(6)
      WRITE(REC(12),210) (A(I), I=1,6)
      PRINT*,' '
      PRINT*, 'RECORDS 0 THROUGH 12:'
      DO 50 I=0,12
        WRITE(6,160) REC(I)
   50 CONTINUE
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 3560
C       [RECORDS 13/14]
      REC(13)='B TOT--.----PO4----.----AL-----.----F------.----NO3----.-
```

```
     *---'
 4280 DO 6 I=1,5
        J=I+33
        CALL READV (VNAME(J),J,A(I))
    6 CONTINUE
      NO3=A(5)
      WRITE(REC(14),210) (A(I), I=1,5)
      PRINT*,' '
      PRINT*, 'RECORDS 0 THROUGH 14:'
      DO 60 I=0,14
        WRITE(6,160) REC(I)
   60 CONTINUE
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 4280
C       [INPUT OF OPTIONAL CONCENTRATION DATA AND SIGMAS]
      REC(15)='$$$$ --- ++++++.+++++ --- ++++++.+++++ --- ++++++.+++++ -
     *-- ++++++.+++++'
 4960 DO 7 I=16, 30
        REC(I)=' '
    7 CONTINUE
      NVAL=0
      IREC=15
      DO 8 I=1, 29
        J=I+38
        CALL READV (VNAME(J),J,AX)
        IF (I.EQ.1) FE2=AX
        IF (I.EQ.2) FE3=AX
        IF (I.EQ.15) NO2=AX
        IF (I.EQ.18) AST=AX
        IF (I.EQ.19) AS3=AX
        IF (I.EQ.20) AS5=AX
        IF (I.EQ.23) SET=AX
        IF (I.EQ.25) SE4=AX
        IF (I.EQ.26) SE6=AX
        IF (I.EQ.28) U4=AX
        IF (I.EQ.29) U6=AX
        IF (AX.EQ.0.) GOTO 8
        NVAL=NVAL+1
        JJ=NVAL-4*INT(REAL(NVAL-1)/4.)
        XIN(JJ)=AX
        VAL(JJ)=TBVAL(I)
        IF (REAL(NVAL)/4. .NE. INT(REAL(NVAL)/4.)) GOTO 8
        IREC=IREC+1
        WRITE(REC(IREC),630) (VAL(K),XIN(K), K=1,JJ)
  630 FORMAT('CUN ',4(1X,I3,1X,F12.5))
    8 CONTINUE
      IF (REAL(NVAL)/4. .NE. INT(REAL(NVAL)/4.)) WRITE(REC(IREC+1),630)
     * (VAL(K),XIN(K), K=1,JJ)
      CALL EHCHEK(EHOPT,EHPHRA)
      PRINT*,' '
      PRINT*, 'FINAL DATA:'
      DO 70 I=0,30
        IF(REC(I).NE.' ') WRITE(6,160) REC(I)
   70 CONTINUE
      PRINT*,' '
      CALL DATAOK(ANSW)
      IF (ANSW.EQ.'N' .OR. ANSW.EQ.'n') GOTO 4960
      PRINT*,' '
      PRINT*, ' Store this data set on disk?'
      CALL YESNO(ANSW)
      IF (ANSW.NE.'N' .AND. ANSW.NE.'n') THEN
        PRINT*,'Data set now being appended to file ',FILNAM
        OPEN (UNIT=11,FILE=FILNAM)
  133   READ (11,120,END=135) ANSW
```

```
        GOTO 133
  135   BACKSPACE (UNIT=11)
        DO 80 I=0,30
          IF(REC(I).NE.' ') THEN
            CALL CHOP(REC(I),FMT,LREC)
            WRITE(11,FMT) REC(I)(1:LREC)
            END IF
   80   CONTINUE
  220   FORMAT(A4)
        WRITE(11,220) '    '
        CLOSE(UNIT=11)
      ELSE
        PRINT*,'Data set has been discarded'
        DO 90 I=0,30
          REC(I)=' '
   90   CONTINUE
        END IF
      GOTO 770
C       [END OF **GIANT** LOOP]
 5710 OPEN (UNIT=12,FILE='READNAME.BAT')
      WRITE(12,230) FILNAM
  230 FORMAT('SET FILNAM=',A20)
      WRITE(12,240)
  240 FORMAT('%PGMNAM% %FILNAM% %PRTOPT%')
      CLOSE(UNIT=12)
      PRINT*,'Exiting this program.  Your data file name is ',FILNAM
      STOP 'WQ4FINPT exited normally.'
