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SOLMNEQ: SOLUTION-MINERAL EQUILIBRIUM COMPUTATIONS

Yousif K. Kharaka, et al

California University

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SOLMNEQ: Solution-Mineral Equilibrium Computations

by

Yousif K. Kharaka and Ivan Barnes

U.S. Geological Survey
Menlo Park, California
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SOLMNEQ is a computer program written in PL/I for the IBM 360 computers. SOLMNEQ computes the equilibrium distribution of 162 inorganic aqueous species generally present in natural waters over the temperature range of 0° to 350°C from the reported chemical analyses, temperature, pH, and Eh (optional). Interpolated dissociation constants of the aqueous complexes and the computed activity coefficients are also used in these computations. States of reactions of the aqueous solutions with respect to 158 solid phases (minerals) are computed from the distribution of aqueous species and an internally consistent set of thermodynamic data. Ionic proportions and subsurface temperature estimates are computed.

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SOLMNEQ: Solution-Mineral Equilibrium Computations[1]

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ABSTRACT

SOLMNEQ is a computer program written in PL/I for the IBM 360 computers. SOLMNEQ computes the equilibrium distribution of 162 inorganic aqueous species generally present in natural waters over the temperature range of 0° to 350°C from the reported chemical analyses, temperature, pH, and Eh (optional). Interpolated dissociation constants of the aqueous complexes and the computed activity coefficients are also used in these computations. States of reactions of the aqueous solutions with respect to 158 solid phases (minerals) are computed from the distribution of aqueous species and an internally consistent set of thermodynamic data. Ionic proportions and subsurface temperature estimates are computed.

[1]This research was sponsored by the U.S. Geological Survey, Department of the Interior, under U.S.G.S. Grant No. 14-08-0001G-45. F.A.F. Berry, principal investigator.

[2]Headquarters at U.S. Geological Survey, Menlo Park, California.

INTRODUCTION

Analyses of states of chemical reaction have been made using equilibrium models (Helgeson and others, 1970; Truesdell, 1973) and models that include departures from equilibrium (Paces, 1968, 1971; Barnes and Clarke, 1969; A. H. Truesdell and B. F. Jones, unpub. data, 1972). The present program, incorporating elements from the earlier cited work, has been expanded to include all inorganic species of major and minor elements generally present in natural waters for which thermodynamic data are available.

SOLMNEQ computes the equilibrium distribution of 162 chemical species in aqueous solution over the temperature range of 0° to 350°C from the properties of the solution and an internally consistent set of thermodynamic data. States of reaction of the aqueous solutions with respect to 158 solid phases (minerals) are also computed.

Uncertainties involved in computations carried out in SOLMNEQ and similar computer programs should be recognized at the outset. Major uncertainties may be imposed by the amount and quality of the thermodynamic and other data available in published literature for the computations of equilibrium constants (K). The uncertainties in the thermodynamic functions depend on the rate and reversibility of the reactions involved. The more rapidly, completely, and reversibly a phase reacts, the less error is to be expected in its thermodynamic functions.

Usefulness of the data analysis is limited also by the completeness and reliability of the reported chemical analysis of the water. Many chemical analyses are limited to the major cations and anions. Uncertainties are imposed by the method of sample collection and treatment and method of analysis (Chave, 1960; Rainwater and Thatcher, 1960; White, 1965; Barnes and others, 1969). An important limitation of many chemical analyses is the extrapolation of the determined pH to the in situ pH of the sample, especially in the case of subsurface water samples. The pH of the sample may change from variations in partial pressures of the gases present (CO_2, H_2S, and others), from precipitation of solid phases (for example, $CaCO_3$, $SrCO_3$), and from reactions of aqueous species produced by changes in the temperature and pressure of the sample. An additional limitation of the data analysis applies to studies of aluminosilicate minerals and minerals containing trace elements. Results of analyses for aluminum in solution in the literature are suspect because of the lack of a sufficiently sensitive analytical method. Trace element analyses are particularly subject to errors from insensitive procedures, sample contamination, and losses during storage and manipulation.

Assumptions used in the calculation of the activity coefficients of the aqueous species and in limiting minerals to end member compositions introduce errors, but generally these errors are minor compared to those mentioned above.

METHOD OF COMPUTATION

SOLMNEQ treats mostly mass action reactions; however, there is an option to calculate the molalities (m) of Fe^{+3}, Cu^{++}, Hg^{++}, and Mn^{++} using electron transfer reactions involving the measured Eh of the aqueous sample. The formal reactions used for the minerals (table 1) are for the complete reactions; no incongruent reactions are used. For albite, for example, the reaction is:

$$NaAlSi_3O_8 + 4H^+ + 4H_2O = Na^+ + Al^{+3} + 3H_4SiO_4 \ . \qquad (1)$$

Activities

The activities (a) of solid phases are taken as unity at all temperatures. The activity of H_2O is computed from the equation (Garrels and Christ, 1965, p. 65)

$$a_{H_2O} = 1 - \underline{0.017} \sum_i m_i \qquad (2)$$

the summation covering the molalities (m_i) of all the species in solution.

The activities of the aqueous species are computed from:

$$a_i = m_i \gamma_i \qquad (3)$$

where γ_i is the activity coefficient of species i. The standard state adopted for the aqueous species is a hypothetical 1 molal solution at 1 atmosphere and at any temperature.

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated.

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA[1]
	A - AQUEOUS COMPLEXES	
1. HCO3-1	$HCO_3^- \rightleftharpoons CO_3^{--} + H^+$	(3)
2. KH2O	$H_2O \rightleftharpoons OH^- + H^+$	Fisher and Barnes (1972)
3. H4SIO4	$H_4SiO_4 \rightleftharpoons H_3SiO_4^- + H^+$	Cobble (1964)
4. CU+2	$Cu^{++} + Fe^{++} \rightleftharpoons Cu^+ + Fe^{+3}$	K (1)
5. FE+3	$Fe^{+3} + \frac{1}{2} H_2O + \frac{1}{8} HS^- \rightleftharpoons Fe^{++} + \frac{1}{8} SO_4^{--} + \frac{9}{8} H^+$	K (1)
6. HG+2	$2 Hg^{++} + 2 Fe^{++} \rightleftharpoons Hg_2^{++} + 2Fe^{+3}$	K (1)
7. MN+3	$Mn^{+3} + Fe^{++} \rightleftharpoons Mn^{++} + Fe^{+3}$	K (1)
8. AS(OH)4-	$As(OH)_4^- \rightleftharpoons As(OH)_3 + OH^-$	D (1)
9. Blank		
10. H2S AQ	$H_2S \rightleftharpoons HS^- + H^+$	(1)
11. ALF+2	$AlF^{+2} \rightleftharpoons Al^{+3} + F^-$	D (3)
12. ALF2+1	$AlF_2^+ \rightleftharpoons Al^{+3} + 2F^-$	D (3)
13. ALF3	$AlF_3 \rightleftharpoons Al^{+3} + 3F^-$	D (3)
14. ALF4-	$AlF_4^- \rightleftharpoons Al^{+3} + 4F^-$	D (3)
15. AL(OH)+2	$Al(OH)^{++} \rightleftharpoons Al^{+3} + OH^-$	(1)
16. AL(OH)2+	$Al(OH)_2^+ \rightleftharpoons Al^{+3} + 2OH^-$	(25) Hem and Roberson (1967)
17. AL(OH)4-	$Al(OH)_4^- \rightleftharpoons Al^{+3} + 4OH^-$	Helgeson (1971c)
18. AL(SO4)+	$Al(SO_4)^+ \rightleftharpoons Al^{+3} + SO_4^{--}$	D (3)
19. ALSO4)2-	$Al(SO_4)_2^- \rightleftharpoons Al^{+3} + 2SO_4^{--}$	D (3)
20. AGCL	$AgCl \rightleftharpoons Ag^+ + Cl^-$	(1)
21. AGCL2-	$AgCl_2^- \rightleftharpoons Ag^+ + 2Cl^-$	(1)
22. AGCL3-2	$AgCl_3^{--} \rightleftharpoons Ag^+ + 3Cl^-$	(1)
23. AGCL4-3	$AgCl_4^{-3} \rightleftharpoons Ag^+ + 4Cl^-$	(1)
24. AG(SO4)-	$Ag(SO_4)^- \rightleftharpoons Ag^+ + SO_4^{--}$	D (3)
25. AGSO42-3	$Ag(SO_4)_2^{-3} \rightleftharpoons Ag^+ + 2SO_4^{--}$	(0)
26. BACO3AQ	$BaCO_3 \rightleftharpoons Ba^{++} + CO_3^{--}$	Kharaka and Merino (unpub. data, 1971)[2]
27. BAHCO3)+	$Ba(HCO_3)^+ \rightleftharpoons Ba^{++} + HCO_3^-$	Kharaka and Merino (unpub. data, 1971)[2]
28. BA(OH)+1	$Ba(OH)^+ \rightleftharpoons Ba^{++} + OH^-$	D (3)
29. BASO4 AQ	$BaSO_4 \rightleftharpoons Ba^{++} + SO_4^{--}$	Kharaka and Merino (unpub. data, 1971)[2]
30. CACO3 AQ	$CaCO_3 \rightleftharpoons Ca^{++} + CO_3^{--}$	(1)
31. CAHCO3)+	$CaHCO_3^+ \rightleftharpoons Ca^{++} + HCO_3^-$	D (Lafon, 1969)
32. CA(OH)+1	$Ca(OH)^+ \rightleftharpoons Ca^{++} + OH^-$	PATHI, Helgeson and others (1970)
33. CAPO4-	$CaPO_4^- \rightleftharpoons Ca^{++} + PO_4^{-3}$	Chughtai and others (1968)
34. CAHPO4	$CaHPO_4 \rightleftharpoons Ca^{++} + HPO_4^{--}$	Chughtai and others (1968)
35. CAH2PO4+	$CaH_2PO_4^+ \rightleftharpoons Ca^{++} + H_2PO_4^-$	Chughtai and others (1968)

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

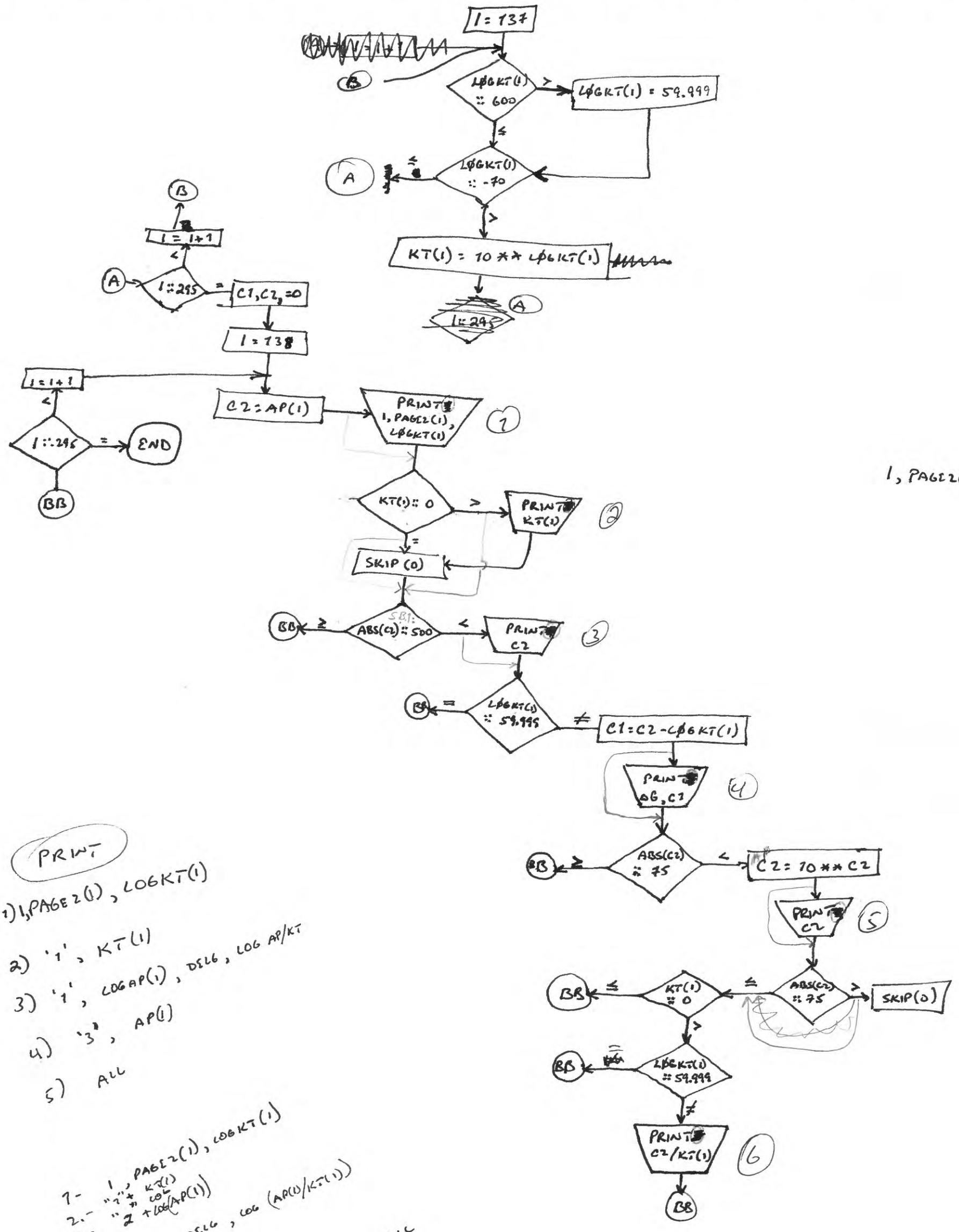
COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
36. CASO4 AQ	$CaSO_4 \rightleftharpoons Ca^{++} + SO_4^{--}$	(1)
37. CUCL	$CuCl \rightleftharpoons Cu^{+} + Cl^{-}$	(0)
38. CUCL2-	$CuCl_2^{-} \rightleftharpoons Cu^{+} + 2Cl^{-}$	(1)
39. CUCL3-2	$CuCl_3^{--} \rightleftharpoons Cu^{+} + 3Cl^{-}$	(1)
40. CUCL+1	$CuCl^{+} \rightleftharpoons Cu^{++} + Cl^{-}$	(1)
41. CUCL2	$CuCl_2 \rightleftharpoons Cu^{++} + 2Cl^{-}$	(1)
42. CUCL3-1	$CuCl_3^{-} \rightleftharpoons Cu^{++} + 3Cl^{-}$	(1)
43. CUCL4-2	$CuCl_4^{--} \rightleftharpoons Cu^{++} + 4Cl^{-}$	(1)
44. CU(OH)+1	$Cu(OH)^{+} \rightleftharpoons Cu^{++} + OH^{-}$	(25) Sillén and Martell (1964)
45. CUSO4AQ	$CuSO_4 \rightleftharpoons Cu^{++} + SO_4^{--}$	D (3)
46. FECL+1	$FeCl^{+} \rightleftharpoons Fe^{++} + Cl^{-}$	(0)
47. FECL2	$FeCl_2 \rightleftharpoons Fe^{++} + 2Cl^{-}$	(0)
48. FECL3-1	$FeCl_3^{-} \rightleftharpoons Fe^{++} + 3Cl^{-}$	(0)
49. FECL4-2	$FeCl_4^{--} \rightleftharpoons Fe^{++} + 4Cl^{-}$	(0)
50. FE(OH)+1	$Fe(OH)^{+} \rightleftharpoons Fe^{++} + OH^{-}$	D (1)
51. FE(OH)2	$Fe(OH)_2 \rightleftharpoons Fe^{++} + 2OH^{-}$	(25) Langmuir (1969)
52. FEOOH-1	$FeOOH^{-} + 3H^{+} \rightleftharpoons Fe^{++} + 2H_2O$	(25) (4)
53. FESO4	$FeSO_4 \rightleftharpoons Fe^{++} + SO_4^{--}$	D (3)
54. FECL+2	$FeCl^{++} \rightleftharpoons Fe^{+3} + Cl^{-}$	(1)
55. FECL2+1	$FeCl_2^{+} \rightleftharpoons Fe^{+3} + 2Cl^{-}$	(1)
56. FECL3	$FeCl_3 \rightleftharpoons Fe^{+3} + 3Cl^{-}$	(1)
57. FECL4-1	$FeCl_4^{-} \rightleftharpoons Fe^{+3} + 4Cl^{-}$	(1)
58. FESO4+1	$FeSO_4^{+} \rightleftharpoons Fe^{+3} + SO_4^{--}$	D (3)
59. FESO4)2-	$Fe(SO_4)_2^{-} \rightleftharpoons Fe^{+3} + 2SO_4^{--}$	(25) (4)
60. FE(OH)+2	$Fe(OH)^{++} \rightleftharpoons Fe^{+3} + OH^{-}$	(1)
61. FE(OH)2+	$Fe(OH)_2^{+} \rightleftharpoons Fe^{+3} + 2OH^{-}$	(25) (4)
62. FE(OH)3	$Fe(OH)_3 \rightleftharpoons Fe^{+3} + 3OH^{-}$	(25) Langmuir (1969)
63. FE(OH)4-	$Fe(OH)_4^{-} \rightleftharpoons Fe^{+3} + 4OH^{-}$	(25) Langmuir (1969)
64. H4(BO4)-	$H_4(BO_4)^{-} \rightleftharpoons H_3BO_3 + OH^{-}$	Mesmer and others (1972)
65. Blank		
66. H3SIO4)-	$H_3SiO_4^{-} \rightleftharpoons H_2SiO_4^{--} + H^{+}$	(3)
67. HAS(OH)4	$HAs(OH)_4 \rightleftharpoons As(OH)_4^{-} + H^{+}$	D (1)
68. HASOH8-2	$HAs(OH)_8^{--} \rightleftharpoons As(OH)_8^{-3} + H^{+}$	D (1)
69. H2ASOH8-	$H_2As(OH)_8^{-} \rightleftharpoons As(OH)_8^{-3} + 2H^{+}$	D (1)
70. H3AS(OH8	$H_3As(OH)_8 \rightleftharpoons As(OH)_8^{-3} + 3H^{+}$	D (1)

Table 1.--List of the aqueous complexes and minerals used in COLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
71. HF	$HF \rightleftharpoons H^+ + F^-$	(3)
72. H2CO3	$H_2CO_3 \rightleftharpoons HCO_3^- + H^+$	(3)
73. HPO4-2	$HPO_4^{--} \rightleftharpoons PO_4^{-3} + H^+$	(3)
74. H2PO4-1	$H_2PO_4^- \rightleftharpoons HPO_4^{--} + H^+$	(3)
75. HS-1	$HS^- \rightleftharpoons H^+ + S^{--}$	Ellis and Giggenbach (1971)
76. HSO4-1	$HSO_4^- \rightleftharpoons H^+ + SO_4^{--}$	(3)
77. HNO_3	$HNO_3 \rightleftharpoons NO_3^- + H^+$	(3)
78. HGCL+1	$HgCl^+ \rightleftharpoons Hg^{++} + Cl^-$	D (1)
79. HGCL2	$HgCl_2 \rightleftharpoons Hg^{++} + 2Cl^-$	D (1)
80. HGCL3-1	$HgCL_3^- \rightleftharpoons Hg^{++} + 3Cl^-$	D (1)
81. HGCL4-2	$HgCl_4^{--} \rightleftharpoons Hg^{++} + 4Cl^-$	D (1)
82. HGSO4	$HgSO_4 \rightleftharpoons Hg^{++} + SO_4^{--}$	(25) (4)
83. HGSH2S)2	$HgS(H_2S)_2 + H^+ \rightleftharpoons Hg^{++} + 2H_2S + HS^-$	D (Barnes and others, 1967)
84. HG(HS)3-	$Hg(HS)_3^- \rightleftharpoons Hg^{++} + 3HS^-$	(25) (Barnes snd others, 1967)
85. HGSHS2-2	$HgS(HS)_2^{--} + H^+ \rightleftharpoons Hg^{++} + 3HS^-$	(25) (Barnes and others, 1967)
86. KCL	$KCl \rightleftharpoons K^+ + Cl^-$	Truesdell and Jones (unpub. data, 1972)
87. HGS2-2	$HgS_2^{--} + 2H^+ \rightleftharpoons Hg^{++} + 2HS^-$	(25) Barnes and others, 1967)
88. KHSO4	$KHSO_4 \rightleftharpoons K^+ + HSO_4^-$	(0)
89. KSO4-1	$KSO_4^- \rightleftharpoons K^+ + SO_4^{--}$	Truesdell and Jones (unpub. data, 1972)
90. KHPO4-1	$KHPO_4^- \rightleftharpoons K^+ + HPO_4^{--}$	(0)
91. LI(OH)	$Li(OH) \rightleftharpoons Li^+ + OH^-$	Sillén and Martell (1964)
92. LI(SO4)-	$Li(SO_4)^- \rightleftharpoons Li^+ + SO_4^{--}$	(25) Sillén and Martell (1964)
93. MGCO3AQ	$MgCO_3 \rightleftharpoons Mg^{++} + CO_3^{--}$	D (Lafon, 1969)
94. MGHCO3)+	$Mg(HCO_3)^+ \rightleftharpoons Mg^{++} + HCO_3^-$	D (Lafon, 1969)
95. MGF 1	$MgF^+ \rightleftharpoons Mg^{++} + F^-$	D (3)
96. MG(OH)+1	$Mg(OH)^+ \rightleftharpoons Mg^{++} + OH^-$	(1)
97. MGSO4AQ	$MgSO_4 \rightleftharpoons Mg^{++} + SO_4^{--}$	(1)
98. MG(PO4)-	$Mg(PO_4)^- \rightleftharpoons Mg^{++} + PO_4^{-3}$	Childs (1970); Chughtai and others (1968)
99. MGHPO4	$MgHPO_4 \rightleftharpoons Mg^{++} + HPO_4^{--}$	Childs (1970); Chughtai and others (1968)
100. MGH2PO4+	$Mg(H_2PO_4)^+ \rightleftharpoons Mg^{++} + H_2PO_4^-$	Childs (1970); Chughtai and others (1968)
101. MNCL+1	$MnCl^+ \rightleftharpoons Mn^{++} + Cl^-$	(0)
102. MNCL2	$MnCl_2 \rightleftharpoons Mn^{++} + 2Cl^-$	(25) (4)
103. MNCL3-1	$MnCl_3^- \rightleftharpoons Mn^{++} + 3Cl^-$	(25) (4)
104. MNCL4-2	$MnCl_4^{--} \rightleftharpoons Mn^{++} + 4Cl^-$	(0)
105. MNHCO3+1	$MnHCO_3^+ \rightleftharpoons Mn^{++} + HCO_3^-$	(0)