      END
      SUBROUTINE DATAOK (ANSW)
C       [SUBROUTINE TO ASK IF DATA JUST CONSTRUCTED IS ACCEPTABLE]
      CHARACTER*1 ANSW
      PRINT*, 'Is this data OK (<Enter>=Yes)?'
      ENTRY YESNO (ANSW)
   10 READ(5,100) ANSW
  100 FORMAT(A1)
      IF(ANSW.EQ.' ') ANSW='Y'
      IF(ANSW.EQ.'Y' .OR. ANSW.EQ.'y' .OR. ANSW.EQ.'N' .OR. ANSW.EQ.'n')
     *  RETURN
      PRINT*, 'Please answer yes or no.'
      GOTO 10
      END
      SUBROUTINE READV(NAME,INDEX,VALUE)
      CHARACTER*20 NAME,LINE
      CHARACTER*4 CDEF(70)
      DIMENSION DEFAULT(70)
      DATA CDEF/2*'0.0 ','00  ',7*'0.0 ','25.0','7.0 ','9.9 ',2*'0.0 ',
     *'0   ','1   ','1.0 ','0   ','1   ','0   ',49*'0.0 '/
      DATA DEFAULT/10*0.0,25.0,7.0,9.9,3*0.0,2*1.0,52*0.0/
      WRITE(6,100)NAME,CDEF(INDEX)
      GOTO 10
      ENTRY READEH(NAME,INDEX,VALUE)
      WRITE(6,130)
   10 READ(5,110) LINE
      IF(LINE(1:1).EQ.' ') THEN
        VALUE=DEFAULT(INDEX)
      ELSE
        READ(LINE,120,ERR=20) VALUE
      END IF
      RETURN
   20 PRINT*,'Your last input was invalid.  Please try again.'
      GOTO 10
  100 FORMAT(' Enter ',A20,/,' Default=',A4)
  110 FORMAT(A20)
  120 FORMAT(F20.0)
  130 FORMAT(' Default=0')
```

```
      END
      SUBROUTINE CHOP(STRING,FMT,K)
      CHARACTER*80 STRING
      CHARACTER*5 FMT
      DO 1 I=80,1,-1
        IF(STRING(I:I).NE.' ') THEN
          K=I
          IF(K.GT.9)THEN
            WRITE(FMT,100)K
          ELSE
            WRITE(FMT,110)K
          END IF
          RETURN
        END IF
    1 CONTINUE
      RETURN
  100 FORMAT('(A',I2,')')
  110 FORMAT('(A',I1,')')
      END
      SUBROUTINE FILCHK(FILNAM,ERCODE)
C     [SUBROUTINE TO CHECK INPUT TO SEE IF IT IS A VALID DOS FILENAME]
      CHARACTER*20 FILNAM
      CHARACTER*17 REFSTR
      INTEGER ERCODE,PER
      DATA REFSTR/'!^&*_+=[]:;<>/\?"'/
      ERCODE=0
      NERR=0
      K=1
   10 IF (FILNAM(K:K).NE.' ' .AND. K.LE.20) THEN
        K=K+1
        GOTO 10
      END IF
      K=K-1
      DO 100 N=1, K
        IF (INDEX(REFSTR,FILNAM(N:N)).EQ.0) GOTO 100
        NERR=1
  100 CONTINUE
      IF (NERR .GT. 0) GOTO 200
      PER=INDEX(FILNAM,'.')
      IF (PER .GT. 9) GOTO 200
      IF (PER .EQ. 0 .AND. K .LT. 9) RETURN
      IF (K-PER .LE. 3) RETURN
  200 PRINT*,'The filename you entered is not a valid DOS file name.'
      ERCODE=1
      RETURN
      END
      SUBROUTINE EHCHEK(EHOPT,EHPHRA)
C     [SUBROUTINE TO CHECK FOR ERRONEOUS EHOPT SETTINGS]
      COMMON/IONS/EHM,DOX,SO4,FET,H2S,NH4,NO3,FE2,FE3,NO2,AST,AS3,AS5,
     *SET,SE4,SE6,UT,U4,U6
      CHARACTER*1 CHAR
      CHARACTER*36 EHPHRA(9)
      INTEGER EHOPT(9)
      REAL NH4,NO2,NO3
      IF (FET.GT.0. .AND. FE2.GT.0. .AND. FE3.LE.0.) FE3=FET-FE2
      IF (FET.GT.0. .AND. FE3.GT.0. .AND. FE2.LE.0.) FE2=FET-FE3
      IF (AST.GT.0. .AND. AS3.GT.0. .AND. AS5.LE.0.) AS5=AST-AS3
      IF (AST.GT.0. .AND. AS5.GT.0. .AND. AS3.LE.0.) AS3=AST-AS5
      IF (SET.GT.0. .AND. SE4.GT.0. .AND. SE6.LE.0.) SE6=SET-SE4
      IF (SET.GT.0. .AND. SE6.GT.0. .AND. SE4.LE.0.) SE4=SET-SE6
      IF (UT.GT.0. .AND. U4.GT.0. .AND. U6.LE.0.) U6=UT-U4
      IF (UT.GT.0. .AND. U6.GT.0. .AND. U4.LE.0.) U4=UT-U6
      IF (EHOPT(1).EQ.1) PRINT*,'**WARNING**  It is invalid to use Eh ca
     *lculated FROM ',EHPHRA(1)(1:23),' to calculate ',EHPHRA(1)
      IF (EHOPT(4).EQ.8) PRINT*,'**WARNING**  It is invalid to use Eh ca
```

```
     *lculated FROM ',EHPHRA(4)(1:23),' to calculate ',EHPHRA(4)
      IF (EHOPT(5).EQ.10) PRINT*,'**WARNING**  It is invalid to use Eh c
     *alculated FROM ',EHPHRA(5)(1:23),' to calculate ',EHPHRA(5)
      IF (EHOPT(8).EQ.5) PRINT*,'**WARNING**  It is invalid to use Eh ca
     *lculated FROM ',EHPHRA(8)(1:23),' to calculate ',EHPHRA(8)
      IF (EHOPT(9).EQ.13) PRINT*,'**WARNING**  It is invalid to use Eh c
     *alculated FROM ',EHPHRA(9)(1:22),' to calculate ',EHPHRA(9)
      DO 10 I=1,9
        IF ((EHOPT(I).EQ.2 .OR. EHOPT(I).EQ.3) .AND. DOX.LE.0.) PRINT*,
     *'**WARNING**  You must have D.O. input to use the Eh calculated fr
     *om D.O.'
   10 CONTINUE
      DO 20 I=1,9
        IF (EHOPT(I).EQ.4 .AND. (NH4.LE.0. .OR. NO3.LE.0.)) PRINT*,'**WA
     *RNING**  You must have NH4 and NO3 input to use the Eh calculated
     *from NH4 and NO3.'
   20 CONTINUE
      DO 30 I=1,9
        IF (EHOPT(I).EQ.5 .AND. (H2S.LE.0. .OR. SO4.LE.0.)) PRINT*,'**WA
     *RNING**  You must have H2S and SO4 input to use the Eh calculated
     *from H2S and SO4.'