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
106. MNSO4AQ	$MnSO_4 \rightleftharpoons Mn^{++} + SO_4^{--}$	D (1)
107. MNCL+2	$MnCl^{++} \rightleftharpoons Mn^{+3} + Cl^-$	(0)
108 MNCL2+1	$MnCl_2^+ \rightleftharpoons Mn^{+3} + 2Cl^-$	(0)
109. MNCL3	$MnCl_3 \rightleftharpoons Mn^{+3} + 3Cl^-$	(0)
110. NACL	$NaCl \rightleftharpoons Na^+ + Cl^-$	Truesdell and Jones (unpub. data, 1972)
111. NACO3-1	$NaCO_3^- \rightleftharpoons Na^+ + CO_3^{--}$	D (Lafon, 1969)
112. NAHCO3	$NaHCO_3 \rightleftharpoons Na^+ + HCO_3^-$	(25) Lafon (1969)
113. NA2CO3AQ	$Na_2CO_3 \rightleftharpoons 2Na^+ + CO_3^{--}$	(25) Garrels and Christ (1965)
114. NA2SO4AQ	$Na_2SO_4 \rightleftharpoons 2Na^+ + SO_4^{--}$	(0)
115. NASO4-1	$NaSO_4^- \rightleftharpoons Na^+ + SO_4^{--}$	D(Lafon, 1969)
116. NAHPO4-1	$NaHPO_4^- \rightleftharpoons Na^+ + HPO_4^{--}$	(0)
117. Blank		
118. NH4OH	$NH_4OH \rightleftharpoons NH_4^+ + OH^-$	Wright and others (1961)
119. NH4PO4-2	$NH_4(PO_4)^{--} \rightleftharpoons NH_4^+ + PO_4^{-3}$	(0)
120. NH4SO4)-	$NH_4(SO_4)^- \rightleftharpoons NH_4^+ + SO_4^{--}$	(0)
121. PBCL+1	$PbCl^+ \rightleftharpoons Pb^{++} + Cl^-$	D (1)
122. PBCL2	$PbCl_2 \rightleftharpoons Pb^{++} + 2Cl^-$	D (1)
123. PBCL3-1	$PbCl_3^- \rightleftharpoons Pb^{++} + 3Cl^-$	D (1)
124. PBCL4-2	$PbCl_4^{--} \rightleftharpoons Pb^{++} + 4Cl^-$	D (1)
125. PBSO4 AQ	$PbSO_4 \rightleftharpoons Pb^{++} + SO_4^{--}$	(0)
126. PBSO42-2	$Pb(SO_4)_2^{--} \rightleftharpoons Pb^{++} + 2SO_4^{--}$	(0)
127. SR(OH)-1	$Sr(OH)^- \rightleftharpoons Sr^{++} + OH^-$	D (3)
128. SRCO3 AQ	$SrCO_3 \rightleftharpoons Sr^{++} + CO_3^{--}$	Kharaka and Merino (unpub. data, 1971)[2]
129. SRHCO3)+	$Sr(HCO_3)^+ \rightleftharpoons Sr^{++} + HCO_3^-$	Kharaka and Merino (unpub. data, 1971)[2]
130. SRSO4 AQ	$SrSO_4 \rightleftharpoons Sr^{++} + SO_4^{--}$	Kharaka and Merino (unpub. data, 1971)[2]
131. ZNCL+1	$ZnCl^+ \rightleftharpoons Zn^{++} + Cl^-$	(1)
132. ZNCL2	$ZnCl_2 \rightleftharpoons Zn^{++} + 2Cl^-$	(1)
133. ZNCL3-1	$ZnCl_3^- \rightleftharpoons Zn^{++} + 3Cl^-$	(1)
134. ZNCL4-2	$ZnCl_4^{--} \rightleftharpoons Zn^{++} + 4Cl^-$	(1)
135. ZNSO4 AQ	$ZnSO_4 \rightleftharpoons Zn^{++} + SO_4^{--}$	(1)
136. ASOH)8-3	$As(OH)_8^{-3} + 2Fe^{++} \rightleftharpoons As(OH)_4^- + 2Fe^{+3} + 4OH^-$	D (1)
137. Blank		
	B - SOLID PHASES[4]	
138. ACMITE	$NaFe(SiO_3)_2 + 4H^+ + 2H_2O \rightleftharpoons Na^+ + Fe^{+3} + 2H_4SiO_4$	(0)
139. AG	$Ag_{(C)} + Fe^{+3} \rightleftharpoons Ag^+ + Fe^{++}$	K(1)
140. AG2S A	$Ag_2S + H^+ \rightleftharpoons 2Ag^+ + HS^-$	K(1)
141. AGCL	$AgCl \rightleftharpoons Ag^+ + Cl^-$	K(1)
142. ADULARIA	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftharpoons K^+ + Al^{+3} + 3H_4SiO_4$	K(1)



I, PAGE2(I), LOGKT(I)

PRINT

1) I, PAGE2(I), LOGKT(I)

2) '1', KT(I)

3) '1', LOGAP(I), DSLG, LOG AP/KT

4) '3', AP(I)

5) ALL

1 - I, PAGE2(I), LOGKT(I)

2 - "1" * KT(I)

3 - "2" + LOG(AP(I))

4 - "3" + DSLG, LOG (AP(I)/KT(I))

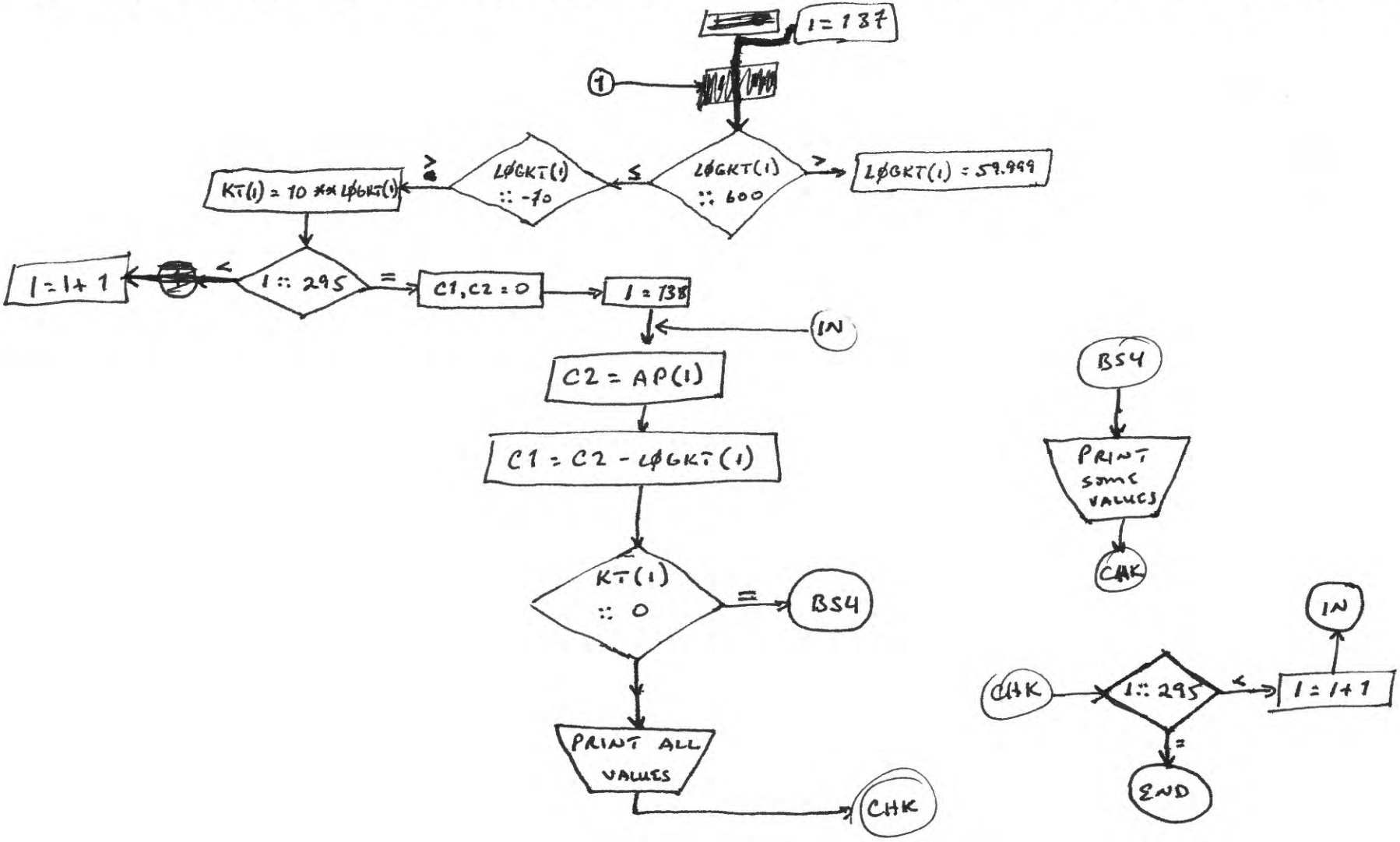
5 - "4" + AP(I)

6 - 5 + AP(I)/KT(I) — ALL

547.1

572.1

584.1


I = 137
1
LOGKT(I) :: 600
>
LOGKT(I) = 59.999
≤
LOGKT(I) :: -10
≥
KT(I) = 10 ** LOGKT(I)
I = I + 1
<
I :: 295
=
C1, C2 = 0
I = 138
IN
C2 = AP(I)
C1 = C2 - LOGKT(I)
KT(I) :: 0
=
BS4
PRINT ALL VALUES
CHK
BS4
PRINT SOME VALUES
CHK
IN
CHK
I :: 295
<
I = I + 1
=
END

141 - 197

2 ITER STANDARD

74

197

387

564

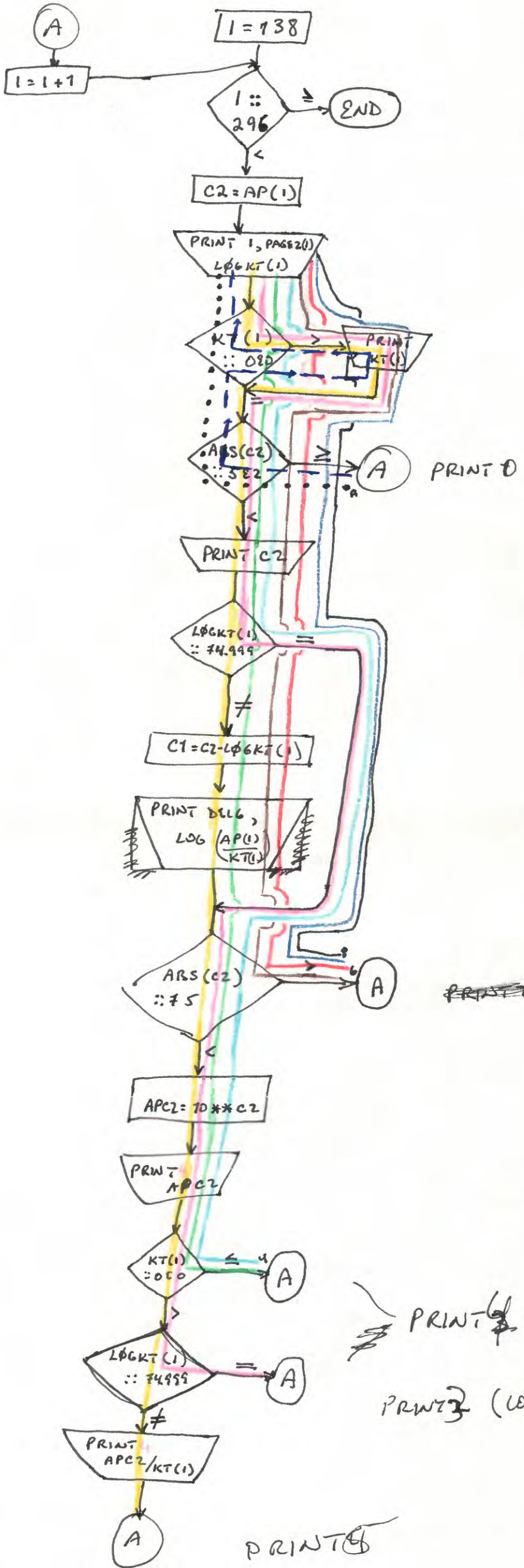

A
I = 138
I = I+1
I :: 296
<
>
END
C2 = AP(1)
PRINT I, PAGE2(I)
LOGKT(I)
KT(I) :: 0&0
<
=
>
PRINT KT(I)
ABS(C2) :: 582
<
=
>
A
PRINT 0
PRINT C2
LOGKT(I) :: 74.999
=
≠
C1 = C2-LOGKT(I)
PRINT DELL, LOG (AP(1)/KT(I))
ABS(C2) :: 75
<
=
>
A
APC2 = 10**C2
PRNT APC2
KT(I) :: 000
<
=
>
A
LOGKT(I) :: 74999
<
=
>
A
PRINT APC2/KT(I)
A
2 LOG ≠
PRINT 7
1 LOG =
PRINT (LOGKT(I) ≠ 7.499587)
PRINT (LOGKT(I) = 7.499587)
PRINT

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
143. AKERMANI	$Ca_2MgSi_2O_7 + 6H^+ + H_2O \rightleftharpoons 2Ca^{++} + Mg^{++} + 2H_4SiO_4$	K (2)
144. ALBITE L	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftharpoons Na^+ + Al^{+3} + 3H_4SiO_4$	K(1)
145. ALBITE H	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftharpoons Na^+ + Al^{+3} + 3H_4SiO_4$	K(1)
146. ALUNITE	$KAl_3(SO_4)_2(OH)_6 \rightleftharpoons K^+ + 3Al^{+3} + 2SO_4^{--} + 6(OH)^-$	K (Hemley and others, 1969)
147. ANALCIME	$NaAlSi_2O_6 \cdot H_2O + 4H^+ + H_2O \rightleftharpoons Na^+ + Al^{+3} + 2H_4SiO_4$	K (1)
148. ANDALUSI	$Al_2SiO_5 + 6H^+ \rightleftharpoons 2Al^{+3} + H_4SiO_4 + H_2O$	K(1)
149. ANHYDRIT	$CaSO_4 \rightleftharpoons Ca^{++} + SO_4^{--}$	K(1)
150. ANNITE	$KFe_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftharpoons K^+ + 3Fe^{++} + Al^{+3} + 3H_4SiO_4$	K (Dick Beane, oral commun., 1972)
151. APATCHLR	$Ca_5(PO_4)_3Cl \rightleftharpoons 5Ca^{++} + 3PO_4^{-3} + Cl^-$	Truesdell & Jones (unpub. data, 1972)
152. APATFLUR	$Ca_5(PO_4)_3F \rightleftharpoons 5Ca^{++} + 3PO_4^{-3} + F^-$	K(3)
153. APATHYDX	$Ca_5(PO_4)_3OH \rightleftharpoons 5Ca^{++} + 3PO_4^{-3} + OH^-$	K(2)
154. ARAGONIT	$CaCO_3 \rightleftharpoons Ca^{++} + CO_3^{--}$	K(1)
155. BARITE	$BaSO_4 \rightleftharpoons Ba^{++} + SO_4^{--}$	K(2)
156. BIOTITE		
157. BOEHMITE	$AlOOH + 3H^+ \rightleftharpoons Al^{+3} + 2H_2O$	K(1)
158. BORNITE	$Cu_5FeS_4 + 4H^+ \rightleftharpoons 5Cu^+ + Fe^{+3} + 4HS^-$	K(1)
159. BRUCITE	$Mg(OH)_2 \rightleftharpoons Mg^{++} + 2OH^-$	K(1)
160. CALCITE	$CaCO_3 \rightleftharpoons Ca^{++} + CO_3^{--}$	K(1)
161. CACL2	$CaCl_2 \rightleftharpoons Ca^{++} + 2Cl^-$	K(1)
162. CAOLIME	$CaO + 2H^+ \rightleftharpoons Ca^{++} + H_2O$	K(1)
163. Ca(OH)2	$Ca(OH)_2 \rightleftharpoons Ca^{++} + 2OH^-$	K(1)
164. CAS	$CaS + H^+ \rightleftharpoons Ca^{++} + HS^-$	K(1)
165. CELESTIT	$SrSO_4 \rightleftharpoons Sr^{++} + SO_4^{--}$	K(1)
166. CHALCEDN	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	Fournier (1973)
167. CHLOR MG	$Mg_5Al_2Si_3O_{10}(OH)_8 + 16H^+ \rightleftharpoons 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4 + 6H_2O$	K (Zen, 1972)
168. CRYSOCOL	$CuSiO_3 \cdot 2H_2O + 2H^+ \rightleftharpoons Cu^{++} + H_4SiO_4 + H_2O$	(0)
169. CRYSOTIL	$Mg_3Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 3Mg^{++} + 2H_4SiO_4 + H_2O$	K(1)
170. CINNABAR	$HgS + H^+ \rightleftharpoons Hg^{++} + HS^-$	K(1)
171. CINABMET	$HgS + H^+ \rightleftharpoons Hg^{++} + HS^-$	K(1)
172. CLINENST	$MgSiO_3 + 2H^+ + H_2O \rightleftharpoons Mg^{++} + H_4SiO_4$	K(1)
173. CLINPTIL	$Na_2Al_2Si_7O_{18} \cdot 6H_2O + 8H^+ + 4H_2O \rightleftharpoons 2Na^+ + 2Al^{+3} + 7H_4SiO_4$	(0)
174. CORUNDUM	$Al_2O_3 + 6H^+ \rightleftharpoons 2Al^{+3} + 3H_2O$	K(1)
175. CRISTOBA	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	Fournier and Rowe (1962)
176. CRISTOBB	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	Fournier (1973)
177. CU	$Cu + Fe^{+3} \rightleftharpoons Cu^+ + Fe^{++}$	K(1)
178. CU2O	$Cu_2O + 2H^+ \rightleftharpoons 2Cu^+ + H_2O$	K(1)
179. CU2S	$Cu_2S + H^+ \rightleftharpoons 2Cu^+ + HS^-$	K(1)
180. CU5FES6	$Cu_5FeS_6 + 6H^+ \rightleftharpoons 5Cu^{++} + Fe^{++} + 6HS^-$	(0)
181. CUFES2	$CuFeS_2 + 2H^+ \rightleftharpoons Cu^{++} + Fe^{++} + 2HS^-$	K(1)
182. CUFES3	$CuFeS_3 + 3H^+ \rightleftharpoons Cu^{++} + Fe^{++} + 3HS^-$	(0)

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
183. CUO	$CuO + 2H^+ \rightleftharpoons Cu^{++} + H_2O$	K(1)
184. CUS	$CuS + H^+ \rightleftharpoons Cu^{++} + HS^-$	K(1)
185. CUMMINGT	$Fe_7Si_8O_{22}(OH)_2 + 14H^+ + 8H_2O \rightleftharpoons 7Fe^{++} + 8H_4SiO_4$	(0)
186. DICKITE	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{+3} + 2H_4SiO_4 + H_2O$	K(1)
187. DIOPSIDE	$CaMgSi_2O_6 + 4H^+ + 2H_2O \rightleftharpoons Ca^{++} + Mg^{++} + 2H_4SiO_4$	K(1)
188. DOLOMITE	$CaMg(CO_3)_2 \rightleftharpoons Ca^{++} + Mg^{++} + 2CO_3^{--}$	K(Lafon, 1969)
189. ENSTATCT	$MgSiO_3 + 2H^+ + H_2O \rightleftharpoons Mg^{++} + H_4SiO_4$	(0)
190. ERIONITE	$CaNaAl_3Si_9O_{24}\cdot 9H_2O + 12H^+ + 3H_2O \rightleftharpoons Ca^{++} + Na^+ + 3Al^{+3} + 9H_4SiO_4$	(0)
191. FAYALITE	$Fe_2SiO_4 + 4H^+ \rightleftharpoons 2Fe^{++} + H_4SiO_4$	K(1)
192. FEASS		(0)
193. FECL2	$FeCl_2 \rightleftharpoons Fe^{++} + 2Cl^-$	K(1)
194. FECL3	$FeCl_3 \rightleftharpoons Fe^{+3} + 3Cl^-$	K(1)
195. FECO3	$FeCO_3 \rightleftharpoons Fe^{++} + CO_3^{--}$	K(1)
196. FEO	$FeO + 2H^+ \rightleftharpoons Fe^{++} + H_2O$	K(1)
197. FE203HEM	$Fe_2O_3 + 6H^+ \rightleftharpoons 2Fe^{+3} + 3H_2O$	K(1)
198. FE203MGH	$Fe_2O_3 + 6H^+ \rightleftharpoons 2Fe^{+3} + 3H_2O$	(25) Langmuir (1969)
199. FE304	$Fe_3O_4 + 8H^+ \rightleftharpoons 2Fe^{+3} + Fe^{++} + 4H_2O$	K(1)
200. FEOH3AM	$Fe(OH)_3 \rightleftharpoons Fe^{+3} + 3OH^-$	K(2)
201. FES2PYR	$4FeS_2 + 4H_2O \rightleftharpoons 4Fe^{++} + 7HS^- + SO_4^{--} + H^+$	K(1)
202. FESTROLT	$FeS + H^+ \rightleftharpoons Fe^{++} + HS^-$	K(1)
203. FESMAKIN	$FeS + H^+ \rightleftharpoons Fe^{++} + HS^-$	(0)
204. FORSTERI	$Mg_2SiO_4 + 4H^+ \rightleftharpoons 2Mg^{++} + H_4SiO_4$	K(1)
205. FLUORITE	$CaF_2 \rightleftharpoons Ca^{++} + 2F^-$	K(1)
206. GOETHITE	$FeOOH + 3H^+ \rightleftharpoons Fe^{+3} + 2H_2O$	K (Langmuir, 1971)
207. GIBBS AM	$Al(OH)_3 \rightleftharpoons Al^{+3} + 3OH^-$	K(3)
208. GIBBS C	$Al(OH)_3 \rightleftharpoons Al^{+3} + 3OH^-$	K(1)
209. GREENALI	$Fe_3Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 3Fe^{++} + 2H_4SiO_4 + H_2O$	(25) Truesdell & Jones (unpub. data,1972)
210. GREIGITE	$Fe_3S_4 + 4H^+ \rightleftharpoons 2Fe^{+3} + Fe^{++} + 4HS^-$	(25) Berner (1967)
211. GYPSUM	$CaSO_4\cdot 2H_2O \rightleftharpoons Ca^{++} + SO_4^{--} + 2H_2O$	K(2)
212. HALITE	$NaCl \rightleftharpoons Na^+ + Cl^-$	K(1)
213. HALLOYSI	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{+3} + 2H_4SiO_4 + H_2O$	K(1)
214. HEULANDI	$CaAl_2Si_7O_{18}\cdot 6H_2O + 8H^+ + 4H_2O \rightleftharpoons Ca^{++} + 7H_4SiO_4 + 2Al^{+3}$	(0)
215. HGO	$HgO + 2H^+ \rightleftharpoons Hg^{++} + H_2O$	K(1)
216. HUNTIT	$CaMg_3(CO_3)_4 \rightleftharpoons Ca^{++} + 3Mg^{++} + 4CO_3^{--}$	K(1)
217. HYDRMAGN	$Mg_4(CO_3)_3(OH)_2\cdot 3H_2O \rightleftharpoons 4Mg^{++} + 3CO_3^{--} + 2(OH)^- + 3H_2O$	(25) Langmuir (1965)
218. ILLITE	$K_{.6}Mg_{.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 8H^+ + 2H_2O \rightleftharpoons 0.6K^+ + 0.25\ Mg^{++} + 2.3\ Al^{+3} + 3.5H_4SiO_4$	K(1)
219. KAOLINIT	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{+3} + 2H_4SiO_4 + H_2O$	K(1)