   30 CONTINUE
      DO 40 I=1,9
        IF (EHOPT(I).EQ.6 .AND. (NO2.LE.0. .OR. NO3.LE.0.)) PRINT*,'**WA
     *RNING**  You must have NO2 and NO3 input to use the Eh calculated
     *from NO2 and NO3.'
   40 CONTINUE
      DO 50 I=1,9
        IF (EHOPT(I).EQ.1 .AND. (FE2.LE.0. .OR. FE3.LE.0.)) PRINT*,'**WA
     *RNING**  You must have FE2 and FE3 input to use the Eh calculated
     *from FE2 and FE3.'
   50 CONTINUE
      DO 60 I=1,9
        IF (EHOPT(I).EQ.8 .AND. (AS3.LE.0. .OR. AS5.LE.0.)) PRINT*,'**WA
     *RNING**  You must have AS3 and AS5 input to use the Eh calculated
     *from AS3 and AS5.'
   60 CONTINUE
      DO 70 I=1,9
        IF (EHOPT(I).EQ.10 .AND. (SE4.LE.0. .OR. SE6.LE.0.)) PRINT*,'**W
     *ARNING**  You must have SE4 and SE6 input to use the Eh calculated
     * from SE4 and SE6.'
   70 CONTINUE
      DO 80 I=1,9
        IF (EHOPT(I).EQ.7 .AND. H2S.LE.0.) PRINT*,'**WARNING**  You must
     * have H2S input to use the Eh calculated from S= and S(s).'
   80 CONTINUE
      DO 90 I=1,9
        IF (EHOPT(I).EQ.13 .AND. (U4.LE.0. .OR. U6.LE.0.)) PRINT*,'**WAR
     *NING**  You must have U4 and U6 input to use the Eh calculated fro
     *m U4 and U6.'
   90 CONTINUE
      DO 100 I=1,9
        IF (EHOPT(I).EQ.0 .AND. EHM.EQ.9.9) PRINT*,'**WARNING**  No inpu
     *t Eh was supplied.  Use of any EHOPT=0 will result in those calcul
     *ations being skipped.'
  100 CONTINUE
      PRINT*, ' '
      PRINT*, 'Eh inconsistency tests completed.'
      PRINT*, ' '
      PRINT*, 'Press <Enter> to continue . . . '
      READ(5,110)CHAR
  110 FORMAT(A1)
      RETURN
      END
```

Attachment F. Program Listing of WQ4F.BAT

```
Echo Off
If Exist Tables.out Erase Tables.out
If %1/==D/ GoTo Test_Input
If %1/==d/ GoTo Test_Input
If %1/==/ GoTo Test_Input
GoTo Copy
:Test_Input
If Not Exist Wateq4f.Dat GoTo Error1
:Test_Output
If Exist Wateq4f.Out GoTo Error4
:Run
Wateq4f
If Not Exist Wateq4f.Out GoTo Error2
If %2/==P/ GoTo Skip1
If %2/==p/ GoTo Skip1
:Quest1
Echo:
Echo
Echo    ╔═══════════════════════════════════════════════════════════════════╗
Echo    ║ This run of WATEQ4F is now complete.  You may either:             ║
Echo    ║     (1) Convert the output file into a directly printable form, or ║
Echo    ║     (2) Quit and examine the file as is.                          ║
Echo    ╚═══════════════════════════════════════════════════════════════════╝
Echo:
Rem  "Query" is a public domain utility that requests and processes keyboard
Rem     input.  Any utility that accomplishes the same thing (e.g. Norton
Rem     Utilities "Ask") may be substituted.  A copy of QUERY.COM is
Rem     included with the WATEQ4F software package.
Rem
Query Please specify either 1 or 2: @12
If ErrorLevel 2 GoTo Exit
If ErrorLevel 1 GoTo Skip1
:Skip1
Basica CCprint
Del Wateq4f.Out
Rename Wateq4f.Prn Wateq4f.Out
If %2/==P/ GoTo Skip2
If %2/==p/ GoTo Skip2
:Quest2
Echo:
Echo
Echo    ╔═══════════════════════════════════════════════════╗
Echo    ║  Conversion of the WATEQ4F.OUT file is now complete.
Echo    ║  Now you may either:                              ║
Echo    ║       (1) Send the file to your printer, or       ║
Echo    ║       (2) Quit and examine the file onscreen.     ║
Echo    ╚═══════════════════════════════════════════════════╝
Echo:
Query Please specify either 1 or 2: @12
If ErrorLevel 2 GoTo Exit
If ErrorLevel 1 GoTo Skip2
:Skip2
Echo:
Echo
Echo    ╔═══════════════════════════════╗
Echo    ║   Printing file WATEQ4F.OUT   . . .
Echo    ╚═══════════════════════════════╝
Echo:
Copy Wateq4f.Out Prn
GoTo Exit
Cls
:Copy
If Not Exist %1 GoTo Error5
If %1==WATEQ4F.DAT GoTo Run
If Exist Wateq4f.Dat GoTo Error3
:Go_Ahead
Copy %1 Wateq4f.Dat > nul
GoTo Test_Output
:Error1
Echo:
```

```
Echo
Echo ┌──────────────────────────────────────────────────────────────────┐
Echo │ There is no file named WATEQ4F.DAT in this directory.  You may either: │
:Jumpin
Echo │                                                                  │
Echo │      (1) Exit this program and restart it, specifying the name of an │
Echo │          existing input data file or copying it to WATEQ4F.DAT, or │
Echo │      (2) Proceed directly to program WQ4FINPT, and create        │
Echo │          WATEQ4F input data sets.                                │
Echo └──────────────────────────────────────────────────────────────────┘
Echo:
Query Please specify either 1 or 2: @12
If ErrorLevel 2 GoTo Create
If ErrorLevel 1 GoTo Exit
:Error2
Cls
Echo:
Echo ┌──────────────────────────────────────────────────────┐
Echo │   Output file WATEQ4F.OUT was not created.  Program terminated. │
Echo └──────────────────────────────────────────────────────┘
GoTo Exit
:Error3
Echo:
Echo ┌──────────────────────────────────────────────────────────────────┐
Echo │ File WATEQ4F.DAT already exists in the current directory.  You can either: │
Echo │       (1) Exit this program and examine the file to see if you want │
Echo │           to rename it or move it into another directory, or      │
Echo │       (2) Overwrite the present contents of file WATEQ4F.DAT     │
Echo │           with the file you have specified.                      │
Echo └──────────────────────────────────────────────────────────────────┘
Echo:
Query Please specify either 1 or 2: @12
If ErrorLevel 2 GoTo Go_Ahead
If ErrorLevel 1 GoTo Exit
:Error4
Echo:
Echo ┌──────────────────────────────────────────────────────────────────┐
Echo │ File WATEQ4F.OUT already exists in the current directory.  You can either: │
Echo │       (1) Exit this program and examine the file to see if you want │
Echo │           to rename it or move it into another directory, or      │
Echo │       (2) Go ahead and execute WATEQ4F, which will overwrite     │
Echo │           the present contents of WATEQ4F.OUT with new data.     │
Echo └──────────────────────────────────────────────────────────────────┘
Echo:
Query Please specify either 1 or 2: @12
If ErrorLevel 2 GoTo Run
If ErrorLevel 1 GoTo Exit
:Error5
Echo:
Echo ┌──────────────────────────────────────────────────────────────────┐
Echo │ The data file whose name you specified does not exist.  You may either: │
GoTo Jumpin
:Create
Echo:
Echo ┌──────────────────────────────────────────────────┐
Echo │   Starting Program WQ4FINPT   .  .  .            │
Echo └──────────────────────────────────────────────────┘
Set Pgmnam=Wq4f
Set Prtopt=%2
Basica Wq4finpt
Readname
:Exit
Set Pgmnam=
Set Prtopt=
Set Filnam=
If Exist Readname.Bat Erase Readname.Bat
```