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
220. KENYAITE	$NaSi_{11}O_{20.5}(OH)_4 \cdot 3H_2O + H^+ + 16.5H_2O \rightleftharpoons Na^+ + 11H_4SiO_4$	(25) Bricker (1969)
221. KYANITE	$Al_2SiO_5 + 6H^+ \rightleftharpoons 2Al^{+3} + H_4SiO_4 + H_2O$	K(1)
222. K2O	$K_2O + 2H^+ \rightleftharpoons 2K^+ + H_2O$	K(1)
223. LARNITE	$Ca_2SiO_4 + 4H^+ \rightleftharpoons 2Ca^{++} + H_4SiO_4$	K(1)
224. LAUMNIT	$CaAl_2Si_4O_{12} \cdot 4H_2O + 8H^+ \rightleftharpoons Ca^{++} + 2Al^{+3} + 4H_4SiO_4$	K (Zen, 1972)
225. LEUCITE	$KAlSi_2O_6 + 4H^+ + 2H_2O \rightleftharpoons K^+ + Al^{+3} + 2H_4SiO_4$	K(1)
226. LEONITE	$MgSO_4K_2SO_4 \cdot 4H_2O \rightleftharpoons Mg^{++} + 2K^{+1} + 2SO_4^{--} + 4H_2O$	(0)
227. MAGADITE	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O \rightleftharpoons Na^+ + 7H_4SiO_4$	(25) Bricker (1969)
228. MAGNESIT	$MgCO_3 \rightleftharpoons Mg^{++} + CO_3^{--}$	K(1)
229. MALACHIT	$Cu_2CO_3(OH)_2 \rightleftharpoons 2Cu^{++} + CO_3^{--} + 2OH^-$	K(3)
230. MARIALIT	$(NaAlSi_3O_8)_3 \cdot NaCl + 12H^+ + 12H_2O \rightleftharpoons 4Na^+ + 3Al^{+3} + 9H_4SiO_4 + Cl^-$	PATHI, Helgeson and others(1970)
231. MEIONITE	$(CaAl_2Si_2O_8)_3 \cdot CaCO_3 + 24H^+ \rightleftharpoons 4Ca^{++} + 6Al^{+3} + 6H_4SiO_4 + CO_3^{--}$	(0)
232. MERWINIT	$Ca_3MgSi_2O_8 + 8H^+ \rightleftharpoons 3Ca^{++} + Mg^{++} + 2H_4SiO_4$	K(1)
233. MGCL2	$MgCl_2 \rightleftharpoons Mg^{++} + 2Cl^-$	K(1)
234. MGFE2O4	$MgFe_2O_4 + 8H^+ \rightleftharpoons Mg^{++} + 2Fe^{+3} + 4H_2O$	K(1)
235. MGOPERIC	$MgO + 2H^+ \rightleftharpoons Mg^{++} + H_2O$	K(1)
236. MICROCLN	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftharpoons K^+ + Al^{+3} + 3H_4SiO_4$	K(1)
237. MIRABILT	$Na_2SO_4 \cdot 10H_2O \rightleftharpoons 2Na^+ + SO_4^{--} + 10H_2O$	K(4)
238. MNCL2	$MnCl_2 \rightleftharpoons Mn^{++} + 2Cl^-$	K(1)
239. MNCO3	$MnCO_3 \rightleftharpoons Mn^{++} + CO_3^{--}$	K(1)
240. MNO	$MnO + 2H^+ \rightleftharpoons Mn^{++} + H_2O$	K(1)
241. MNO2	$MnO_2 + 4H^+ + Mn^{++} \rightleftharpoons 2Mn^{+3} + 2H_2O$	PATHI, Helgeson and others(1970)
242. MNS	$MnS + H^+ \rightleftharpoons Mn^{++} + HS^-$	K(1)
243. MONTICEL	$CaMgSiO_4 + 4H^+ \rightleftharpoons Ca^{++} + Mg^{++} + H_4SiO_4$	K(1)
244. MONTCA	$Ca_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.324\ H^+ + 2.678\ H_2O \rightleftharpoons .167\ Ca^{++} + 2.33\ Al^{+3} + 3.67\ H_4SiO_4$	K(1)
245. MONT K	$K_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32\ H^+ + 2.68\ H_2O \rightleftharpoons .33K^+ + 2.33\ Al^{+3} + 3.67\ H_4SiO_4$	K(1)
246. MONT MG	$Mg_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.324\ H^+ + 2.678\ H_2O \rightleftharpoons .167\ Mg^{++} + 2.33\ Al^{+3} + 3.67\ H_4SiO_4$	K(1)
247. MONTNA	$Na_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.324\ H^+ + 2.678\ H_2O \rightleftharpoons .33\ Na^+ + 2.33\ Al^{+3} + 3.67\ H_4SiO_4$	K(1)
248. MONTCANA		(0)
249. MONTSEAW		(0)
250. MORDENIT	$CaAl_2Si_{10}O_{24} \cdot 7H_2O + 8H^+ + 9H_2O \rightleftharpoons Ca^{++} + 2Al^{+3} + 10H_4SiO_4$	(0)
251. MUSCOVIT	$K\ Al_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftharpoons K^+ + 3Al^{+3} + 3H_4SiO_4$	K (Zen, 1972)
252. NA2O	$Na_2O + 2H^+ \rightleftharpoons 2Na^+ + H_2O$	K(1)
253. Na2SO4	$Na_2SO_4 \rightleftharpoons 2Na^+ + SO_4^{--}$	K(1)
254. NAHCOLIT	$NaHCO_3 \rightleftharpoons Na^+ + HCO_3^-$	K(3)
255. NATRON	$Na_2CO_3 \cdot 10H_2O \rightleftharpoons 2Na^+ + CO_3^{--} + 10H_2O$	K(3)
256. NATRTHRM	$Na_2CO_3 \cdot H_2O \rightleftharpoons 2Na^+ + CO_3^{--} + H_2O$	K(3)
257. NEPHELIN	$NaAlSiO_4 + 4H^+ \rightleftharpoons Na^+ + Al^{+3} + H_4SiO_4$	K(2)
258. NESQUEHN	$MgCO_3 \cdot 3H_2O \rightleftharpoons Mg^{++} + CO_3^{--} + 3H_2O$	K(3)
259. NICOLITE		(0)
260. PYRX		

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

PUTER NO. AND NAME	REACTION	SOURCE OF DATA
261. PBCL2	$PbCl_2 \rightleftharpoons Pb^{++} + 2\ Cl^-$	K(1)
262. PBCO3	$PbCO_3 \rightleftharpoons Pb^{++} + CO_3^{--}$	K(1)
263. PBCLITHR	$PbO + 2H^+ \rightleftharpoons Pb^{++} + H_2O$	K(1)
264. PBOMASIC	$PbO + 2H^+ \rightleftharpoons Pb^{++} + H_2O$	K(1)
265. PBS	$PbS + H^+ \rightleftharpoons Pb^{++} + HS^-$	K(1)
266. PBSO4	$PbSO_4 \rightleftharpoons Pb^{++} + SO_4^{--}$	K(1)
267. PHILLIPS	$Na_{.5}K_{.5}AlSi_3O_8 \cdot H_2O + 4H^+ + 3H_2O \rightleftharpoons .5Na^+ + .5K^+ + Al^{+3} + 3H_4SiO_4$	(25)Truesdell & Jones (unpub. data, 1972)
268. PHLOGPTF	$K\ Mg_3\ AlSi_3O_{10}\ F_2 + 8H^+ + 2H_2O \rightleftharpoons K^+ + 3Mg^{++} + Al^{+3} + 3H_4SiO_4 + 2F^-$	K(2)
269. PLAG(AN)	$CaAl_2Si_2O_8 + 8H^+ \rightleftharpoons Ca^{++} + 2Al^{+3} + 2H_4SiO_4$	K(1)
270. PREHNITE	$Ca_2Al_2Si_3O_{10}(OH)_2 + 10\ H^+ \rightleftharpoons 2Ca^{++} + 2Al^{+3} + 3H_4SiO_4$	K(2)
271. PYROPHYL	$Al_2Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftharpoons 2Al^{+3} + 4H_4SiO_4$	K (Zen, 1972)
272. QUARTZ	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	Morey and others (1962)
273. SANADNHI	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftharpoons K^+ + Al^{+3} + 3H_4SiO_4$	K(1)
274. SEPIOLIT	$Mg_2Si_3O_8 \cdot 2H_2O + 4H^+ + 2H_2O \rightleftharpoons 2Mg^{++} + 3H_4SiO_4$	PATHI, Helgeson and others (1970)
275. SILICAAM	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	K(1)
276. SILICGEL	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4$	Fournier (1973)
277. SILLIMAN	$Al_2SiO_5 + 6H^+ \rightleftharpoons 2Al^{+3} + H_4SiO_4 + H_2O$	K(1)
278. SPINEL	$MgAl_2O_4 + 8H^+ \rightleftharpoons Mg^{++} + 2Al^{+3} + 4H_2O$	K(1)
279. SRCO3	$SrCO_3 \rightleftharpoons Sr^{++} + CO_3^{--}$	K(2)
280. STRENGIT	$FePO_4 \cdot 2H_2O \rightleftharpoons Fe^{+3} + PO_4^{-3} + 2H_2O$	K(3)
281. SYLVITE	$KCl \rightleftharpoons K^+ + Cl^-$	K(1)
282. TALC	$Mg_3Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftharpoons 3Mg^{++} + 4H_4SiO_4$	K(1)
283. TREMOLIT	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 14H^+ + 8H_2O \rightleftharpoons 2Ca^{++} + 5Mg^{++} + 8H_4SiO_4$	K(1)
284. TRONA	$Na_2CO_3NaHCO_3 \cdot 2H_2O \rightleftharpoons 3Na^+ + HCO_3^- + CO_3^{--} + 2H_2O$	(25)Truesdell & Jones (unpub. data, 1972)
285. WAIRAKIT	$CaAl_2Si_4O_{12} \cdot 2H_2O + 8H^+ + 2H_2O \rightleftharpoons Ca^{++} + 2Al^{+3} + 4H_4SiO_4$	K (Zen, 1972)
286. WITHERIT	$BaCO_3 \rightleftharpoons Ba^{++} + CO_3^{--}$	K(1)
287. WALLOSTO	$CaSiO_3 + 2H^+ + H_2O \rightleftharpoons Ca^{++} + H_4SiO_4$	K(1)
288. ZNCO3	$ZnCO_3 \rightleftharpoons Zn^{++} + CO_3^{--}$	K(1)
289. ZNO	$ZnO + 2H^+ \rightleftharpoons Zn^{++} + H_2O$	K(1)
290. ZNS	$ZnS + H^+ \rightleftharpoons Zn^{++} + HS^-$	K(1)
291. ZNSO4	$ZnSO_4 \rightleftharpoons Zn^{++} + SO_4^{--}$	K(1)
292. ZOISITE	$Ca_2Al_3Si_3O_{12}OH + 13H^+ \rightleftharpoons 2Ca^{++} + 3Al^{+3} + 3H_4SiO_4 + H_2O$	K (Zen, 1972)
293. VIVIANIT	$Fe_3(PO_4)_2 \cdot 8H_2O \rightleftharpoons 3Fe^{++} + 2PO_4^{-3} + 8H_2O$	(25) Nriagu (1972)
294. Blank		
295. Blank		

Table 1.--List of the aqueous complexes and minerals used in SOLMNEQ. The source of data for the log (KT) values of the given reactions is indicated--Continued

COMPUTER NO. AND NAME	REACTION	SOURCE OF DATA
	C - OXIDATION-REDUCTION REACTION	
296. FE2 TO FE3	$Fe^{++} \rightleftharpoons Fe^{+3} + e^-$	K(1)
297. CU1 TO CU2	$Cu^{+} \rightleftharpoons Cu^{++} + e^-$	K(1)
298. HG222HG2	$Hg_2^{++} \rightleftharpoons 2Hg^{++} + 2e^-$	K(1)
299. MN2 TO MN3	$Mn^{++} \rightleftharpoons Mn^{+3} + e^-$	K(1)

[1] (0) No data available; (1) Helgeson (1969). Log KT values were extrapolated and interpolated to temperatures of App. 2A. These values were generally checked using DQUANT; (2) Robie and Waldbaum (1968); (3) Naumov and others (1971); (4) NBS Technical Note 270-3 and 4 (1968 and 1969); (25) log KT computed at 25°C and assumed constant at other temperatures; D(X) log KT values generated with DQUANT (Helgeson, 1971b). Input data for DQUANT obtained from reference (X); K(X) log KT values generated with KELYCOB (Helgeson, 1971a). Input data for KELYCOB obtained from reference (X). Conventional heat capacities for aqueous species were calculated from average heat capacities (Cobble, 1964; Helgeson, unpub. data).

[2] Estimated from correlation plots of electronegativities, and ionic radii of cations versus pK (Garrels and Christ, 1965). For $SrSO_4$, ΔG°_f from Lieser (1965), S° estimates from correlation plots (Helgeson, 1969).

[3] Log KT values for Mg-phosphate complexes are equal to those of Ca (Ghughtai, 1968) but with variations shown by Childs (1971) at 51°C.

[4] Log KT values for minerals were generated with KELYCOB. ΔH°_f, S° for the minerals were generally obtained from Helgeson, 1969; these values are generally similar to the values of Robie and Waldbaum (1968) and Naumov and others (1971). Cp power functions for minerals were obtained from Kelley (1960, or (3), or estimated (see text).

Activity coefficients

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

$$\text{Log } \gamma_i(T,I) = \frac{-A(T)\ \nu_i^2\ I^{1/2}}{1 + a_i^o B(T)\ I^{1/2}} + B^{\cdot}(T)\ I \qquad (4)$$

where

a_i^o is the distance of the nearest approach of ions in solution,

A(T) is a molal Debye-Hückel coefficient at temperature T,

B(T) is a molal Debye-Hückel coefficient at temperature T,

ν_i is the charge of the ith ion,

I is the ionic strength, and

B$^{\cdot}$ is a deviation function.

The Debye-Hückel coefficients A and B are given by

$$A(T) = \frac{1.8246X10^{6}(\rho(T))^{1/2}}{(\varepsilon(T)T)^{3/2}} \qquad (5)$$

and

$$B(T) = \frac{50.29X10^{8}(\rho(T))^{1/2}}{(\varepsilon(T)T)^{1/2}} \qquad (6)$$

where ρ and ε are the density and the dielectric constant of water at temperature T.

The ionic strength (I) of a given solution is given by

$$I \equiv 1/2 \sum_{i} m_i \nu_i^2 \ . \qquad (7)$$

The density of water is computed from the equations of Keenan and Keyes (1936, p. 21). The dielectric constant of water is calculated to 100°C from the equation of Wyman and Ingalls as cited by Harned and Owen (1958, p. 159); it is calculated at higher temperatures from the function of Akerlof and Oshry (1950). (See Appendix 1.)

The a^{o} values used (App. 2B) are from Kielland (1937). Arbitrary a^{o} values of 4.0, 5.0, and 6.0 were assigned respectively to those monovalent, divalent and trivalent species in solution not reported by Kielland.

The values for the deviation function, B', reported in this program as a function of temperature (App. 2D) are from Helgeson (1969). SOLMNEQ computes B' by linear interpolation of the values in Appendix 2D. This method has been discussed in detail by Helgeson (1969). The B' values used in this program are for NaCl solutions, a close approximation for the majority of natural waters. The presence of appreciable amounts of divalent and trivalent cations and anions in solution with their higher degree of hydration will make the γ_i obtained slightly lower than the true values.

The activity coefficients of all neutral species are assumed equal to the activity coefficients of dissolved CO_2 in NaCl solutions (Helgeson, 1967). SOLMNEQ computes γ_{CO_2} at the temperature and ionic strength (up to 3 molal) of the solution by linear interpolation of γ_{CO_2} values as a function of temperature and ionic strength of an equivalent solution (App. 2C after Helgeson, 1969). Helgeson computed γ_{CO_2} from Ellis and Golding (1963) using

$$\gamma_{CO_2}(T) = k_m/k \tag{8}$$

where k and k_m are the Henry's law coefficients in pure water and in a sodium chloride solution of molality, m, at temperature T. SOLMNEQ has an option by which the activity coefficients of the neutral species may be given as unity.

Equilibrium constants

The equilibrium constant (K) of a reaction such as reaction (1) is given by:

$$K_{albite} = \frac{a_{Na^+} \cdot a_{Al^{+3}} \cdot \left(a_{H_4SiO_4}\right)^3}{a_{alb} \cdot \left(a_{H^+}\right)^4 \cdot \left(a_{H_2O}\right)^4} \qquad (9)$$

where a_i is the activity of the ith species at equilibrium.

The equilibrium constants for the reactions shown on table 1 are punched as part of the object deck. The K(T) values reported (App. 2A) at intervals of 25°C from 0-200°C and at intervals of 50°C from 200-350°C were computed assuming a constant pressure of 1 atmosphere. Pressures normally encountered in natural systems will not significantly affect these computations (Helgeson, 1969). The equilibrium constants were obtained by the following methods, which are listed in decreasing order of reliability:

1. Reported experimental data (solubility, free energy, and other data) over the temperature range considered in this program.
2. Computed using KELYCOB (Program No. 0802 D/E, Helgeson, 1971a). KELYCOB computes the equilibrium constants as well as the standard entropies, enthalpies, free energies, and heat capacities of a given reaction (log K_r, ΔS°_r, ΔH°_r, ΔG°_r, and $\Delta C^\circ_{p,r}$) as a function of temperature and pressure. The Maier-Kelley ($a + bT + cT^{-2}$, Kelley, 1960) heat capacity power functions, the standard enthalpies of formation

Δ = Delta

(ΔH°_{f}) and the standard entropies (S°_{i}) of all the components involved are used as input to this program. KELYCOB computes the K(T) values from an integrated form of the Van't Hoff's equation (Helgeson, 1969).

$$\log K(T) = \log K_{298.15} - \frac{\Delta H^{\circ}_{r}}{2.303R}\left(\frac{1}{T} - \frac{1}{298.15}\right) - \frac{1}{2.303RT} \int_{298.15}^{T} \Delta C^{\circ}_{p,r}(T)dT + \frac{1}{2.303R} \int_{298.15}^{T} \Delta C^{\circ}_{p,r}(T)d\ln T \quad (10)$$

KELYCOB was used to generate log K values at 25°C intervals from 0°C to 350°C for most of the hydrolysis reactions reported on table 1. A number of log K values for the dissociation reactions of aqueous complexes were also obtained by this method.

The heat capacity power function for many minerals reported in this program are not known. These were approximated by summing up the heat capacity power functions for the oxides. Ice (9.0 Cal $mole^{-1}deg^{-1}$) was used to represent H_2O in these approximations (Helgeson, 1969).

3. Computed using DQUANT (Program No. 0405 AR, Helgeson, 1971b). This program requires only that $\Delta H^\circ_r\ (T_r)$ and $\Delta S^\circ_r\ (T_r)$ be known; it was used where no heat capacity data of any kind were available for one or more of the species involved in the reaction. This last condition covers most of the aqueous reactions reported on table 1. DQUANT computes K(T) values by evaluating (Helgeson, 1967)

$$\log K(T) = \frac{\Delta S^\circ_r(T_r)}{2.303RT}\left[T_r - \frac{\theta}{W}\left(1 - \exp[\exp\,(b + aT) - c + (T - T_r)/\theta]\right)\right] - \frac{\Delta H^\circ_r(T_r)}{2.303RT} \qquad (11)$$

where

θ, w, a, b, and c are temperature independent constants characteristic of the solvent,

R is the gas constant.

DQUANT assumes that $\Delta C^{o}_{p,r}$ changes monotonically but nonlinearly with temperature. Dissociation constants computed from this program are often much closer approximations of actual dissociation constants at higher temperatures than those computed assuming $\Delta C^{o}_{p,r}(T) = 0$ or $\Delta C^{o}_{p,r}(T) =$ a constant (Helgeson, 1969). K(T) values obtained with DQUANT are reasonable approximations only to $\sim$ 200°C.

A correction factor was applied to some of the K(T) values generated with DQUANT at temperatures higher than 200°C. These factors were applied only to those complexes where experimental values for similar species are available. Even with the application of these correction factors, the errors involved in the values of K(T) at temperatures higher than 200°C are large; this introduces large uncertainties in computations carried out with SOLMNEQ at temperatures higher than $\sim$ 200°C.

4. Reported experimental data over a restricted temperature range which were extrapolated to cover the temperature range considered. Some K values are known or could only be calculated at 25°C; these have been assumed constant over the temperature range of the program.

5. No K(T) values could be obtained for a number of minerals and aqueous species incorporated in SOLMNEQ. A dummy value of log K equal to 999.99 is used for these minerals and species. This value is so high that the species and minerals involved do not affect the results obtained with SOLMNEQ.

Values of log K for aqueous complexes and minerals at any desired temperature can be computed from data in Appendix 2A by the subroutine (TLUV) (P. C. Doherty, oral commun., 1972). The interpolation of the log K values (see listing, App. 1) is by:

$$Y = a + bX + cX^2 + dX^3 \qquad (12)$$

where

X is the independent variable (= the reported values of log K at the specified temperatures),

Y is the dependent variable (= the interpolated value of log K at the sample temperature), and

a, b, c, and d are constants.

This subroutine is more than adequate to interpolate the log K values between the reported intervals (25°C from 0°C-200°C and 50°C from 200-350°C).

Oxidation-reduction reactions

The distribution of Fe^{+3}, Cu^{++}, Hg^{++}, and Mn^{+3} in SOLMNEQ may be computed using equations involving electron transfer reactions such as

$$Fe^{++} = Fe^{+3} + e^{-} \tag{13}$$

where e^{-} represents an electron. The concentration of Fe^{+3} ($m_{Fe}+3$) may be calculated from the following equation if the Eh of the solution and $m_{Fe^{++}}$ are known:

$$Eh(T) = E^{\circ}(T) + \frac{RT}{nF} \ln \frac{m_{Fe^{+3}} \cdot \gamma_{Fe^{+3}}}{m_{Fe^{++}} \cdot \gamma_{Fe^{++}}} \tag{14}$$

where

Eh(T) is the oxidation potential at the measured temperature referred to the hydrogen half cell,

E° is the potential of the half cell in which all reactants and products are in their standard states,

n is the number of electrons (e) involved; it is equal to unity for reaction (13), and

F is the Faraday constant.

$$E^{\circ} = \frac{\Delta G_r^{\circ}(T)}{nF} \tag{15}$$

The standard free energies for the four oxidation-reduction reactions (ΔG°_{r} 296, 297, 298, and 299) at the same temperatures as for log K are included in Appendix 2A. They are interpolated to the specified temperature of the sample by Lagrange subroutine (TLUV).

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

Computations based on measured Eh have been kept to a minimum in this program because Barnes and Clarke (1969) showed that the measured Eh is quantitatively related only to the behavior of iron species.

Distribution of species in solution

The distribution of species in the aqueous solution is computed from the reported chemical analysis of the water sample together with field measurements of its temperature, pH, and Eh. The interpolated dissociation constants of the aqueous complexes (K_{diss}) and the computed activity coefficients (γ) are also utilized in these computations.

The chemical analysis may contain the total concentrations of all or part of the following list of elements and ions: Ca, Mg, Na, K, Cl, SO_4, HCO_3, SiO_2, Ag, Al, Ba, Cu, Fe, Hg, Li, Mn, Pb, Sr, Zn, $As(OH)_4$, PO_4, F, H_3BO_3, NH_3, H_2S, CO_3, and NO_3. It is not necessary to distribute the alkalinity of the sample between HCO_3 and CO_3; SOLMNEQ computes the concentration of these and other species contributing to the reported alkalinity.

The concentration units, for the purpose of this program, may be in ppm (parts per million) or mg/l (milligrams/liter) or moles/l (moles/liter) or meq/l (millequivalent/liter). The computations in SOLMNEQ are carried out after converting the concentration units reported to molalities.

The distribution of species in the aqueous phase is computed using mass action reactions for all the aqueous complexes reported in table 1, oxidation-reduction reactions, and mass balance relationships. The mass balance relationships are of the type

$$m_{i,t} = \sum_i n_i m_i \qquad (16)$$

where

$m_{i,t}$ is the total reported or computed molality of the ith ion (for example, total molality of Ca),

$\sum_i n_i m_i$ is the summation of the molalities of Ca^{++} and all the aqueous complexes containing Ca (for example, $CaCO_{3(aq)}$, and $CaHCO_3^-$, and $CaSO_{4(aq)}$), and

n_i is the number of molecules of (i) appearing in the aqueous complex.

For a more detailed and specific examination of distribution of species see the listing of SOLMNEQ (App. 1).

Iteration cycles are used to solve for the distribution of carbonate, sulphate, fluoride, phosphate, and chloride species. The iteration cycles are carried out whenever the computed $m_{i,t}$ (equation 16) of any of these five ligands differs by more than 0.5 percent from their analyzed values. Most water samples will probably converge to meet the above requirement within about 20 iterative cycles. The cutoff number in SOLMNEQ is 100 cycles.

Gibbs free energy functions

The Gibbs free energy for many hydrolysis reactions in natural systems may be obtained (Garrels and Christ, 1965; Barnes and Clarke, 1969) from

$$\Delta G_r = -RT \ln Q \tag{17}$$

where ΔG_r is the Gibbs free energy of reaction and Q is the reaction quotient. Q is equal to the activity product (AP) and is given for reaction (1) by

$$Q = AP = \frac{\bar{a}_{Na^+} \cdot \bar{a}_{Al^{+3}} \cdot \bar{a}_{H_4SiO_4}}{\left(\bar{a}_{H^+}\right)^4 \cdot \left(\bar{a}_{H_2O}\right)^4 \cdot \bar{a}_{Alb.}} \tag{18}$$

where $(\bar{a})$ is the actual activity of the species in the given solution at the specified temperature and pressure. The value of $\bar{a}_{Alb.}$ is assumed to be unity.

The Gibbs free energy difference between the actual and equilibrium states is given by

$$\Delta G_{diff} = RT \ln (Q/K) \qquad (19)$$

All the reactions used in SOLMNEQ (table 1) have the solid on the left side of the reaction equation. As a consequence, the following relations hold:

$$\Delta G_{diff} < 0 \qquad (20)$$

The reaction tends to proceed spontaneously from left to right. The solid cannot precipitate from this solution because of undersaturation.

$$G_{diff} > 0 \qquad (21)$$

The reaction tends to proceed spontaneously from right to left. The solid cannot dissolve in the solution because of supersaturation.

$$G_{diff} = 0 \qquad (22)$$

The reaction is at equilibrium and neither dissolution nor precipitation should take place.

The fact that the free energy difference of a given reaction (ΔG_{diff}) indicates that it should proceed from left to right or vice versa, does not mean that the reaction will indeed proceed in the specified direction. The only definitive statements that can be made are that the solution is supersaturated, saturated or undersaturated with respect to the solid. Evaluation of this type should not, by themselves alone, be interpreted to indicate presence or absence of specific mineral species. It is possible for a given solution to be supersaturated (unstable but persistent condition) with respect to a mineral by a number of kilocalories without precipitation (Barnes and Clarke, 1969). The computation of Gibbs free energy difference for minerals may be a useful guide for application of methods of identifying mineral species expected to be present in the system under study.

INPUT

Input to SOLMNEQ consists of fixed (card Nos. 1 through 6) and optional (card Nos. 7 through 9) data as follows:

Card No.	Data	Format
1	Sample description (may be blank)	A(80)
2	TEMP (temp. in °C), PH, EHM (Measured Eh in volts if available; otherwise put 9.000 E0), and FLAG for concentration units (PPM or MG/L or MOL/L or MEQ/L).	E(6,1), X(1), E(6,2), X(1), E(8,3), X(1), A(5)
3	Total concentration of Ca, Mg, Na, K, Cl, SO_4, HCO_3, and SiO_2	8(E(8,3), X(1))
4	Total concentration of Ag, Al, Ba, Cu, Fe, Hg, Li, and Mn	8(E(8,3), X(1))
5	Total concentration of Pb, Sr, Zn, $AS(OH)_4$, PO_4, F, H_3BO_3, and NH_3	8(E(8,3), X(1)
6	Total concentration of H_2S, CO_3 and NO_3	3(E(8,3), X(1)

6 + N (N=0 to 3)	Optional data including DENS (density if ≠ 1.0), EHMC (the EMF in volts of the Eh cell including the Calomel reference electrode), EMFZSCE (the EMF in volts of the Eh cell calibrated using Zobell's solution). The values of FLAG1-5 may be changed from "0" to "1". To suppress the printout of "TABLES" and "RATIOS" put INFORM=1, and RATIO=1. These cards may also be used to temporarily supercede the log (KT) values of any species in table 1, for example, "LOGKT(36)= "	Data directed format. For example, FLAG1=1,------, INFORM=1; Separate the data with commas and end with semicolon.
6+N+1	Blank card separating every sample, and at end of last sample.	Blank

The total concentrations used in SOLMNEQ should be for the species mentioned in cards 3 through 6 and in the specified order. Zeros, in the appropriate format, must be used for the concentrations of those species appearing in cards 3 through 6 but not reported in the chemical analyses of the sample.

FLAG1 through FLAG5 are dummy identifiers which have been initialized in SOLMNEQ as = 0. The value of any one of these FLAGs, however, may be changed to (1) if an alternate specified method of computation is desired. SOLMNEQ equates the activity coefficient of the neutral species in solution to the computed activity coefficient of dissolved carbon dioxide. The activity coefficient of the neutral species will be = 1.0 when FLAG1=1.

If the Eh of the sample is known and it is desired that the concentration of any or all of the species Cu^{++}, Fe^{+3}, Hg^{++}, and Mn^{+3} be computed from equations similar to equation 14, then put FLAG2 through FLAG5 = 1. The concentrations of these species, otherwise, will be computed from equations 4, 5, 6, and 7 (table 1), respectively.

It should be noted that the input value to be assigned to the concentration units variable (FLAG) must be punched left-justified in the appropriate field.

OUTPUT (RESULTS)

A printout from SOLMNEQ for a test sample of sea water composition (after Goldberg, 1963) is shown on Appendix 3. Table 2 gives the list of identifiers used in SOLMNEQ and their significance. A typical printout includes a listing of SOLMNEQ, a printout of the data file (TABLES) as well as the results of the computations. SOLMNEQ (see Appendix 1 for listing) is written for the IBM 360 computer and conforms to PL/1 language as given in the IBM reference manual (IBM GC28-6594, 1972).

Table 2.--List of identifiers used in COLMNEQ and their significance

PL/1 Identifier	Text Symbol	Significance
A	A	Molal Debye-Hückel coefficient defined in equation (5)
AGTOT,..., XTOT	-----	Total analyzed concentration of Ag; X is for the species shown on the input section
AH2O	a_{H_2O}	Activity of water
ALFA(0:161)	a_i	Array for the activity of the aqueous species shown on App. 2B.
ANALCO3	-----	Total concentration of all the carbonate species in solution.
ANALM(0:161)	m_i	Array for the analyzed molality of the aqueous species shown on Table 1.
AP(138:295)	AP = Q	Array for the activity product of minerals in solution defined in equation (18).
B	B	Molal Debye-Hückel coefficient defined in equation (5).
BDAT(10)	-----	Array for $\dot{B}$ (see below) as a function of temperature (App. 2D)
BDOT	$\dot{B}$	Deviation function defined in equation (4).
C	2.303	Conversion factor from (ln) to (log 10).
CO2TIT	-----	Analyzed molality of (CO_3^{--} + HCO_3^-)
CO3TOT	-----	Computed molalities of CO_3^{--}, HCO_3^- and H_2CO_3
CO3CALC	$m_{CO_3^-}$	Computed molality of CO_3^{--}
CUNITS(0:161)	ppm or mg/l,--etc.	Reported concentration units
DENS	ρ	Density of water
DHA(0:161)	a°	Array for the distance of the nearest approach of ions in solutions
EHM	Ehm	Measured Eh oxidation potential
EHMC	EHMC	Emf of the Eh Cell including the Calomel reference electrode
EMFZSCE	EMFZSCE	Emf of the Eh Cell calibrated using Zobell's solution
EPMAN	-----	Total milliequivalent of anions/liter
EPMCAT	-----	Total milliequivalent of cations/liter
F	F	The Faraday constant
FLAG, FLAG1-5	-----	See input
G = GAMMACO2(0:3,10)	γ_{CO_2}	Array for the activity coefficient of dissolved CO_2 as a function of an equivalent NaCl solution and temp. (App. 2C)
GAMMA(0:161)	γ_i	Array for the activity coefficients of the dissolved species
GFW(0:161)	GFW	Array for the gram formula weight of the aqueous species (App. 2B)
INFORM	-----	See input

Table 2.--List of identifiers used in SOLMNEQ and their significance (continued)

PL/1 Identifier	Text Symbol	Significance
KT(295)	K(T)	Array for the equilibrium constants for the reactions of Table 1
LH2O	Log a_{H_2O}	Log (activity of water)
LKT(299,11)	Log K	Array for the log of the equilibrium constants as a function of temperature for the reactions of Table 2. LKT(296:299,11) is ΔG°_r for reactions 296, -7, -8, and -9 (Table 1)
LOGKT(299)	log K(T)	Log (K) above at temperature T. LOGKT (296:299) is $\Delta G^\circ_r(T)$ for the reactions 296, -7, -8, and -9
M(0:161)	m_i	Array for the molality of the aqueous species (App. 2B)
M NACLE	m_{NaCl}	Molality of an equivalent NaCl solution
MU	I	Ionic strength of the sample defined in equation (7)
NAME1(0:161)	-----	Array for the numbers and the names of the aqueous species of App. 2B
PAGE2(299)	-----	Array for the numbers and the names of the aqueous complexes and minerals of App. 2A
PCO2	P_{CO_2}	Partial pressure of $CO_{2(g)}$ in atmospheres that would be in equilibrium with the solution
PH	pH	pH = -log a_{H+}
PH2O	P_{H_2O}	Partial pressure of $H_2O_{(g)}$ in atmospheres that would be in equilibrium with the solution
R	R	Gas constant
S1, S2, S3, S4, and S5	$\Sigma_i \nu_i m_i$	Summations of the molalities of carbonate, sulphate, flouride, phosphate and cloride ligands respectively in all the aqueous species
T	T	Temperature, degrees Kelvin
TABLES	-----	Name of file containing Appendix 2
TCO2(10)	-----	Array for the 10 temperatures (App. 2C&D) for the reported values of $\gamma_{CO_2(aq)}$ and B
TEMP	t	Temperature, degrees Centigrade
TEMPH	a_{H+}	10^{-pH}
TK(11)	-----	Array for the 11 temperatures (App. 2A) for which the values of log KT are given
Y1-Y24	-----	Statement labels used to bypass the species of an element not included in the reported analyses
Z(0:161)	ν_i	Array for the charge of the aqueous species (App. 2B)

The data file "TABLES" (App. 2) consists of the following:

1. A two-dimensional array (App. 2A) of log KT (299, 11) values at the 11 specified temperatures. The reaction numbers as well as the aqueous complexes (Nos. 1 through 136) and minerals (137 through 295) are also indicated. Dummy values of 999.99 appear where no thermodynamic data are available. The values reported for the reaction numbers 296 through 299 are the standard free energies of reaction ($\Delta G_r^o(T)$) for the indicated oxidation-reduction reactions at the specified temperatures. Table 1 gives the names of the species, the reactions, and the source of log K values.
2. A list of the aqueous species involved in the computations (App. 2B). This consists of the program number, name, charge (Z), distance of the nearest approach (DHA), and gram formula weight (GFW) of the species.
3. A two-dimensional array of the activity coefficient of the dissolved CO_2 (γ_{CO_2}) as a function of temperature and an equivalent NaCl solution (Helgeson, 1969) (App. 2C).
4. A one-dimensional array of B˙ (BDOT) as a function of temperature (Helgeson, 1969) (App. 2D).

The results of the computatations carried out by this program and appearing in the printout (App. 3) consist of the following:

1. A list consisting of information read into SOLMNEQ (sample description, concentration units, pH, Eh (if measured), and temperature), the computed value of Eh (computed from field measurements; a dummy value of 9.0000 is printed when no Eh data are available), total milliequivalent of cations (MEQ/L CAT) and anions (MEQ/L AN) computed from the analytical data (ANAL...) and from the calculated molalities (CALC...), the ionic strength of solution (I), the molality and ppm of the dissolved CO_2, and the partial pressures, in atmospheres, of $CO_{2(g)}(P_{CO_2})$ and $H_2O_{(g)}(P_{H_2O})$ in equilibrium with the solution.
2. A table showing the distribution of species in solution. This consists of the index number and name of the species (0 to 161), reported and computed ppm (ANAL PPM, CALC PPM), reported and computed mg/l (ANAL MG/L, CALC MG/L), reported and computed molality (ANAL MOLAL, CALC MOLAL), activity (ALFA), activity coefficient (GAMMA), and -log activity (PION).

   This table can be used to calculate the degree of complexing in the solution under study.
3. Ratios of a number of cations and anions of importance in geochemical processes. These consist of the mole ratios

of cations and anions which may aid in deciphering the origin of the water samples (White, 1965; Kharaka, 1971) and logs of the activity ratios of a number of cations used to study the stability fields of minerals. The subsurface temperature of a geothermal reservoir is computed by six different geochemical methods (see App. 1 for the details of computations). A number of criteria for selecting the most probable temperature are also printed. (Fournier and Truesdell, 1973; and references cited therein).

The computation and printout of these ratios and temperatures may be suppressed by inputting "RATIO = 1" in the optional data.

4. A table showing the states of reactions for 158 minerals considered. The "DELG" column gives the (ΔG_{diff}), in kilocalories, of equation 19. A positive (DELG) value indicates that the solution is supersaturated with respect to the given mineral; a negative (DELG) value indicates undersaturation with respect to it. This table also shows the mineral name and its computer numbers, AP = Q (equation 19), the value of K at temperature T, log (AP), log (KT), AP/KT and log AP/KT. The activity product (AP) and LOG(AP) as well as (AP/KT), DELG and LOG AP/KT of a mineral which contains a species not reported in the chemical analyses of the water sample will be blank. However, an arbitrary value may be assigned to the concentration of any desired species. A dummy value of 59.9990 is printed for the LOG KT

(9.9770E + 59 for KT) where these are unknown. The log (KT) of a number of minerals (for example, kenyaite, magadiite) is known only at 25°C; it is assumed constant at other temperatures. The "DELG" values obtained for these minerals will not be too significant if the temperature of the sample varies by more than about 10°C from 25°C.

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

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APPENDIX 1. LISTING OF SOLMNEQ

```
/*
   ************************************************************************

   THIS PROGRAM IS WRITTEN FOR THE IBM 360 COMPUTER & CONFORMS TO
   PL/1 LANGUAGE AS GIVEN IN THE IBMGC28-6594REFERENCE MANUAL.THIS
   PROGRAM WAS WRITTEN BY YOUSIF K.KHARAKA,U.CALIFORNIA,BERKELEY,
   WHILE WORKING AT U.S.GEOLOGICAL SURVEY.SOLMNEQ WAS BASED IN PART
   ON WATCHEM & WATEQ. THIS VERSION WAS COMPLETED AUGUST/1972.

   ************************************************************************
                                                                        */
SOLMNEQ: PROCEDURE OPTIONS (MAIN);
/*
.........................................................................

     PURPOSE :
     TABLE-LOOK-UP AND LAGRANGE INTERPOLATION SUBROUTINE
     DESCRIPTION OF PARAMETERS
         X - THE VALUE OF THE INDEPENDENT VARIABLE (FOR WHICH THE
             VALUE OF THE DEPENDENT VARIABLE AND/OR ITS DERIVATIVES
             ARE DESIRED).
        XT - TABLE OF 'X' VALUES IN ASCENDING ORDER.
        YT - TABLE OF CORRESPONDING 'Y' VALUES.
         N - NUMBER OF ENTRIES IN THE TABLE. (DIMENSION OF XT AND YT
             MUST BE AT LEAST N)
         Y - COMPUTED VALUE OF DEPENDENT VARIABLE CORRESPONDING TO X.

.........................................................................
                                                                        */
TLUV:       PROCEDURE(XT,YT,X,Y);
            DECLARE (LO,UP,DIF,MID,K,N)   FIXED BINARY (31),
            (X,Y(299),XT(11),YT(299,11)) FLOAT DEC(16),
            (W(10),C(4)) FLOAT DECIMAL (16) STATIC;
            N=11;
            LO=1;
            UP=N;
            MID=1;
            IF X > XT(N) THEN DO;
            PUT EDIT ('X-OUT IN TLU, X=',X,'XT(N)=',XT(N))
                     (SKIP(3),X(3),A,E(13,6),X(2),A,E(13,6));
            GO TO START;
            MID=N-1;
            GOTO BSTEP;
            END;
            IF X < XT(1) THEN DO;
            PUT EDIT ('X-OUT IN TLU, X=',X,'XT(1)=',XT(1))
                     (SKIP(3),X(3),A,E(13,6),X(2),A,E(13,6));
            GO TO START;
            MID=3;
            GOTO BSTEP;
```

```
            END;
ASTEP:      DIF=UP-LO;
            IF DIF > 2 THEN MID=(UP+LO+1)/2;
            ELSE IF DIF = 0 THEN GOTO BSTEP;
            ELSE MID=LO+1;
            IF X = XT(MID) THEN GOTO BSTEP;
            IF X > XT(MID) THEN DO;
            LO=MID;
            GOTO ASTEP;
            END;
            IF X = XT(MID-1) THEN DO;
            MID=MID-1;
            GOTO BSTEP;
            END;
            IF X < XT(MID-1) THEN DO;
            UP=MID;
            GOTO ASTEP;
            END;
BSTEP:      K=MID-2;
            IF K < 1 THEN K=1;
            IF (K+3) > N THEN K=N-3;
            W(1)=X-XT(K);
            W(2)=X-XT(K+1);
            W(3)=X-XT(K+2);
            W(4)=X-XT(K+3);
            W(5)=XT(K)-XT(K+1);
            W(6)=XT(K)-XT(K+2);
            W(7)=XT(K)-XT(K+3);
            W(8)=XT(K+1)-XT(K+2);
            W(9)=XT(K+1)-XT(K+3);
            W(10)=XT(K+2)-XT(K+3);
            DO I=1 TO 299;
            C(1)=YT(I,K)/(W(5)*W(6)*W(7));
            C(2)=-YT(I,K+1)/(W(5)*W(8)*W(9));
            C(3)=YT(I,K+2)/(W(6)*W(8)*W(10));
            C(4)=-YT(I,K+3)/(W(7)*W(9)*W(10));
             Y(I)=C(1)*W(2)*W(3)*W(4)
               +C(2)*W(1)*W(3)*W(4)
               +C(3)*W(1)*W(2)*W(4)
               +C(4)*W(1)*W(2)*W(3);
            END;
            RETURN;
            END TLUV;
      ON CONVERSION BEGIN;
      PUT FILE (SYSPRINT) EDIT ('INPUT CONVERSION ERROR IN I= ',I,
      ONCHAR,ONSOURCE)
        (SKIP (5) ,A,X(3),F(3),X(3),A,X(2),A); ONCHAR='0';  END;
   GET FILE(TABLES) EDIT((I,PAGE1(I),Z(I),DHA(I),GFW(I) DO J=0 TO 161))
```

```
        (F(3),X(1),A(8),X(1),F(2),X(1),F(3,1),X(1),F(8,4),SKIP );
      GET FILE(TABLES) EDIT((I,PAGE2(I),LKT(I,* ) DO J=1 TO 299))
   (SKIP,F(3),X(1),A(8),7(X(1),F(7,2)),SKIP,X(13),4(F(7,2),X(1)));
      GET FILE(TABLES) EDIT((I,GAMACO2(I,* ) DO J=0 TO 3))
   (SKIP,F(1),10(X(1),F(4,2)));
      GET FILE(TABLES) EDIT((BDAT(I) DO I=1 TO 10))
   (SKIP,10(F(5,3),X(1)));
      GET FILE(TABLES) EDIT((TK(I) DO I=1 TO 11))
   (SKIP,F(3,1),3(X(1),F(4,1)),7(X(1),F(5,1)));
      GET FILE(TABLES) EDIT((ICO2(I) DO I=1 TO 10))
   (SKIP,F(3,1),2(X(1),F(4,1)),7(X(1),F(5,1)));
      OPEN FILE(SYSPRINT)PRINT LINESIZE(132);
      ON ENDFILE (SYSIN) GO TO EOF;
      ON CONVERSION BEGIN;
      PUT FILE (SYSPRINT) EDIT ('INPUT CONVERSION ERROR',ONCHAR,
      ONSOURCE) (PAGE,A,X(2),A,X(2),A)
         ((CARD(I) DO I=1 TO N)) (SKIP,A);
      GO TO START; END;
      C=2.302585; F=23.0603; R=1.98719E-3;
START: CUNITS,ALFA,M=0E0;
      EHM,EHMC,EMFZSCE =9E0;
      N=1;DENS=1E0;    LOGKT=0E0;    KT=0E0;
     RATIO,INFORM,FLAG1,FLAG2,FLAG3,FLAG4,FLAG5=0;
CREED: GET FILE(SYSIN) EDIT (CARD(N))(A(80));
         IF CARD(N)¬=' ' THEN DO;
         N=N+1; GO TO CREED; END;
      N=N-1;       LONG='';
      DO  I=2 TO 6; LONG=LONG||CARD(I);   END;
         DO I=0 TO 6,11,12,13,14,15,17,20,21,22,24,25,26,27,28,29,30,
      31,32,97,135;
      CUNITS(I)=999999E0;        END;
      GET STRING(LONG) EDIT (TEMP,PH,EHM,FLAG,(CUNITS(I)
         DO I=0 TO 6,11,12,13,14,15,17,20,21,22,24,25,26,27,28,29,30,
  31,32,97,135))(E(6,1),X(1),E(6,2),X(1),E(8,3),X(1),A(5),X(52),
      8(E(8,3),X(1)),X(8),8(F(8,3),X(1)),X(8),8(E(8,3),X(1)),X(8),
      3(E(8,3),X(1)));
      IF CUNITS(I)>6.0E5 THEN DO;
         PUT EDIT('INSUFFICIENT NUMBER OF INPUT DATA ITEMS IN THE',
                  'FOLLOWING SET:') (PAGE,2 A)
         ((CARD(I) DO I=1 TO N)) (SKIP,A);
      GO TO START; END;
 /*CALLING THE LOGKT VALUES WHICH ARE INTERPOLATED BY LAGRANGE SUBROUT-
     INE FROM A LOGKT VS TEMPERATURE TABLE                              */
       CALL TLUV(TK,LKT,TEMP,LOGKT);
      LONG='';
      DO  I=7 TO N; LONG=LONG||CARD(I);   END;
        IF  N>6 THEN GET STRING(LONG)DATA;
      DO I=1 TO 136;
```

```
      IF LOGKT(I) <-7.0E1  THEN   LOGKT(I)=-7.0E1;
      IF LOGKT(I) > 2.0E2  THEN   LOGKT(I)=2.0E1;
    KT(I) =1E1**(LOGKT(I));              END;
/* PRINT OF TABLES. LOG(KT),LIST OF AQUEOUS SPECIES,GAMMA CO2 & BDOT.
       IF PRINT OUT OF TABLES NOT REQUIRED PUT INFORM=1   */
      IF INFORM=0 THEN DO;
      PUT SKIP EDIT('**  TABLE OF LOG(KT) FOR THE AQUEOUS COMPLEXES &',
    ' MINERALS  **') (X(40) ,2 A);
      PUT SKIP (2);
 PUT SKIP EDIT('I','PAGE2','0C','25C','50C','75C','100C','125C','150C',
        '200C','250C','300C','350C')(X(1),A,X(4),A,X(6),4(A,X(8)),
                                     6(A,X(7)),A);
      PUT SKIP (2);
           DO I=1 TO 299;
      PUT SKIP EDIT(I,PAGE2(I),LKT(I,* ))(F(3),X(1),A,X(2),F(7,2),
       10(X(4),F(7,2)));
      END;
      PUT PAGE EDIT ('* LIST OF AQUEOUS SPECIES *',
      '**  GAMMA CO2 AS A FUNCTION OF TEMP. & EQ. NACL  **')(X(3),A,
      X(30),A);
   PUT SKIP(3) EDIT ('I','PAGE1','Z','DHA','GFW','EMNACL','0C','25C',
                '50C','100C','150C','200C','250C','270C','300C','350C')
                     (X(1),A,X(3),A,X(6),A,X(2),A,X(5),A,X(15),A,X(3),
                      A,X(4),2(A,X(3)),7(A,X(2)),A);
      PUT SKIP (2);
      DO I=0 TO 161;
      PUT SKIP EDIT (I,PAGE1(I),Z(I),DHA(I),GFW(I))
                     (F(3),X(2),A,F(4),F(5,1),F(11,5));
       IF I<4 THEN PUT EDIT(I,GAMACO2(I,* )) (COL(47),F(2),X(3),
       10 F(6,2));
       END;
      PUT SKIP (3) EDIT('BDOT=')(COL(40),A);
      DO I=1 TO 10;
      PUT EDIT(BDAT(I)) (F(7,3));
      END;            END;
/* CALCULATION OF EH FROM FIELD DATA  */
      IF EMFZSCE=9E0 THEN C1=.2145E0-7.6E-4*(TEMP-25E0);
         ELSE C1=4.28E-1-2.2E-3*(TEMP-25E0)-EMFZSCE;
      IF EHMC <9E0
         THEN EHM = EHMC+C1 ;
/* CALCULATION OF ANALYZED MOLALITY  */
         C3=0E0; DO I=0 TO 161;
         IF FLAG='PPM  ' THEN C3=C3+1E-6*CUNITS(I)*DENS;
         ELSE IF FLAG='MG/L ' THEN C3=C3+1E-6*CUNITS(I);
         ELSE IF FLAG ='MOL/L' THEN C3=C3+1E-3*CUNITS(I)*GFW(I);
         ELSE IF FLAG='MEQ/L' & Z(I)¬=0 THEN
          C3=C3+1E-6*CUNITS(I)*GFW(I)/ABS(Z(I)); END;
      IF FLAG='PPM  ' THEN M=1E-3*CUNITS*DENS/(GFW*(DENS-C3));
```

```
      ELSE IF FLAG='MG/L ' THEN M=1E-3*CUNITS/(GFW*(DENS-C3));
      ELSE IF FLAG='MOL/L' THEN M=CUNITS/(DENS-C3);
      ELSE IF FLAG='MEQ/L' THEN DO I=0 TO 161;
         IF Z(I)¬=0 THEN M(I)=1E-3*CUNITS(I)/(ABS(Z(I))*(DENS-C3));END;
         ANALM = M; EPMCAT,EPMAN =0E0;
/* CALCULATION OF CATION-ANION BALANCE */
      DO I=0 TO 161;
         IF Z(I)>0 THEN EPMCAT = EPMCAT+Z(I)* M(I) ;
         ELSE EPMAN = EPMAN-Z(I)*M(I)  ; END;
      EPMCAT=EPMCAT*(DENS-C3);
      EPMAN =EPMAN *(DENS-C3);
/* TEMP. EFFECTS ON DEBYE-HUCKEL SOLVENT CONSTANTS  */
      S1  = 374.11E0-TEMP;
      S2  = S1**.333333E0 ;
      S3  = SQRT((1E0+.1342489E0*S2-3.946263E-3*S1)/(3.1975E0-
            .3151548E0*S2-1.203374E-3*S1+7.48908E-13*S1**4));
      T=TEMP+273.16E0;
      IF T < 373.16E0
         THEN C1=87.74E0-TEMP*(TEMP*(1.41E-6*TEMP-9.398E-4)+ .4008E0);
         ELSE C1=5321E0/T+233.76E0-T*(T*(8.292E-7*T-1.417E-3)+.9297E0);
      C1 =SQRT(C1*T);
      A  =  18246E2*S3/C1**3 ;
      B  =  50.29*S3/C1 ;
/*          ***  CALCULATION OF PH2O  ***    */
PH2OC1=-1.87E0+3.74E0*(1.152894E0-.745794E0*LOG(654.2906E0/(TEMP+
266.778E0)+SQRT((654.2906E0/(TEMP+266.778E0))**2-1E0))) ;
PH2OC2=PH2OC1**2*(3.4969E0-PH2OC1**2)/(.30231574E0+.3377565E-2*TEMP) ;
LOG10PH2O=1.0642332E0+4.16385282E0*(TEMP-187E0)/(TEMP+237.098157E0)-
1.0137921E0*(1E0+5.83531E-4*TEMP)*3.97307778E-3*((1E-2*TEMP-1.87E0)-
1E-2*PH2OC2)*(3.4969E0-(1E-2*TEMP-1.87E0-1E-2*PH2OC2)**2) ;
PH2O= 10E0**LOG10PH2O ;
/* INITIALIZE STARTING VALUES FOR ITERATIVE LOOP AND CONSTANT GAMMAS */
      CATOT=M(0); MGTOT=M(1); NATOT=M(2);
      KTOT=M(3); CLTOT=M(4); SO4TOT,SO4ITR=M(5);
      HCO3TOT=M(6); SITOT=M(11); AGTOT=M(12);
      ALTOT=M(13); BATOT=M(14); CUTOT=M(15);
      FETOT=M(17); HGTOT=M(20); LITOT=M(21);
      MNTOT=M(22); PBTOT=M(24); SRTOT=M(25);
      ZNTOT=M(26); ASTOT=M(27); PTOT,PITR=M(28);
      FTOT=M(29); BTOT=M(30) ;    NH3TOT=M(31);
      H2STOT=M(32); CO2TIT,CO2TOT=M(6)+M(97);
      TENPH=1E1**(-PH);
      PUT PAGE EDIT (CARD(1)) (A);
  PUT SKIP EDIT('ITER','S1-ANALCO3','S2-ANALSO4','S3-ANALF',
      'S4-ANALPO4','S5-ANALCL')
         (SKIP(2),X(2),A,X(9),A,X(10),A,3(X(11),A));
      ITER=0; RBIT='1'B; DO WHILE(RBIT); ITER=ITER+1;
 /*CALC. OF TOTAL MOLALITY & AH2O  */
```

```
      C1=0E0; DO I=0 TO 8,10,12 TO 30,32 TO 161;
      C1=C1+M(I); END;
      AH2O=1E0-1.7E-2*C1; LH2O=LOG10(AH2O);
/* THE FOLLOWING ROUTINE ESTIMATES THE GAMMA OF CO2 BY LINEAR INTERPO-
   LATION BETWEEN THE KNOWN VALUES OF GAMMA CO2 GIVEN AS A FUNCTION OF
   TEMPERATURE AND EQUIVALENT MNACL(NACLE) */
/* CALCULATION OF THE IONIC STRENGTH (I), EQUIVALENT MNACLE=I*/
      MU=0E0;
      DO I=0 TO 161;
      MU=MU+M(I)*Z(I)**2;
      END;
      MU=.5E0*MU;
      MUHALF=SQRT(MU);
      MNACLE=MU;
      IF MNACLE>3.0E0 THEN MNACLE=3.0E0;
      G=GAMACO2;
      MJ=TRUNC(MNACLE);
      DO I=1 TO 10;
      IF TEMP> TCO2(I)  THEN
         GO TO SKIP;
      IF TEMP=TCO2(I) THEN
         DO;   GT1=G(MJ,I);        GT2=G(MJ+1,I); MJ=MJ+1;     END;
      IF TEMP=TCO2(I) THEN GO TO OUTB;
      GT1=G(MJ,I-1)+(TEMP-TCO2(I-1))*(G(MJ,I)-G(MJ,I-1)) / (TCO2(I)-
        TCO2(I-1));
      GO TO OUT;
SKIP: END;
OUT: MJ=MJ+1;
      GT2=G(MJ,I-1)+(TEMP-TCO2(I-1))*(G(MJ,I)-G(MJ,I-1))/(TCO2(I)-
          TCO2(I-1));
OUTB:  GTM=GT1+(MNACLE-(MJ-1))*(GT2-GT1);
/* CALCULATION OF ACTIVITY COEFFICIENTS. GAMMA FOR NEUTRAL SPECIES=
   GAMMA CO2,THEY ARE =1.0 IF FLAG1=1.GAMMA FOR CHARCHED SPECIES IS BY
   BDOT METHOD,HELGESON,1969. */
      IF TEMP > 300E0 THEN
         BDOT = 0E0;
      ELSE DO J = 1 TO 9;
      IF TEMP = TCO2(J) THEN
         BDOT = BDAT(J);
      ELSE IF TEMP > TCO2(J) THEN GO TO ADD;
       ELSE BDOT = BDAT(J-1)+(TEMP-TCO2(J-1))*(BDAT(J)-BDAT(J-1))/
                 (TCO2(J)-TCO2(J-1));
      GO TO CONTINU ;
ADD:  END;
CONTINU:  DO I=0 TO 161;
      IF Z(I)¬=0 THEN
         GAMMA(I)=1E1**(-A*MUHALF*Z(I)**2/(1E0+DHA(I)*B*MUHALF)
         +BDOT*MU);
```

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 ELSE IF Z(I)=0 & FLAG1=0 THEN GAMMA(I)=GTM;
      ELSE IF Z(I)=0 & FLAG1=1 THEN GAMMA(I)=1E0;    END;
/* CALCULATION OF A NUMBER OF ANION ACTIVITIES */
      DO I=4,5,29,135;
         ALFA(I)=M(I)*GAMMA(I); END;
/* CO2 SPECIES  */
Y1:   IF CUNITS(6)<=0E1 & CUNITS(97)<=0E1 THEN GO TO Y2;
      M(6)=CO2TOT/(1E0+((GAMMA(6)*TENPH)/(KT(72)* GAMMA(96))+((KT(1)*
         GAMMA(6))/(GAMMA(97)* TENPH))));
      ALFA(6)=M(6)*GAMMA(6);
      M(97)=(KT(1)*ALFA(6))/(GAMMA(97)*TENPH);
      ALFA(97)=M(97)*GAMMA(97);
      M(96)=(ALFA(6)*TENPH)/(KT(72)*GAMMA(96)) ;
      ALFA(96)=M(96)*GAMMA(96);
/* SULPHUR SPECIES  */
Y2:   IF CUNITS(32) <=0E1 THEN GO TO Y3;
      M(100)=H2STOT/(1E0+((GAMMA(100)*TENPH)/(KT(10)*GAMMA(32))+
               ((KT(75)*GAMMA(100))/(GAMMA(101)*TENPH))));
      ALFA(100)=GAMMA(100)*M(100);
      M(32)=(ALFA(100)*TENPH)/(KT(10)*GAMMA(32));
      ALFA(32)=GAMMA(32)*M(32);
      M(101)=(KT(75)*ALFA(100))/(GAMMA(101)*TENPH);
      ALFA(101)=M(101)*GAMMA(101);
Y3:   IF CUNITS(5) <=0E1 THEN GO TO Y4;
       M(102)=SO4ITR/(1E0+(((KT(76)*GAMMA(102))/(GAMMA(5)*TENPH))));
      ALFA(102)=M(102)*GAMMA(102);
      M(5)=(KT(76)*ALFA(102))/(GAMMA(5)*TENPH);
      ALFA(5)=M(5)*GAMMA(5);
/* SILICA SPECIES  */
Y4:   IF CUNITS(11) <=0E1 THEN GO TO Y5;
      M(90)=SITOT/(1E0+((GAMMA(90)*TENPH)/(KT(3)*GAMMA(10))+((KT(66)
         *GAMMA(90))/(GAMMA(89)*TENPH))));
      ALFA(90)=GAMMA(90)*M(90);
      M(10)=(ALFA(90)*TENPH)/(KT(3)*GAMMA(10));
      ALFA(10)=M(10)*GAMMA(10);
      M(89)=(KT(66)*ALFA(90))/(GAMMA(89)*TENPH);
      ALFA(89)=M(89)*GAMMA(89);
  /*   ACTIVITY OF OH,H+,HF,   AND HNO3          */
Y5:   ALFA(8)=(AH2O*KT(2))/TENPH;
      M(8)=ALFA(8)/GAMMA(8);
      M(7)=TENPH/GAMMA(7);
      ALFA(7)=TENPH;
      M(95)=(TENPH*ALFA(29))/(GAMMA(95)*KT(71));
      ALFA(95)=M(95)*GAMMA(95);
       M(103)=(TENPH*ALFA(135))/(GAMMA(103)*KT(77));
      IF ITER=1  THEN   M(135)=M(135)-M(103);
      ALFA(103)=M(103)*GAMMA(103);
/* BORON SPECIES */
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      IF CUNITS(30) <=0E1 THEN GO TO Y6;
       M(30)=BTOT/(1E0+((GAMMA(30)*ALFA(8))/(KT(64)*GAMMA(88))));
       ALFA(30)=M(30)*GAMMA(30);
       M(88)=(ALFA(30)*ALFA(8))/(KT(64)*GAMMA(88));
       ALFA(88)=M(88)*GAMMA(88);
/* PHOSPHATE SPECIES  */
Y6:   IF CUNITS(28) <=0E1 THEN GO TO Y7;
       M(98)=PITR/(1E0+((GAMMA(98)*TENPH)/(KT(74)*GAMMA(99))+((KT(73)*
             GAMMA(98))/(GAMMA(28)*TENPH))));
       ALFA(98)=M(98)*GAMMA(98);
       M(99)=(ALFA(98)*TENPH)/(KT(74)*GAMMA(99));
       M(28)=(KT(73)*ALFA(98))/(GAMMA(28)*TENPH);
       ALFA(99)=M(99)*GAMMA(99);
       ALFA(28)=M(28)*GAMMA(28);
/* NITROGEN SPECIES */
Y7:   IF CUNITS(31) <=0E1 THEN GO TO Y8;
       M(144)=ALFA(8)/(KT(118)*GAMMA(144));
       M(145)=ALFA(28)/(KT(119)*GAMMA(145));
       M(146)=ALFA(5)/(KT(120)*GAMMA(146));
       M(143)=NH3TOT/(1E0+GAMMA(143)*(M(144)+M(145)+M(146)));
       ALFA(143),C1= M(143)*GAMMA(143);
       DO I=144 TO 146;
       M(I)=M(I)*C1;
       ALFA(I)=M(I)*GAMMA(I); END;
/* CA SPECIES  */
Y8:   IF CUNITS(0) <=0E1  THEN GO TO Y9;
       M(54)=ALFA(97)/(KT(30)*GAMMA(54));
       M(55)=ALFA(6)/(KT(31)*GAMMA(55));
       M(56)=ALFA(8)/(KT(32)*GAMMA(56));
       M(57)=ALFA(28)/(KT(33)*GAMMA(57));
       M(58)=ALFA(98)/(KT(34)*GAMMA(58));
       M(59)=ALFA(99)/(KT(35)*GAMMA(59));
       M(60)=ALFA(5)/(KT(36)*GAMMA(60));
       M(0)=CATOT /(1E0+GAMMA(0)*(M(54)+M(55)+M(56)+M(57)+M(58)+M(59)+
          M(60)));
       ALFA(0),C1=M(0)*GAMMA(0);
       DO I=54 TO 60;
       M(I)=C1*M(I);
       ALFA(I)=M(I)*GAMMA(I);
       END;
/* MG SPECIES  */
Y9:   IF CUNITS(1) <=0E1  THEN GO TO Y10;
       M(119)=ALFA(97)/(KT(93)*GAMMA(119));
       M(120)=ALFA(6)/(KT(94)*GAMMA(120));
       M(121)=ALFA(29)/(KT(95)*GAMMA(121));
       M(122)=ALFA(8)/(KT(96)*GAMMA(122));
       M(123)=ALFA(5)/(KT(97)*GAMMA(123));
       M(124)=ALFA(28)/(KT(98)*GAMMA(124));
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      M(125)=ALFA(98)/(KT(99)*GAMMA(125));
      M(126)=ALFA(99)/(KT(100)*GAMMA(126));
      M(1)=MGTOT/(1E0+GAMMA(1)*(M(119)+M(120)+M(121)+M(122)+M(123)+
           M(124)+M(125)+M(126)));
      ALFA(1),C1=M(1)*GAMMA(1);
      DO I=119 TO 126;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);
      END;
/* NA SPECIES  */
Y10: IF CUNITS(2) <=0E1  THEN GO TO Y11;
      M(136)=ALFA(4)/(KT(110)*GAMMA(136));
      M(137)=ALFA(97)/(KT(111)*GAMMA(137));
      M(138)=ALFA(6)/(KT(112)*GAMMA(138));
      M(139)=(M(2)*GAMMA(2)*ALFA(97))/(KT(113)*GAMMA(139));
      M(140)=(M(2)*GAMMA(2)*ALFA(5))/(KT(114)*GAMMA(140));
      M(141)=ALFA(5)/(KT(115)*GAMMA(141));
      M(142)=ALFA(98)/(KT(116)*GAMMA(142));
      M(2)=NATOT/(1E0+GAMMA(2)*(M(136)+M(137)+M(138)+M(139)+M(140)+
                                M(141)+M(142)));
         ALFA(2),C1=M(2)*GAMMA(2);
      DO I=136 TO 142;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I); END;
/* K SPECIES  */
Y11: IF CUNITS(3) <=0E1  THEN GO TO Y12;
      M(112)=ALFA(4)/(KT(86)*GAMMA(112));
      M(114)=ALFA(102)/(KT(88)*GAMMA(114));
      M(115)=ALFA(5)/(KT(89)*GAMMA(115));
      M(116)=ALFA(98)/(KT(90)*GAMMA(116));
      M(3)=KTOT/(1E0+GAMMA(3)*(M(112)+M(114)+M(115)+M(116)));
      ALFA(3),C1=M(3)*GAMMA(3);
      DO I=112,114 TO 116;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I); END;
/* AG SPECIES */
Y12: IF CUNITS(12) <=0E1 THEN GO TO Y13;
      M(42)=ALFA(4)/(KT(20)*GAMMA(42));
      M(43)=ALFA(4)**2/(KT(21)*GAMMA(43));
      M(44)=ALFA(4)**3/(KT(22)*GAMMA(44));
      M(45)=ALFA(4)**4/(KT(23)*GAMMA(45));
      M(46)=ALFA(5)/(KT(24)*GAMMA(46));
      M(47)=ALFA(5)**2/(KT(25)*GAMMA(47));
      M(12)=AGTOT/(1E0+GAMMA(12)*(M(42)+M(43)+M(44)+M(45)+M(46)+
                                  M(47)));
      ALFA(12),C1=M(12)*GAMMA(12);
      DO I=42 TO 47;
      M(I)=M(I)*C1;
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      ALFA(I)=M(I)*GAMMA(I); END;
/* AL SPECIES  */
Y13: IF CUNITS(13) <=0E1 THEN GO TO Y14;
      M(33)=ALFA(29)/(KT(11)*GAMMA(33));
      M(34)=ALFA(29)**2/(KT(12)*GAMMA(34));
      M(35)=ALFA(29)**3/(KT(13)*GAMMA(35));
      M(36)=ALFA(29)**4/(KT(14)*GAMMA(36));
      M(37)=ALFA(8)/(KT(15)*GAMMA(37));
      M(38)=ALFA(8)**2/(KT(16)*GAMMA(38));
      M(39)=ALFA(8)**4/(KT(17)*GAMMA(39));
      M(40)=ALFA(5)/(KT(18)*GAMMA(40));
      M(41)=ALFA(5)**2/(KT(19)*GAMMA(41));
      M(13)=ALTOT/(1E0+GAMMA(13)*(M(33)+M(34)+M(35)+M(36)+M(37)+M(38)
         +M(39)+M(40)+M(41)));
      ALFA(13),C1=M(13)*GAMMA(13);
      DO I=33 TO 41;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);  END;
/* FE SPECIES  */
Y14: IF CUNITS(17) <=0E1 THEN GO TO Y15;
      M(70)=ALFA(4)/(KT(46)*GAMMA(70));
      M(71)=ALFA(4)**2/(KT(47)*GAMMA(71));
      M(72)=ALFA(4)**3/(KT(48)*GAMMA(72));
      M(73)=ALFA(4)**4/(KT(49)*GAMMA(73));
      M(74)=ALFA(8)/(KT(50)*GAMMA(74));
      M(75)=ALFA(8)**2/(KT(51)*GAMMA(75));
      M(76)=AH2O/(KT(52)*TENPH**3*GAMMA(76));
      M(77)=ALFA(5)/(KT(53)*GAMMA(77));
/* IF FE+3 IS TO BE CALCULATED FROM EH MEASUREMENTS THEN PUT FLAG2=1,
   IF FROM THE REACTION FE+3 + 1/2H2O +1/8HS- =FE++ +1/8SO4 +9/8H+ THEN
   FLAG2=0 */
      IF EHM <9E0 & FLAG2=1 THEN    DO;
      C1=1E1**((EHM*F-LOGKT(296))/(2.303*R*T));
         M(18)=C1 / GAMMA(18);        END;
      ELSE IF CUNITS(32)=0E1 THEN   M(18)=0E1;
      ELSE IF FLAG2 =0 THEN
         M(18)=(ALFA(5)**.125*TENPH**1.125)/(KT(5)*SQRT(AH2O)*
         ALFA(100)**.125*GAMMA(18));
      M(78)=ALFA(4)/(KT(54)*GAMMA(78));
      M(79)=ALFA(4)**2/(KT(55)*GAMMA(79));
      M(80)=ALFA(4)**3/(KT(56)*GAMMA(80));
      M(81)=ALFA(4)**4/(KT(57)*GAMMA(81));
      M(82)=ALFA(5)/(KT(58)*GAMMA(82));
      M(83)=ALFA(5)**2/(KT(59)*GAMMA(83));
      M(84)=ALFA(8)/(KT(60)*GAMMA(84));
      M(85)=ALFA(8)**2/(KT(61)*GAMMA(85));
      M(86)=ALFA(8)**3/(KT(62)*GAMMA(86));
      M(87)=ALFA(8)**4/(KT(63)*GAMMA(87));
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      DO I=78 TO 87;
      M(I)=M(I)*M(18)*GAMMA(18); END;
      M(17)=FETOT/(1E0+GAMMA(17)*(M(18)+M(70)+M(72)+M(73)+M(74)+M(71)
          +M(75)+M(76)+M(77)+M(78)+M(79)+M(80)+M(81)+M(82)+M(83)+M(84)
          +M(85)+M(86)+M(87)));
      ALFA(17),C2=M(17)*GAMMA(17);
      DO I=18,70 TO 87;
      M(I)=M(I)*C2;
         ALFA(I)=M(I)*GAMMA(I); END;
/* BA SPECIES  */
Y15: IF CUNITS(14) <=0E1 THEN GO TO Y16;
      M(50)=ALFA(7)/(KT(26)*GAMMA(50));
      M(51)=ALFA (6)/(KT(27)*GAMMA(51));
      M(52)=ALFA(8)/(KT(28)*GAMMA(52));
      M(53)=ALFA(5)/(KT(29)*GAMMA(53));
      M(14)=BATOT/(1E0+GAMMA(14)*(M(50)+M(51)+M(52)+M(53)));
      ALFA(14),C1=M(14)*GAMMA(14);
      DO I=50 TO 53;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I); END;
/* CU SPECIES  */
Y16: IF CUNITS(15) <=0E1 THEN GO TO Y17;
      M(61)=ALFA(4)/(KT(37)*GAMMA(61));
      M(62)=ALFA(4)**2/(KT(38)*GAMMA(62));
      M(63)=ALFA(4)**3/(KT(39)*GAMMA(63));
/* IF CU++ IS TO BE CALCULATED FROM EH MEASUREMENTS THEN FLAG3=1, IF
   FROM CU++ +FE++ = CU+ +FE+3, THEN FLAG3=0 */
         IF EHM <9E0 & FLAG3=1 THEN  DO;
      C1=1E1**((EHM*F-LOGKT(297))/(2.303*R*T));
      M(16)=C1/GAMMA(18);          END;
      ELSE IF CUNITS(32)=0E1 THEN M(16)=0E1;
      ELSE IF CUNITS(17)=0E1 THEN M(16)=0E1;
      ELSE IF FLAG3=0 THEN
      M(16)=ALFA(18)/(KT(4)*ALFA(17)*GAMMA(16));
      M(64)=ALFA(4)/(KT(40)*GAMMA(64));
      M(65)=ALFA(4)**2/(KT(41)*GAMMA(65));
      M(66)=ALFA(4)**3/(KT(42)*GAMMA(66));
      M(67)=ALFA(4)**4/(KT(43)*GAMMA(67));
      M(68)=ALFA(8)/(KT(44)*GAMMA(68));
      M(69)=ALFA(5)/(KT(45)*GAMMA(69));
      DO I=64 TO 69;
      M(I)=M(I)*M(16)*GAMMA(16); END;
      M(15)=CUTOT/(1E0+GAMMA(15)*(M(16) +M(61)+M(62)+M(63)+M(64)+M(65)+
                                  M(66)+M(67)+M(68)+M(69)));
      ALFA(15),C2=M(15)*GAMMA(15);
      DO I=16,61 TO 69;
      M(I)=M(I)*C2;
      ALFA(I)=M(I)*GAMMA(I); END;
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/* HG SPECIES  */
Y17: IF CUNITS(20) <=0E1 THEN GO TO Y18;
      M(104)=ALFA(4)/(KT(78)*GAMMA(104));
      M(105)=ALFA(4)**2/(KT(79)*GAMMA(105));
      M(106)=ALFA(4)**3/(KT(80)*GAMMA(106));
      M(107)=ALFA(4)**4/(KT(81)*GAMMA(107));
      M(108)=ALFA(5)/(KT(82)*GAMMA(108));
      M(109)=(ALFA(32)**2*ALFA(100))/(KT(83)*GAMMA(109)*TENPH);
      M(110)=ALFA(100)**3/(KT(84)*GAMMA(110));
      M(111)=ALFA(100)**3/(KT(85)*GAMMA(111)*TENPH);
      M(113)=ALFA(100)**2/(KT(87)*GAMMA(113)*TENPH**2);
      KT(6)=-KT(6);
/* IF HG++ IS TO BE CALCULATED FROM EH THEN FAG4=1,IF FROM 2HG++ +2FE++
   =HG2++ +2FE+3 THEN FLAG4=0 */
      IF EHM<9E0 & FLAG4=1 THEN DO;
      C1=1E1**(((EHM*F-LOGKT(298))*2)/(2.303*R*T));
        M(19)=C1*M(20)*GAMMA(20)/GAMMA(19);        END;
      ELSE IF CUNITS(32)=0E1 THEN M(19)=0E1;
      ELSE IF CUNITS(17)=0E1 THEN M(19)=0E1;
      ELSE IF FLAG4=0 THEN
     M(19)=(GAMMA(19)*ALFA(18)**2)/(KT(6)*M(20)*GAMMA(20)*ALFA(17)**2);
      M(20)=HGTOT/(1E0+GAMMA(20)*(M(19)+M(104)+M(105)+M(106)+M(107)+
        M(108)+M(109)+M(110)+M(111)+M(113)));
      ALFA(20),C2=M(20)*GAMMA(20);
      DO I=19,104 TO 111,113;
      M(I)=M(I)*C2;
      ALFA(I)=M(I)*GAMMA(I);       END;
/* LI SPECIES   */
Y18: IF CUNITS(21) <=0E1 THEN GO TO Y19;
      M(117)=ALFA(8)/(KT(91)*GAMMA(117));
      M(118)=ALFA(5)/(KT(92)*GAMMA(118));
      M(21)=LITOT/(1E0+GAMMA(21)*(M(117)+M(118)));
      ALFA(21),C1=M(21)*GAMMA(21);
      DO I=117 TO 118;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);  END;
/* MN SPECIES   */
Y19: IF CUNITS(22) <=0E1 THEN GO TO Y20;
      M(127)=ALFA(4)/(KT(101)*GAMMA(127));
      M(128)=ALFA(4)**2/(KT(102)*GAMMA(128));
      M(129)=ALFA(4)**3/(KT(103)*GAMMA(129));
      M(130)=ALFA(4)**4/(KT(104)*GAMMA(130));
      M(131)=ALFA(6)/(KT(105)*GAMMA(131));
      M(132)=ALFA(5)/(KT(106)*GAMMA(132));
/* IF MN+++ IS TO BE CALCULATED FROM EH THEN FLAG5=1, IF FROM MN+++ +
   FE++ = MN++ +FE+3 THEN FLAG5=0 */
      IF EHM < 9E0 & FLAG5=1 THEN DO;
      C1=1E1**((EHM*F-LOGKT(299))/(2.303*R*T));
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      M(23)=C1/GAMMA(22);          END;
      ELSE IF CUNITS(32)=0E1 THEN M(23)=0E1;
      ELSE IF CUNITS(17)=0E1 THEN M(23)=0E1;
         ELSE IF FLAG4=0 THEN
      M(23)=ALFA(18)/(KT(7)*ALFA(17)*GAMMA(23));
      M(133)=ALFA(4)/(KT(107)*GAMMA(133));
      M(134)=ALFA(4)**2/(KT(108)*GAMMA(134));
      DO I=133 TO 134;
      M(I)=M(I)*M(23)*GAMMA(23);  END;
      M(22)=MNTOT/(1E0+GAMMA(22)*(M(23)+M(127)+M(128)+M(129)+M(130)+
                M(131)+M(132)+M(133)+M(134)));
      ALFA(22),C2=M(22)*GAMMA(22);
      DO I=23,127 TO 134;
      M(I)=M(I)*C2;
      ALFA(I)=M(I)*GAMMA(I); END;
/* PB SPECIES    */
Y20: IF CUNITS(24) <=0E1 THEN GO TO Y21;
      M(147)=ALFA(4)/(KT(121)*GAMMA(147));
      M(148)=ALFA(4)**2/(KT(122)*GAMMA(148));
      M(149)=ALFA(4)**3/(KT(123)*GAMMA(149));
      M(150)=ALFA(4)**4/(KT(124)*GAMMA(150));
      M(151)=ALFA(5)/(KT(125)*GAMMA(151));
      M(152)=ALFA(5)**2/(KT(126)*GAMMA(152));
      M(24)=PBTOT/(1E0+GAMMA(24)*(M(147)+M(148)+M(149)+M(150)+M(151)+
         M(152)));
      ALFA(24),C1=M(24)*GAMMA(24);
      DO I=147 TO 152;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);  END;
/* SR SPECIES    */
Y21: IF CUNITS(25) <=0E1 THEN GO TO Y22;
      M(153)=ALFA(8)/(KT(127)*GAMMA(153));
      M(154)=ALFA(97)/(KT(128)*GAMMA(154));
      M(155)=ALFA(6)/(KT(129)*GAMMA(155));
      M(156)=ALFA(5)/(KT(130)*GAMMA(156));
      M(25)=SRTOT/(1E0+GAMMA(25)*(M(153)+M(154)+M(155)+M(156)));
      ALFA(25), C1= M(25)*GAMMA(25);
      DO I = 153 TO 156;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);  END;
/* ZN SPECIES    */
Y22: IF CUNITS(26) <=0E1 THEN GO TO Y23;
      M(157)=ALFA(4)/(KT(131)*GAMMA(157));
      M(158)=ALFA(4)**2/(KT(132)*GAMMA(158));
      M(159)=ALFA(4)**3/(KT(133)*GAMMA(159));
      M(160)=ALFA(4)**4/(KT(134)*GAMMA(160));
      M(161)=ALFA(5)/(KT(135)*GAMMA(161));
      M(26)=ZNTOT/(1E0+GAMMA(26)*(M(157)+M(158)+M(159)+M(160)+M(161)));
```

```
      ALFA(26),C1=M(26)*GAMMA(26);
      DO I=157 TO 161;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I);    END;
/* AS SPECIES    */
Y23: IF CUNITS(27) <=0E1 THEN GO TO Y24;
      M(48)=KT(8)/ALFA(8)*GAMMA(48);
      M(91)=TENPH/(KT(67)*GAMMA(91));
         IF ALFA(17) ¬=0E1 THEN DO;
      M(49)=(ALFA(18)**2*ALFA(8)**4)/(ALFA(17)**2*GAMMA(49)); END;
      M(92)=TENPH/(KT(68)*GAMMA(92));
      M(93)=TENPH**2/(KT(69)*GAMMA(93));
      M(94)=TENPH**3/(KT(70)*GAMMA(94));
      DO I=92 TO 94;
      M(I)=M(I)*M(49)*GAMMA(49);    END;
      M(27)=ASTOT/(1E0+GAMMA(27)*(M(48)+M(91)+M(92)+M(93)+M(94)+
       M(49)));
      ALFA(27),C1=M(27)*GAMMA(27);
      DO I=48,49,91 TO 94;
      M(I)=M(I)*C1;
      ALFA(I)=M(I)*GAMMA(I); END;
/* SUMMATION OF ANION SPECIES    */
Y24:          S1=M(6)+M(97)+M(50)+M(51)+M(54)+M(55)+M(119)+M(120)
           +M(131)+M(137)+M(138)+M(139)+M(154)+M(155);
      S2=M(5)+M(40)+2*M(41)+M(46)+2*M(47)+M(53)+M(60)+M(69)+M(77)+M(82)
         +2*M(83)+M(102)+M(108)+2*M(109)+M(110)+2*M(111)+M(114)+
         M(115)+M(118)+M(123)+M(132)+M(140)+M(141)+M(146)+M(151)+
         M(156)+M(161)+2*M(152);
      S3=M(29)+M(33)+2*M(34)+3*M(35)+4*M(36)+M(121)+M(95);
      S4=M(28)+M(57)+M(58)+M(59)+M(98)+M(99)+M(116)+M(124)+M(125)+
        M(126)+M(142)+M(145);
      S5=M(4)+M(42)+2*M(43)+3*M(44)+4*M(45)+M(61)+2*M(62)+3*M(63)+M(64)
           +2*M(65)+3*M(66)+4*M(67)+M(70)+2*M(71)+3*M(72)+4*M(73)+M(78)
           +2*M(79)+3*M(80)+4*M(81)+M(104)+2*M(105)+3*M(106)+4*
         M(107)+M(127)+2*M(128)+3*M(129)+4*M(130)+M(133)+2*M(134)
                  +M(136)+M(147)+2*M(148)+3*M(149)+4*M(150)+M(157)+2*
         M(158)+3*M(159)+4*M(160);
      ANALCO3=CO2TIT-4E0*M(27)-3E0*M(28)-M(37)-2E0*M(38)-4E0*M(39)-3E0*
        M(48)-8E0*M(49)-M(52)-M(56)-M(68)-M(74)-2E0*M(75)-M(76)-M(84)
          -2E0*M(85)-3E0*M(86)-4E0*M(87)-M(88)-2E0*M(89)-M(90)-3E0*M(91)
            -7E0*M(92)-6*M(93)-5E0*M(94)-2E0*M(98)-M(99)-M(100)-2E0*
       M(101)-M(102)-M(117)-M(122)-M(144)-M(153);
/* ITERATION TESTS    */
      RBIT='0'B;
      IF S1¬> 0E0 THEN ANALCO3=0E0;
      ELSE IF ABS(S1-ANALCO3)>5E-3*ANALCO3 THEN DO;
   CO2TOT=.5E0*(M(6)+M(96)+M(97))*(1E0+ANALCO3/S1);
      RBIT='1'B; END;
```

```
      IF S2¬=0E0 THEN
      IF ABS(S2-SO4TOT)>5E-3*SO4TOT THEN DO;
      SO4ITR=SO4ITR-0.5*((S2-SO4TOT)/S2)*SO4ITR;
      RBIT='1'B;  END;
      IF S3 ¬=0E0 THEN
      IF ABS(S3-FTOT)>5E-3*FTOT THEN DO;
      M(29)=M(29)-0.5*((S3-FTOT)/S3)*M(29);
      RBIT='1'B;  END;
      IF S4¬=0E0 THEN
      IF ABS(S4-PTOT)>5E-3*PTOT THEN DO;
      PITR=PITR-0.5*((S4-PTOT)/S4)*PITR;
      RBIT='1'B;  END;
      IF ABS(S5-CLTOT)>5E-3*CLTOT  THEN DO;
      M(4)=M(4)-0.5*((S5-CLTOT)/S5)*M(4);
      RBIT='1'B;  END;
      PUT EDIT (ITER,S1-ANALCO3,S2-SO4TOT,S3-FTOT,S4-PTOT,S5-CLTOT)
      (SKIP,F(5),E(21,5),4 E(20,5));
/*  ITERATION MONITOR   */
      IF ITER >100 THEN RBIT='0'B;                END;
/* PRINT OF INPUT   */
      LONG=DATE;
      PUT PAGE EDIT(CARD(1),'DATE=')(A,X(9),A)((SUBSTR(LONG,N,2),'/'
         DO N=3,5),SUBSTR (LONG,1,2)) (A);
      PUT SKIP;
      IF EMFZSCE<9E0 THEN PUT EDIT('EMFZSCE=',EMFZSCE)(X(5),A,F(10.6));
      IF  FLAG='PPM  ' THEN PUT EDIT('DATA IN PPM')(X(5),A);
   ELSE IF FLAG='MG/L ' THEN PUT EDIT('DATA IN MG/L')(X(5),A);
      ELSE IF FLAG='MOL/L' THEN PUT EDIT('DATA IN MOLES/L')(X(5),A);
      ELSE IF FLAG='MEQ/L' THEN PUT EDIT('DATA IN MEQ/L')(X(5),A);
      PUT EDIT('ANAL MEQ/L CAT=',1E3*EPMCAT,'ANAL MEQ/L AN=',1E3*EPMAN)
                  (SKIP(1),A,F(10,4),X(3),A,F(10,4));
/* RECALCULATION OF CATION-ANION BALANCE   */
      EPMCAT,EPMAN=0E0;
      DO I=0 TO 161;
      IF Z(I)>0 THEN EPMCAT=EPMCAT+Z(I)*M(I);
      ELSE EPMAN=EPMAN-Z(I)*M(I);
         END;
      EPMCAT=EPMCAT*(DENS-C3);
      EPMAN =EPMAN *(DENS-C3);
/* CALCULATION OF PCO2  */
      PCO2=0E0;
      IF ALFA(96)>0E0 THEN
      PCO2=1E1**(LOG10(ALFA(96))-2385.73E0/T-1.5264E-2*T+14.0184E0+MU
         *(0.119-8.33E-4*TEMP+6.66E-6*TEMP**2));
/* PRINT OF SOLUTE DATA   */
      PUT EDIT('PH','EH','T','ION STRENGTH','PCO2 ATM','CO2 TOT',
         'PPM CO2 TOT',PH,EHM,TEMP,MU,PCO2,CO2TOT,4.401E4*CO2TOT)
         (SKIP(3),X(3),2(A,X(9)),A,X(5),A,X(8),A,X(5),A,X(7),A,SKIP,
      *
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      F(6,2),X(2),F(10,4),X(2),F(8,2),X(2),F(13,5),X(2),F(14,7),
     X(2),F(13,6),X(2),F(13,6))
    ('CALC MEQ/L CAT','CALC MEQ/L AN',PAGE1(9),'CO3CALC','PH2O ATM',
    'DENSITY','TDS MG/L',1E3*EPMCAT,1E3*EPMAN,AH2O,M(97),PH2O,DENS,
    1E6*C3) (SKIP(2),A,X(5),A,X(6),A,X(5),A,X(3),A,X(2),A,
      X(4),A,SKIP,F(12,3),X(7),F(12,3),
    F(11,4),E(17,4),2(F(9,4)),F(13,2))
    ('ION','ANAL PPM','CALC PPM','ANAL MG/L','CALC MG/L','ANAL MOLAL'
         ,'CALC MOLAL','ALFA' ,'GAMMA','P ION')(SKIP(2),X(8),A,X(9)
       ,A,X(6),4(A,X(4)),A,X(5),A,2(X(8),A));
    PUT SKIP (2);
    DO I=0 TO 161;
    IF ALFA(I)> 0E0 THEN C1=-LOG10(ALFA(I));
       ELSE C1=0E0;
    PUT SKIP EDIT(I,PAGE1(I),Z(I))(F(3),X(2),A(8),F(3));
    IF CUNITS(I)>0E0 & FLAG='PPM  ' THEN PUT EDIT(CUNITS(I))
        (F(13,4));
ELSE IF CUNITS(I)>0E0 & FLAG='MG/L ' THEN DO ;
    CU=CUNITS(I)/DENS;
    PUT EDIT (CU) (F(13,4));          END;
    S1=1E3*M(I)*GFW(I)*(DENS-C3)/DENS;
    IF S1>0E0 THEN PUT EDIT(S1) (COL(30),F(13,4));
    IF CUNITS(I)>0E0 & FLAG='MG/L ' THEN PUT EDIT(CUNITS(I))
      (COL(43),F(13,4));
ELSE IF CUNITS(I)>0E0 & FLAG='PPM  ' THEN DO ;
    CU=CUNITS(I)*DENS;
    PUT EDIT (CU) (COL(43),F(13,4));       END;
    S2=S1*DENS;
    IF S2>0E0 THEN PUT EDIT (S2) (COL(56),F(13,4));
    IF ANALM(I)>0E0 THEN PUT EDIT (ANALM(I))(COL(69),F(13,4));
    IF M(I)> 0E0 THEN PUT EDIT (M(I)) (COL(82),F(13,4));
    IF ALFA(I)>0E0 THEN PUT EDIT (ALFA(I))(COL(95),F(13,4));
    PUT EDIT (GAMMA(I)) (COL(108),F(12,6));
    IF C1>0E0 THEN PUT EDIT (C1) (COL(120),F(11,4));
    END;
  /*
    ***************************************************************

  CALCULATION OF ION ACTIVITY PRODUCTS IN TERMS OF LOGS.THE ACTIVITY
  PRODUCT (AP) OF A MINERAL WHICH CONTAINS A SPECIES NOT GIVEN IN THE
  CHEMICAL ANALYSIS OF THE WATER SAMPLE WILL BE 'BLANK'.HOWEVER AN
  ARBITRARY VALUE MAY BE ASSIGNED TO THE CONCENTRATION OF ANY DESIRED
  SPECIES. THE SPECIES APPEARING IN THE (AP) EQUATIONS ARE 0 TO 6,8,9,
  10,12 TO 18,20,22 TO 29,97,100.

    ***************************************************************
                                                                  */
    DO I=0 TO 29,97,100;
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      IF ALFA(I)>0E0 THEN
      ALFA(I)=LOG10(ALFA(I));
      ELSE ALFA(I)=-2E4;  END;
/* IF YOU DO NOT WANT PRINT OUT OF MOLE RATIOS,LOG OF ACTIVITY RATIOS
,GAMMA CO2,BOOT,A & B THEN PUT RATIO=1          */
      IF RATIO=0 THEN DO;
      PUT SKIP(5) EDIT ('MOLE RATIOS BASED ON ANALYTICAL MOLALITY',
      'CL/CA','CL/MG','CL/NA ','CL/K','CL/AL',
     'CL/FE','CL/SO4','CL/HCO3','CA/MG','SQRT(CA)/NA')
     (A,SKIP(2),6(X(8),A),X(7),A,X(6),A,X(5),A,X(4),A) ;
      J=1;  DO I=0,1,2,3,13,17,5;
      IF ANALM(I)>0E0 THEN PUT EDIT (CLTOT/ANALM(I)) (COL(J),E(13,4));
            J=J+13;  END;
      IF CO2TIT>0E0 THEN PUT EDIT(CLTOT/CO2TIT)(COL(J),E(13,4));
      IF ANALM(1)>0E0 THEN PUT EDIT (ANALM(0)/ANALM(1))
             (COL(105),E(13,4));
     IF ANALM(2)>0E0 THEN PUT EDIT(SQRT(ANALM(0))/ANALM(2))
             (COL(118),E(13,4));
      PUT SKIP(2) EDIT('NH3/NA','LI/NA','K/NA','MG/CA','SR/CA','BA/CA',
      'SO4/CL','HCO3/CL','F/CL','B/CL' ) (10(X(8),A));
      IF ANALM(2)>0E0 THEN PUT SKIP EDIT (ANALM(31)/ANALM(2),ANALM(21)/
      ANALM(2),ANALM(3)/ANALM(2))(X(2),3(E(13,4)));
      IF ANALM(0)>0E0 THEN PUT EDIT (ANALM(1)/ANALM(0),ANALM(25)/
      ANALM(0),ANALM(14)/ANALM(0))(3(E(13,4)));
      IF ANALM(4) >0E0 & CO2TIT>0E0 THEN PUT EDIT (ANALM(5)/CLTOT,
      CO2TIT/CLTOT,FTOT/CLTOT, BTOT/CLTOT) (2(E(14,4)),2(E(12,4)));
      PUT SKIP(2) EDIT('LOG OF ACTIVITY RATIOS','CA/H2','MG/H2','NA/H'
          ,'K/H','AL/H3','FE/H2','CA/MG','NA/K') (A,SKIP(2),X(7),8(A,
          X(12)));
      C1=-PH;  J=1;  N=13;
      DO I=0,1,2,3,13,17;  C2=ALFA(I);
      IF C1>-9E18 C2>-9E1 THEN DO;
      IF I=13 THEN C2=C2-3E0*C1;
      ELSE IF I=2| I=3 THEN C2=C2-C1;
      ELSE C2=C2-2E0*C1;
      PUT EDIT(C2) (COL(J),F(N,4));  END;
      IF I=0 THEN DO;  J=14; N=16; END;
      ELSE J=J+16; END;
      IF ALFA(0)>-9E1&ALFA(1)>-9E1 THEN PUT EDIT(ALFA(0)-ALFA(1)) (COL
         (97),F(16,4));
      IF ALFA(2)>-9E1&ALFA(3)>-9E1 THEN PUT EDIT(ALFA(2)-ALFA(3))(COL
         (114),F(16,4));
/*    *** CALCULATION OF THE SUBSURFACE TEMPERATURE 'SUBT' OF THE
          SAMPLE FROM THE CHEMICAL DATA     ***     */
      SUBT1,SUBT2,SUBT3,SUBT4,SUBT5,SUBT6,CO,CA1,CA2=0E0;
      IF CUNITS(11)>0E0 THEN DO;
      IF FLAG='MG/L ' THEN CO=CUNITS(11)/DENS;
      ELSE IF FLAG='PPM  ' THEN  CO=CUNITS(11);
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      SUBT1=1.309E3/(5.19E0-LOG10(CO))-273.16E0;
      SUBT2=1.522E3/(5.75E0-LOG10(CO))-273.16E0;
      SUBT3=0.704E3/(4.45E0-LOG10(CO))-273.16E0; END;
      IF ANALM(2)>0E0 & ANALM(3)>0E0 THEN
      SUBT4=0.777E3/(0.47E0+LOG10((ANALM(2)/ANALM(3))))-273.16E0;
     DO I=0,2,3;
     IF ANALM(I)>0E0 THEN
      ANALM(I)=LOG10(ANALM(I)); END; ANALM(0)=0.5*ANALM(0);
      IF ABS(ANALM(0))>0E0 & ABS(ANALM(2))>0E0 & ABS(ANALM(3))>0E0
      THEN DO;              PUT EDIT ('LOG(NA/K)+1/3LOG(SQRT(CA)/NA) =',
      ANALM(2)-ANALM(3)+(1E0/3E0)*(ANALM(0)-ANALM(2)),
      'LOG(NA/K)+4/3LOG(SQRT(CA)/NA) =',ANALM(2)-ANALM(3)+(4E0/3E0)*
      (ANALM(0)-ANALM(2)))        (SKIP(2),A,E(10,3),X(5),A,E(10,3));
   CA1=ANALM(2)-ANALM(3)+(1E0/3E0)*(ANALM(0)-ANALM(2));
   CA2=ANALM(2)-ANALM(3)+(4E0/3E0)*(ANALM(0)-ANALM(2));    END;
      IF ABS(CA1)>0E0 & ABS(CA2)>0E0 THEN DO;
      SUBT5=1.656E3/(2.258E0+CA1)-273.16E0;
      SUBT6=1.656E3/(2.258E0+CA2)-273.16E0;    END;
      PUT EDIT('SUBSURFACE TEMPERATURE (OC) FROM CHEMICAL DATA',
      'QTZ TEMP (CONDUCTIVE)=',SUBT1,'QTZ TEMP (ADIABATIC)=',
      SUBT2,'AM.SILICA TEMP=',SUBT3,'LOG(NA/K) TEMP=',SUBT4,
      'LOG(NA/K)+1/3LOG(SQRT(CA)/NA) TEMP=',SUBT5,
      'LOG(NA/K)+4/3LOG(SQRT(CA)/NA) TEMP=',SUBT6)
      (SKIP(3),A,SKIP(2),A,F(10,1),X(5),A,F(10,1),
       SKIP(1),A,F(10,1),X(5),A,F(10,1),
       SKIP(1),A,F(10,1),X(5),A,F(10,1));
      PUT EDIT ('IF THE SPRING IS BOILING OR STEAM IS LOST DURING',
                ' RODUCTION THEN SELECT QTZ TEMP ADIABATIC ELSE',
               ' SELECT QTZ TEMP CONDUCTIVE','AM.SILICA TEMP SHOULD',
               ' BE CONSIDERED IF SAMPLE IS SATURATED WITH AM.SILICA',
               ' I.E. IF DELG OF MIN.NO.275 IS POSITIVE','NA/K TEMP',
               ' IS USEFUL IF CONC. OF CA IS LOW (MORE DECS) VS NA',
                'USE --4/3LOG-- TEMP IF <100 ELSE USE--1/3- TEMP',
                'READ FOURNIER & TRUESDELL 1973')
               (SKIP(2),3(A),SKIP,3(A),SKIP,2(A),SKIP,A,SKIP,A);
      END;
/* ACTIVITY PRODUCTS OF PHASES   */
      AP(138)=ALFA(2)+ALFA(18)+2E0*ALFA(10)+4E0*PH-2E0*LH2O;
      AP(139)=ALFA(12)+ALFA(17)-ALFA(18);
      AP(140)=2E0*ALFA(12)+ALFA(100)+PH;
      AP(141)=ALFA(12)+ALFA(4);
      AP(142)=ALFA(3)+ALFA(13)+3E0*ALFA(10)+4E0*PH-4E0*LH2O;
      AP(143)=2E0*ALFA(0)+ALFA(1)+2E0*ALFA(10)+6E0*PH-LH2O;
      AP(144)=ALFA(2)+ALFA(13)+3E0*ALFA(10)+4E0*PH-4E0*LH2O;
      AP(145)=ALFA(2)+ALFA(13)+3E0*ALFA(10)+4E0*PH-4E0*LH2O;
      AP(146)=ALFA(3)+3E0*ALFA(13)+2E0*ALFA(5)+6E0*ALFA(8);
      AP(147)=ALFA(2)+ALFA(13)+2E0*ALFA(10)+4E0*PH-LH2O;
      AP(148)=2E0*ALFA(13)+ALFA(10)+LH2O+6E0*PH;
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 AP(149)=ALFA(0)+ALFA(5);
 AP(150)=ALFA(3)+3E0*ALFA(17)+ALFA(13)+3E0*ALFA(10)+10E0*PH;
 AP(151)=5E0*ALFA(0)+3E0*ALFA(28)+ALFA(4);
 AP(152)=5E0*ALFA(0)+3E0*ALFA(28)+ALFA(29);
 AP(153)=5E0*ALFA(0)+3E0*ALFA(28)+ALFA(8);
 AP(154)=ALFA(0)+ALFA(97);
 AP(155)=ALFA(14)+ALFA(5);
 AP(156)=999.9E0;
 AP(157)=ALFA(13)+2E0*LH2O+3E0*PH;
 AP(158)=5E0*ALFA(15)+ALFA(18)+4E0*ALFA(100)+4E0*PH;
 AP(159)=ALFA(1)+2E0*ALFA(8);
 AP(160)=ALFA(0)+ALFA(97);
 AP(161)=ALFA(0)+2E0*ALFA(4);
 AP(162)=ALFA(0)+LH2O+2E0*PH;
 AP(163)=ALFA(0)+2E0*ALFA(8);
 AP(164)=ALFA(0)+ALFA(100)+PH;
 AP(165)=ALFA(25)+ALFA(5);
 AP(166)=ALFA(10)-2E0*LH2O;
AP(167)=5E0*ALFA(1)+2E0*ALFA(13)+3E0*ALFA(10)+6E0*LH2O+16E0*PH;
 AP(168)=ALFA(16)+ALFA(10)+LH2O+2E0*PH;
AP(169)=3E0*ALFA(1)+2E0*ALFA(10)+LH2O+6E0*PH;
 AP(170)=ALFA(20)+ALFA(100)+PH;
 AP(171)=ALFA(20)+ALFA(100)+PH;
 AP(172)=ALFA(1)+ALFA(10)+2E0*PH-LH2O;
 AP(173)=2E0*ALFA(2)+2E0*ALFA(13)+7E0*ALFA(10)+8E0*PH-4E0*LH2O;
 AP(174)=2E0*ALFA(13)+3E0*LH2O+6E0*PH;
AP(175)=ALFA(10)-2E0*LH2O;
 AP(176)=ALFA(10)-2E0*LH2O;
AP(177)=ALFA(15)+ALFA(17)-ALFA(18);
 AP(178)=2E0*ALFA(15)+LH2O+2E0*PH;
 AP(179)=2E0*ALFA(15)+ALFA(100)+PH;
 AP(180)=5E0*ALFA(16)+ALFA(17)+6E0*ALFA(100)+6E0*PH;
 AP(181)=ALFA(16)+ALFA(17)+2E0*ALFA(100)+2E0*PH;
AP(182)=ALFA(16)+2E0*ALFA(17)+3E0*ALFA(100)+3E0*PH;
 AP(183)=ALFA(16)+LH2O+2E0*PH;
 AP(184)=ALFA(16)+ALFA(100)+PH;
 AP(185)=7E0*ALFA(17)+8E0*ALFA(10)+14E0*PH-8E0*LH2O;
 AP(186)=2E0*ALFA(13)+2E0*ALFA(10)+LH2O+6E0*PH;
 AP(187)=ALFA(0)+ALFA(1)+2E0*ALFA(10)+4E0*PH-2E0*LH2O;
 AP(188)=ALFA(0)+ALFA(1)+2E0*ALFA(97);
 AP(189)=ALFA(1)+ALFA(10)+2E0*PH-LH2O;
 AP(190)=ALFA(0)+ALFA(2)+3E0*ALFA(13)+9E0*ALFA(10)+12E0*PH-3E0*
                                                        LH2O;
 AP(191)=2E0*ALFA(17)+ALFA(10)+4E0*PH;
 AP(192)=999.9E0;
 AP(193)=ALFA(17)+2E0*ALFA(4);
 AP(194)=ALFA(18)+3E0*ALFA(4);
 AP(195)=ALFA(17)+ALFA(97);
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```
 AP(196)=ALFA(17)+LH2O+2E0*PH;
 AP(197)=2E0*ALFA(18)+3E0*LH2O+6E0*PH;
 AP(198)=2E0*ALFA(18)+3E0*LH2O+6E0*PH;
 AP(199)=2E0*ALFA(18)+ALFA(17)+4E0*LH2O+8E0*PH;
 AP(200)=ALFA(18)+3E0*ALFA(8);
 AP(201)=4E0*ALFA(17)+7E0*ALFA(100)+ALFA(5)-PH-4E0*LH2O;
AP(202)=ALFA(17)+ALFA(100)+PH;
 AP(203)=ALFA(17)+ALFA(100)+PH;
AP(204)=2E0*ALFA(1)+ALFA(10)+4E0*PH;
 AP(205)=ALFA(0)+2E0*ALFA(29);
 AP(206)=ALFA(18)+2E0*LH2O+3E0*PH;
 AP(207)=ALFA(13)+3E0*ALFA(8);
 AP(208)=ALFA(13)+3E0*ALFA(8);
AP(209)=3E0*ALFA(17)+2E0*ALFA(10)+LH2O+6E0*PH;
 AP(210)=2E0*ALFA(18)+ALFA(17)+4E0*ALFA(100)+4E0*PH;
 AP(211)=ALFA(0)+ALFA(5)+2E0*LH2O;
 AP(212)=ALFA(2)+ALFA(4);
 AP(213)=2E0*ALFA(13)+2E0*ALFA(10)+LH2O+6E0*PH;
 AP(214)=ALFA(0)+2E0*ALFA(13)+7E0*ALFA(10)+8E0*PH-4E0*LH2O;
 AP(215)=ALFA(20)+LH2O+2E0*PH;
 AP(216)=ALFA(0)+3E0*ALFA(1)+4E0*ALFA(97);
 AP(217)=4E0*ALFA(1)+3E0*ALFA(97)+2E0*ALFA(8)+3E0*LH2O;
 AP(218)=.6E0*ALFA(3)+.25E0*ALFA(1)+2.3E0*ALFA(13)+3.5E0*ALFA(10)+
    8E0*PH-2E0*LH2O;
 AP(219)=2E0*ALFA(13)+2E0*ALFA(10)+LH2O+6E0*PH;
AP(220)=ALFA(2)+11E0*ALFA(10)+PH-16.5E0*LH2O;
 AP(221)=2E0*ALFA(13)+ALFA(10)+LH2O+6E0*PH;
 AP(222)=2E0*ALFA(3)+LH2O+2E0*PH;
 AP(223)=2E0*ALFA(0)+ALFA(10)+4E0*PH;
 AP(224)=ALFA(0)+2E0*ALFA(13)+4E0*ALFA(10)+8E0*PH;
 AP(225)=ALFA(3)+ALFA(13)+2E0*ALFA(10)+4E0*PH-2E0*LH2O;
 AP(226)=ALFA(1)+2E0*ALFA(3)+2E0*ALFA(5)+4E0*LH2O;
 AP(227)=ALFA(2)+7E0*ALFA(10)+PH-9E0*LH2O;
 AP(228)=ALFA(1)+ALFA(97);
 AP(229)=2E0*ALFA(16)+ALFA(97)+2E0*ALFA(8);
 AP(230)=4E0*ALFA(2)+3E0*ALFA(13)+9E0*ALFA(10)+ALFA(4)+12E0*PH-
   12E0*LH2O;
 AP(231)=4E0*ALFA(0)+6E0*ALFA(13)+6E0*ALFA(10)+ALFA(97)+24E0*PH;
 AP(232)=3E0*ALFA(0)+ALFA(1)+2E0*ALFA(10)+8E0*PH;
 AP(233)=ALFA(1)+2E0*ALFA(4) ;
 AP(234)=ALFA(1)+2E0*ALFA(18)+4E0*LH2O+8E0*PH;
 AP(235)=ALFA(1)+LH2O+2E0*PH;
 AP(236)=ALFA(3)+ALFA(13)+3E0*ALFA(10)+4E0*PH-4E0*LH2O;
 AP(237)=2E0*ALFA(2)+ALFA(5)+10E0*LH2O;
 AP(238)=ALFA(22)+2E0*ALFA(4);
 AP(239)=ALFA(22)+ALFA(97);
 AP(240)=ALFA(22)+LH2O+2E0*PH;
 AP(241)=2E0*ALFA(23)+2E0*LH2O-ALFA(22)+4E0*PH;
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AP(242)=ALFA(22)+ALFA(100)+PH;
AP(243)=ALFA(0)+ALFA(1)+ALFA(10)+4E0*PH;
AP(244)=.167E0*ALFA(0)+2.33E0*ALFA(13)+3.67E0*ALFA(10)+7.324*PH
   -2.678E0*LH2O;
AP(245)=.33E0*ALFA(3)+2.33E0*ALFA(13)+3.67E0*ALFA(10)+7.32E0*PH-
   2.68*LH2O;
AP(246)=.167E0*ALFA(1)+2.33E0*ALFA(13)+3.67E0*ALFA(10)+7.32E0*PH
   -2.678E0*LH2O;
AP(247)=.33E0*ALFA(2)+2.33E0*ALFA(13)+3.67E0*ALFA(10)+7.32E0*PH
                                          -2.678E0*LH2O;
AP(248)=999.9E0;
AP(249)=999.9E0;
AP(250)=ALFA(0)+2E0*ALFA(13)+10E0*ALFA(10)+8E0*PH-9E0*LH2O;
AP(251)=ALFA(3)+3E0*ALFA(13)+3E0*ALFA(10)+10E0*PH;
AP(252)=2E0*ALFA(2)+LH2O+2E0*PH;
AP(253)=2E0*ALFA(2)+ALFA(5);
AP(254)=ALFA(2)+ALFA(6);
AP(255)=2E0*ALFA(2)+ALFA(97)+10E0*LH2O;
AP(256)=2E0*ALFA(2)+ALFA(97)+LH2O;
AP(257)=ALFA(2)+ALFA(13)+ALFA(10)+4E0*PH;
AP(258)=ALFA(1)+ALFA(97)+3E0*LH2O;
AP(259)=999.9E0;
AP(260)=999.9E0;
AP(261)=ALFA(24)+2E0*ALFA(4);
AP(262)=ALFA(24)+ALFA(97);
AP(263)=ALFA(24)+LH2O+2E0*PH;
AP(264)=ALFA(24)+LH2O+2E0*PH;
AP(265)=ALFA(24)+ALFA(100)+PH;
AP(266)=ALFA(24)+ALFA(5);
AP(267)=.5E0*ALFA(2)+.5E0*ALFA(3)+ALFA(13)+3E0*ALFA(10)+4E0*PH
     -3E0*LH2O;
AP(268)=ALFA(3)+3E0*ALFA(1)+ALFA(13)+3E0*ALFA(10)+2E0*ALFA(29)
                                        +8E0*PH-2E0*LH2O;
AP(269)=ALFA(0)+2E0*ALFA(13)+2E0*ALFA(10)+8E0*PH;
AP(270)=2E0*ALFA(0)+2E0*ALFA(13)+3E0*ALFA(10)+10E0*PH;
AP(271)=2E0*ALFA(13)+4E0*ALFA(10)+6E0*PH-4E0*LH2O;
AP(272)=ALFA(10)-2E0*LH2O;
AP(273)=ALFA(3)+ALFA(13)+3E0*ALFA(10)+4E0*PH-4E0*LH2O;
AP(274)=2E0*ALFA(1)+3E0*ALFA(10)+4E0*PH-2E0*LH2O;
AP(275)=ALFA(10)-2E0*LH2O;
AP(276)=ALFA(10)-2E0*LH2O;
AP(277)=2E0*ALFA(13)+ALFA(10)+LH2O+6E0*PH;
AP(278)=ALFA(1)+2E0*ALFA(13)+4E0*LH2O+8E0*PH;
AP(279)=ALFA(25)+ALFA(97);
AP(280)=ALFA(18)+ALFA(28)+2E0*LH2O;
AP(281)=ALFA(3)+ALFA(4);
AP(282)=3E0*ALFA(1)+4E0*ALFA(10)+6E0*PH-4E0*LH2O;
AP(283)=2E0*ALFA(0)+5E0*ALFA(1)+8E0*ALFA(10)+14E0*PH-8E0*LH2O;
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   AP(284)=3E0*ALFA(2)+ALFA(6)+ALFA(97)+2E0*LH2O;
   AP(285)=ALFA(0)+2E0*ALFA(13)+4E0*ALFA(10)+8E0*PH-2E0*LH2O;
   AP(286)=ALFA(14)+ALFA(97);
   AP(287)=ALFA(0)+ALFA(10)+2E0*PH-LH2O;
   AP(288)=ALFA(26)+ALFA(97);
   AP(289)=ALFA(26)+LH2O+2E0*PH;
   AP(290)=ALFA(26)+ALFA(100)+PH;
   AP(291)=ALFA(26)+ALFA(5);
   AP(292)=2E0*ALFA(0)+3E0*ALFA(13)+3E0*ALFA(10)+LH2O+13E0*PH;
   AP(293)=3E0*ALFA(17)+2E0*ALFA(28)+8E0*LH2O;
   AP(294)=999.9E0;
   AP(295)=999.9E0;
   PUT PAGE EDIT (CARD(1)) (A)
      ('PHASE','AP',' KT ','LOG AP','LOG KT',  'AP/KT'  ,'DELG',
    'LOG AP/KT')
     (SKIP(2),X(6),A,X(8),A,X(12),A,X(9),A,X(6),A,X(8),A,X(9),A,
   X(6),A);
   PUT SKIP (2);
   DO I=137 TO 221,223 TO 295;
   IF LOGKT(I) > 6.0E2  THEN   LOGKT(I)=5.9999E1;
   IF LOGKT(I) >-7.0E1  THEN  DO;
 KT(I) =1E1**(LOGKT(I));            END;   END;
   C1,C2=0E0;
   DO I=138 TO 295;
   C2=AP(I);
   PUT SKIP EDIT(I,PAGE2(I),LOGKT(I))(F(3),X(1),A,COL(57),F(9,4));
   IF KT(I)>0E0 THEN PUT SKIP(0) EDIT(KT(I)) (COL(30),E(11,4));
   IF KT(I)=0E0 THEN PUT SKIP(0);
   IF ABS(C2) <5E2 THEN DO;
         PUT EDIT (C2) (COL(45),F(9,4));
   IF LOGKT(I) ¬=5.9999E1  THEN DO;
   C1=C2-LOGKT(I);
   PUT EDIT (2.302585E0*R*T*C1,C1) (COL(85),F(9,4),F(13,4));  END;
  IF ABS(C2)<75E0 THEN DO; C2=1E1**C2;
   PUT SKIP(0) EDIT (C2) (COL(15),E(11,4));
  IF ABS(C2)>75E0 THEN PUT SKIP(0);
  IF KT(I)>0E0 & LOGKT(I)¬=5.9999E1 THEN PUT EDIT(C2/KT(I))
                                    (COL(69),E(12,4));
   END; END; END;
PUT SKIP(5) EDIT('**DUMMY VALUE FOR LOGKT=59.9990,KT=9.9770E+59**')
   (X(20),A);
   GO TO START;
/*  DECLARE STATEMENTS  */
   DCL LONG CHAR(800) VAR,CARD(10) CHAR(80),FLAG CHAR(5),TABLES
      FILE ,                (PAGE1(0:161),PAGE2(299)) CHAR(8),
         (J,MJ,I,ITER,N,RATIO,INFORM )      FIXED BIN (31), RBIT
      BIT(1),(A,AH2O,DENS,ANALCO3,LH2O,SO4ITR,B,C,C1,C2,C3, EHM,
    EHMC,EMFZSCE, EPMAN,EPMCAT,F,CU,PITR ,CO3CALC ,MU,MUHALF,PCO2,
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        PH,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,HCO3TOT,SITOT,AGTOT,
       ALTOT,BATOT,CUTOT,FETOT,HGTOT,LITOT,MNTOT,PBTOT,SRTOT,ZNTOT,
       ASTOT,PTOT,FTOT,BTOT,NH3TOT,H2STOT,CO2TIT,CO2TOT,TENPH,R,T,
      TEMP,S1,S2,S3,S4,S5,ALFA(0:161),M(0:161),ANALM(0:161),
      CUNITS(0:161),GAMMA(0:161),TK(11),LKT(299,11)) FLOAT(16),
      (DHA(0:161),GFW(0:161),LOGKT(299),KT(295),AP(138:295),
      GAMACO2(0:3,10),G(0:3,10),TCO2(10),MNACLE,BDOT,BDAT(10),
     SUBT1,SUBT2,SUBT3,SUBT4,SUBT5,SUBT6,CO,CA1,CA2,
     GT1,GT2,GTM,PH2O,PH2OC1,PH2OC2,LOG10PH2O) FLOAT (16),
     (Z(0:161),FLAG1,FLAG2,FLAG3,FLAG4,FLAG5) FIXED BIN(31);
EOF: END SOLMNEQ;
```

APPENDIX 2A. TABLE OF LOG(KT) FOR THE AQUEOUS COMPLEXES & MINERALS

I	PAGE2	0C	25C	50C	75C	100C	125C	150C	200C	250C	300C	350C
1	HCO3 -1	-10.61	-10.33	-10.18	-10.14	-10.14	-10.21	-10.34	-10.71	-11.20	-11.78	-12.43
2	KH2O	-14.94	-14.00	-13.26	-12.70	-12.26	-11.91	-11.64	-11.26	-11.05	-11.04	-11.42
3	H4SIO4	-10.20	-9.63	-9.30	-9.11	-9.03	-9.03	-9.10	-9.36	-9.63	-10.20	-11.00
4	CU +2	-11.09	-10.35	-9.72	-9.16	-8.68	-8.25	-7.86	-7.21	-6.66	-6.20	-5.80
5	FE +3	8.95	8.82	8.69	8.58	8.47	8.36	8.27	8.09	7.92	7.77	7.63
6	HG +2	6.11	4.67	3.46	2.44	1.56	0.80	0.13	-0.97	-1.85	-2.56	-3.14
7	MN +3	13.23	11.95	10.86	9.94	9.14	8.44	7.83	6.80	5.98	5.31	4.74
8	AS(OH)4-	-5.29	-4.83	-4.45	-4.12	-3.83	-3.57	-3.34	-2.96	-2.63	-2.34	-2.03
9		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
10	H2S AQ	-7.50	-6.99	-6.77	-6.67	-6.63	-6.66	-6.72	-6.69	-7.35	-8.05	-9.05
11	ALF +2	-6.94	-6.97	-7.07	-7.22	-7.43	-7.71	-8.04	-8.92	-10.25	-12.52	-17.53
12	ALF2 +1	-12.54	-12.60	-12.78	-13.06	-13.45	-13.94	-14.55	-16.16	-18.57	-22.70	-31.77
13	ALF3	-16.60	-16.65	-16.86	-17.21	-17.70	-18.32	-19.09	-21.16	-24.28	-29.61	-41.38
14	ALF4 -	-19.00	-19.04	-19.26	-19.64	-20.18	-20.88	-21.75	-24.08	-27.59	-33.63	-46.95
15	AL(OH)+2	-9.23	-9.25	-9.41	-9.65	-10.00	-10.36	-10.84	-11.90	-13.10	-14.70	-17.00
16	AL(OH)2+	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99	-18.99
17	AL(OH)4-	-33.55	-32.73	-32.26	-32.10	-32.10	-32.30	-32.40	-32.80	-33.50	-34.30	-35.20
18	AL(SO4)+	-2.89	-3.02	-3.17	-3.35	-3.54	-3.77	-4.02	-4.65	-5.53	-6.77	-10.05
19	ALSO4)2-	-4.73	-4.90	-5.10	-5.35	-5.63	-5.96	-6.33	-7.27	-8.58	-10.76	-15.43
20	AGCL	-3.48	-3.31	-3.17	-3.06	-2.99	-2.94	-2.91	-2.93	-3.05	-3.38	-4.22
21	AGCL2 -	-5.54	-5.24	-5.01	-4.84	-4.71	-4.61	-4.56	-4.56	-4.73	-5.19	-6.43
22	AGCL3 -2	-5.53	-5.29	-5.12	-5.00	-4.92	-4.89	-4.89	-5.07	-5.35	-6.07	-7.82
23	AGCL4 -3	-5.73	-5.51	-5.38	-5.30	-5.26	-5.28	-5.31	-5.60	-6.00	-6.90	-8.50
24	AG(SO4)-	-1.22	-1.31	-1.41	-1.51	-1.62	-1.75	-1.89	-2.23	-2.69	-3.44	-5.02
25	AGSO42-3	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
26	BACO3 AQ	-2.40	-2.50	-2.60	-2.70	-2.85	-3.00	-3.20	-3.60	-4.10	-4.70	-5.30
27	BAHCO3)+	-1.18	-1.44	-1.70	-2.00	-2.27	-2.60	-2.88	-3.62	-4.60	-5.60	-6.80
28	BA(OH)+1	-2.17	-2.22	-2.30	-2.40	-2.51	-2.64	-2.79	-3.18	-3.73	-4.64	-6.62
29	BASO4 AQ	-2.39	-2.31	-2.26	-2.23	-2.23	-2.24	-2.26	-2.38	-2.59	-3.01	-3.60
30	CACO3 AQ	-2.99	-3.20	-3.40	-3.65	-3.90	-4.15	-4.50	-5.20	-5.90	-6.45	-7.00
31	CAHCO3)+	-0.86	-1.26	-1.64	-2.03	-2.43	-2.84	-3.27	-4.24	-5.50	-7.00	-8.80
32	CA(OH)+1	-1.15	-1.23	-1.35	-1.50	-1.62	-1.78	-1.95	-2.30	-2.70	-3.20	-3.90
33	CAPO4 -	-6.31	-6.47	-6.69	-6.95	-7.23	-7.65	-8.09	-9.19	-10.77	-13.41	-19.11
34	CAHPO4	-2.41	-2.61	-2.82	-3.05	-3.29	-3.57	-3.87	-4.58	-5.56	-7.13	-10.46
35	CAH2PO4+	-1.23	-1.44	-1.65	-1.87	-2.10	-2.34	-2.60	-3.21	-4.01	-5.27	-7.90
36	CASO4 AQ	-2.30	-2.30	-2.40	-2.55	-2.70	-2.90	-3.10	-3.60	-4.10	-4.50	-5.00
37	CUCL	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
38	CUCL2 -	-4.99	-4.94	-4.94	-4.98	-5.06	-5.19	-5.35	-5.82	-6.57	-7.40	-8.80
39	CUCL3 -2	-5.15	-5.14	-5.18	-5.27	-5.39	-5.56	-5.78	-6.36	-7.25	-8.30	-10.50
40	CUCL +1	-0.53	-0.02	-0.54	-1.04	-1.54	-2.05	-2.58	-3.73	-4.80	-6.00	-7.30
41	CUCL2	1.38	0.71	0.08	-0.53	-1.13	-1.73	-2.34	-3.67	-4.90	-6.50	-8.50
42	CUCL3 -1	3.18	2.30	1.49	0.72	-0.02	-0.76	-1.50	-3.08	-4.60	-6.50	-9.00
43	CUCL4 -2	5.75	4.60	3.56	2.58	1.65	0.74	-0.16	-2.04	-3.90	-6.10	-8.70
44	CU(OH)+1	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37	-6.37
45	CUSO4 AQ	-2.19	-2.25	-2.34	-2.44	-2.56	-2.70	-2.86	-3.26	-3.84	-4.79	-6.84
46	FECL +1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
47	FECL2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
48	FECL3 -1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
49	FECL4 -2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
50	FE(OH)+1	-5.90	-5.70	-5.56	-5.48	-5.45	-5.46	-5.51	-5.76	-6.26	-7.23	-9.53
51	FE(OH)2	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40	-10.40
52	FEOOH -1	30.70	30.70	30.70	30.70	30.70	30.70	30.70	30.70	30.70	30.70	30.70
53	FESO4	-2.41	-2.43	-2.48	-2.54	-2.63	-2.73	-2.86	-3.19	-3.69	-4.53	-6.37

54	FECL +2	-0.98	-1.48	-1.96	-2.44	-2.93	-3.44	-3.98	-5.19	-6.20	-7.59	-8.10
55	FECL2 +1	-1.64	-2.13	-2.62	-3.12	-3.62	-4.16	-4.72	-6.01	-7.10	-7.70	-9.00
56	FECL3	-0.48	-1.13	-1.75	-2.37	-2.99	-3.63	-4.30	-5.70	-7.10	-8.00	-9.30
57	FECL4 -1	1.67	0.79	-0.04	-0.84	-1.63	-2.42	-3.23	-4.90	-6.60	-7.80	-9.10
58	FESO4 +1	-3.78	-4.15	-4.54	-4.96	-5.41	-5.90	-6.44	-7.70	-9.42	-12.15	-17.02
59	FESO4)2-	9.30	9.30	9.30	9.30	9.30	9.30	9.30	9.30	9.30	9.30	9.30
60	FE(OH)+2	-11.89	-11.80	-11.76	-11.75	-11.76	-11.80	-11.88	-12.07	-12.38	-13.38	-15.00
61	FE(OH)2+	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10	-20.10
62	FE(OH)3	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50	-28.50
63	FE(OH)4-	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00	-34.00
64	H4(BO4)-	-5.45	-4.77	-4.20	-3.72	-3.32	-2.99	-2.71	-2.27	-1.98	-1.80	-1.70
65		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
66	H3SIO4)-	-12.20	-11.70	-11.30	-11.10	-11.00	-11.00	-11.00	-11.00	-11.50	-12.00	-13.00
67	HAS(OH)4	-9.69	-9.23	-8.87	-8.61	-8.43	-8.32	-8.28	-8.40	-8.84	-9.87	-12.50
68	HASOH8-2	-12.03	-11.69	-11.48	-11.39	-11.39	-11.48	-11.67	-12.34	-13.55	-15.85	-21.17
69	H2ASOH8-	-30.82	-30.07	-29.64	-29.49	-29.59	-29.93	-30.52	-32.47	-35.88	-42.40	-56.75
70	H3AS(OH8	-51.78	-50.70	-50.16	-50.08	-50.44	-51.20	-52.36	-56.07	-62.33	-73.74	-99.81
71	HF AQ	-2.99	-3.18	-3.38	-3.61	-3.84	-4.09	-4.33	-4.86	-5.40	-5.00	-6.50
72	H2CO3	-6.53	-6.37	-6.31	-6.33	-6.41	-6.54	-6.71	-7.13	-7.66	-8.26	-8.11
73	HPO4 -2	-12.62	-12.34	-12.18	-12.14	-12.10	-12.14	-12.20	-12.45	-12.80	-13.30	-13.80
74	H2PO4 -1	-7.32	-7.21	-7.19	-7.27	-7.36	-7.54	-7.73	-8.25	-8.85	-9.50	-10.20
75	HS -1	-17.50	-17.00	-16.70	-16.30	-16.10	-15.80	-15.40	-15.10	-14.80	-14.60	-14.40
76	HSO4 -1	-1.63	-1.95	-2.29	-2.64	-3.00	-3.37	-3.74	-4.51	-5.29	-6.08	-6.88
77	HNO3 AQ	1.67	1.43	1.17	0.90	0.62	0.34	0.05	-0.55	-1.17	-1.80	-2.45
78	HGCL +1	-6.59	-6.25	-5.99	-5.80	-5.65	-5.56	-5.51	-5.54	-5.78	-6.39	-8.00
79	HGCL2	-14.18	-13.26	-12.51	-11.91	-11.42	-11.03	-10.73	-10.36	-10.34	-10.84	-12.63
80	HGCL3 -1	-16.40	-15.36	-14.50	-13.81	-13.26	-12.82	-12.48	-12.09	-12.10	-12.73	-14.91
81	HGCL4 -2	-15.85	-14.92	-14.18	-13.59	-13.13	-12.79	-12.54	-12.34	-12.58	-13.53	-16.35
82	HGSO4	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40	-1.40
83	HGSH2S)2	-38.50	-35.63	-33.25	-31.26	-29.58	-28.16	-26.97	-25.15	-24.04	-23.83	-25.50
84	HG(HS)3-	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20	-43.20
85	HGSHS2-2	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20	-36.20
86	KCL	2.30	2.00	1.80	1.60	1.40	1.20	1.00	0.60	-0.15	-0.60	-1.70
87	HGS2 -2	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70	-38.70
88	KHSO4	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
89	KSO4 -1	-0.65	-0.83	-1.00	-1.15	-1.30	-1.45	-1.60	-1.93	-2.35	-2.75	-3.10
90	KHPO4 -1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
91	LI(OH)	-0.26	-0.18	-0.20	-0.26	-0.34	-0.42	-0.50	-0.68	-0.87	-1.07	-1.30
92	LI(SO4)-	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
93	MGCO3 AQ	-3.41	-3.40	-3.42	-3.47	-3.55	-3.65	-3.78	-4.16	-4.73	-5.40	-6.10
94	MGHCO3)+	-0.24	-0.90	-1.52	-2.14	-2.76	-3.40	-4.06	-5.50	-7.40	-9.60	-12.80
95	MGF +1	-1.54	-1.82	-2.11	-2.41	-2.72	-3.05	-3.40	-4.21	-5.28	-6.96	-10.46
96	MG(OH)+1	-2.58	-2.60	-2.70	-2.90	-3.10	-3.33	-3.60	-4.10	-4.65	-5.15	-5.70
97	MGSO4 AQ	-2.05	-2.25	-2.60	-2.90	-3.20	-3.55	-3.90	-4.80	-5.70	-6.40	-7.00
98	MG(PO4)-	-6.31	-6.47	-6.69	-6.95	-7.23	-7.65	-8.09	-9.19	-10.77	-13.41	-19.11
99	MGHPO4	-2.91	-3.11	-3.32	-3.55	-3.79	-4.07	-4.37	-5.08	-6.06	-7.63	-11.00
100	MGH2PO4+	-1.23	-1.44	-1.65	-1.87	-2.10	-2.34	-2.60	-3.21	-4.01	-5.27	-7.90
101	MNCL +1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
102	MNCL2	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26	-0.26
103	MNCL3 -1	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23
104	MNCL4 -2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
105	MNHCO3+1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
106	MNSO4 AQ	-2.03	-2.25	-2.48	-2.73	-2.99	-3.28	-3.59	-4.32	-5.30	-6.87	-10.16
107	MNCL +2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
108	MNCL2 +1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
109	MNCL3	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
110	NACL	1.00	0.95	0.80	0.70	0.65	0.55	0.45	0.15	-0.25	-0.95	-2.00
111	NACO3 -1	-0.71	-1.27	-1.81	-2.35	-2.89	-3.45	-4.04	-5.36	-7.05	-9.62	-14.90
112	NAHCO3	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
113	NA2CO3AQ	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68

114	NA2SO4AQ	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
115	NASO4 -1	-0.77	-1.06	-1.35	-1.64	-1.93	-2.24	-2.57	-3.30	-4.26	-5.72	-8.75
116	NAHPO4-1	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
117		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
118	NH4OH	-4.87	-4.75	-4.70	-4.75	-4.85	-4.95	-5.10	-5.53	-6.00	-6.75	-8.00
119	NH4PO4-2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
120	NH4SO4)-	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
121	PBCL +1	-1.59	-1.60	-1.63	-1.68	-1.73	-1.80	-1.89	-2.11	-2.44	-2.99	-4.21
122	PBCL2	-1.73	-1.79	-1.86	-1.95	-2.05	-2.17	-2.30	-2.63	-3.11	-3.89	-5.58
123	PBCL3 -1	-1.56	-1.69	-1.83	-1.98	-2.14	-2.32	-2.51	-2.98	-3.62	-4.64	-6.81
124	PBCL4 -2	-1.17	-1.39	-1.61	-1.83	-2.07	-2.32	-2.58	-3.20	-4.02	-5.29	-7.95
125	PBSO4 AQ	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
126	PBSO42-2	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
127	SR(OH)-1	-0.75	-0.82	-0.89	-0.97	-1.06	-1.15	-1.25	-1.50	-1.83	-2.35	-3.46
128	SRCO3 AQ	-2.70	-2.85	-3.00	-3.10	-3.25	-3.40	-3.60	-4.00	-4.50	-5.10	-5.70
129	SRHCO3)+	-0.86	-1.26	-1.64	-2.03	-2.43	-2.84	-3.27	-4.24	-5.50	-7.00	-8.80
130	SRSO4 AQ	-2.12	-2.20	-2.29	-2.40	-2.52	-2.67	-2.84	-3.25	-3.84	-4.81	-6.30
131	ZNCL +1	0.06	-0.43	-0.90	-1.36	-1.82	-2.29	-2.78	-3.86	-4.80	-6.00	-7.60
132	ZNCL2	-0.07	-0.61	-1.12	-1.63	-2.13	-2.65	-3.19	-4.38	-5.50	-6.90	-8.50
133	ZNCL3 -1	0.07	-0.53	-1.11	-1.67	-2.24	-2.82	-3.42	-4.74	-6.00	-7.70	-9.10
134	ZNCL4 -2	0.49	-0.20	-0.86	-1.51	-2.15	-2.80	-3.47	-4.95	-6.40	-8.30	-10.90
135	ZNSO4 AQ	-2.11	-2.36	-2.61	-2.88	-3.17	-3.48	-3.82	-4.62	-5.69	-7.38	-10.94
136	ASOH)8-3	-53.97	-50.79	-48.25	-46.25	-44.68	-43.50	-42.66	-41.97	-42.75	-45.99	-55.51
137		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
138	ACMITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
139	AG	-1.53	-0.48	0.41	1.18	1.85	2.44	2.97	3.86	4.58	5.19	5.71
140	AG2S A	-23.40	-21.44	-19.83	-18.51	-17.40	-16.48	-15.70	-14.47	-13.58	-12.93	-12.45
141	AGCL	-10.82	-9.74	-8.87	-8.17	-7.60	-7.13	-6.75	-6.18	-5.80	-5.55	-5.40
142	ADULARIA	2.16	1.26	0.54	-0.35	-0.51	-0.91	-1.24	-1.76	-2.14	-2.43	-2.65
143	AKERMANI	50.53	45.74	41.71	38.28	35.32	32.75	30.49	26.71	23.68	21.20	19.13
144	ALBITE L	5.17	3.94	2.95	2.14	1.47	0.91	0.44	-0.30	-0.85	-1.27	-1.59
145	ALBITE H	6.42	5.00	3.85	2.91	2.12	1.46	0.90	0.01	-0.66	-1.18	-1.59
146	ALUNITE	-87.84	-85.53	-84.06	-83.21	-82.83	-82.82	-83.11	-84.29	-86.06	-88.19	-90.54
147	ANALCIME	11.15	9.36	7.95	6.77	5.79	4.97	4.29	3.21	2.43	1.86	1.45
148	ANDALUSI	16.02	12.56	9.70	7.30	5.26	3.51	2.01	-0.46	-2.38	-3.90	-5.13
149	ANHYDRIT	-4.46	-4.65	-4.91	-5.23	-5.59	-5.97	-6.37	-7.20	-8.05	-8.90	-9.74
150	ANNITE	30.92	26.50	22.87	19.84	17.28	15.11	13.23	10.20	7.87	6.04	4.57
151	APATCHLR	-64.90	-66.15	-67.40	-68.65	-69.90	-71.15	-72.40	-74.90	-77.40	-79.80	-82.40
152	APATFLUR	-72.19	-71.58	-71.86	-72.77	-74.16	-75.89	-77.88	-82.39	-87.31	-92.42	-97.61
153	APATHYDX	-60.83	-61.16	-62.25	-63.86	-65.86	-68.13	-70.60	-75.93	-81.52	-87.20	-92.87
154	ARAGONIT	-8.21	-8.32	-8.56	-8.89	-9.30	-9.75	-10.24	-11.28	-12.37	-13.47	-14.57
155	BARITE	-10.19	-9.70	-9.41	-9.27	-9.24	-9.29	-9.41	-9.80	-10.31	-10.90	-11.53
156	BIOTITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
157	BOEHMITE	10.50	8.59	7.01	5.69	4.58	3.63	2.81	1.48	0.46	-0.34	-0.98
158	BORNITE	-124.86	-115.29	-107.36	-100.72	-95.10	-90.29	-86.14	-79.42	-74.25	-70.22	-67.03
159	BRUCITE	-11.33	-11.21	-11.21	-11.30	-11.46	-11.67	-11.91	-12.49	-13.13	-13.81	-14.51
160	CALCITE	-8.24	-8.36	-8.61	-8.96	-9.38	-9.84	-10.34	-11.40	-12.51	-13.63	-14.74
161	CACL2	12.75	11.49	10.32	9.23	8.19	7.21	6.29	4.57	3.00	1.56	0.23
162	CAO LIME	35.74	32.63	30.00	27.76	25.83	24.14	22.65	20.16	18.15	16.49	15.11
163	CA(OH)2	-5.15	-5.36	-5.65	-5.99	-6.38	-6.79	-7.22	-8.10	-9.00	-9.90	-10.78
164	CAS	13.19	11.90	10.75	9.71	8.77	7.90	7.10	5.66	4.40	3.27	2.26
165	CELESTIT	-6.39	-6.40	-6.51	-6.69	-6.93	-7.21	-7.52	-8.19	-8.91	-9.65	-10.39
166	CHALCEDY	-3.87	-3.55	-3.29	-3.06	-2.84	-2.63	-2.46	-2.18	-1.90	-1.59	-1.15
167	CHLOR MG	67.86	59.02	51.84	45.93	41.01	36.90	33.42	27.93	23.90	20.89	18.63
168	CRYSOCOL	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
169	CRYSOTIL	35.79	32.21	29.26	26.81	24.75	23.00	21.50	19.08	17.23	15.80	14.67
170	CINNABAR	-43.23	-39.78	-36.95	-34.61	-32.63	-30.96	-29.54	-27.26	-25.54	-24.24	-23.23
171	CINABMET	-41.67	-38.42	-35.75	-33.54	-31.69	-30.12	-28.79	-26.67	-25.09	-23.90	-22.99
172	CLINENST	12.72	11.36	10.23	9.28	8.48	7.78	7.18	6.19	5.41	4.79	4.27
173	CLINPTIL	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99

174	CORUNDUM	21.56	17.60	14.31	11.54	9.19	7.18	5.43	2.58	0.35	-1.41	-2.84
175	CRISTOBA	-3.66	-3.36	-3.10	-2.87	-2.66	-2.46	-2.29	-2.02	-1.76	-1.47	-1.06
176	CRISTOBB	-3.05	-2.81	-2.61	-2.44	-2.25	-2.11	-1.97	-1.77	-1.56	-1.14	-0.83
177	CU	3.85	4.34	4.76	5.13	5.46	5.76	6.02	6.49	6.89	7.23	7.53
178	CU2O	-1.87	-1.49	-1.14	-0.81	-0.50	-0.20	0.08	0.59	1.06	1.48	1.88
179	CU2S	-37.97	-34.68	-31.93	-29.61	-27.63	-25.97	-24.43	-21.99	-20.07	-18.53	-17.21
180	CU5FES6	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
181	CUFES2	-46.89	-44.04	-41.72	-39.83	-38.26	-36.95	-35.85	-34.15	-32.94	-32.07	-31.45
182	CUFE2S3	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
183	CUO	8.90	7.84	6.95	6.20	5.56	5.01	4.53	3.74	3.12	2.62	2.22
184	CUS	-23.61	-22.05	-20.79	-19.75	-18.90	-18.18	-17.59	-16.67	-16.00	-15.53	-15.20
185	CUMMINGT	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
186	DICKITE	11.26	8.57	6.38	4.59	3.10	1.85	0.79	-0.68	-2.11	-3.04	-3.74
187	DIOPSIDE	22.05	19.86	18.05	16.52	15.22	14.09	13.11	11.48	10.19	9.14	8.27
188	DOLOMITE	-16.61	-17.00	-17.61	-18.38	-19.26	-20.22	-21.23	-23.34	-25.49	-27.64	-29.76
189	ENSTATIT	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
190	ERIONITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
191	FAYALITE	19.70	17.22	15.17	13.44	11.96	10.69	9.59	7.78	6.36	5.22	4.29
192	FEASS	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
193	FECL2	9.12	7.90	6.76	5.70	4.70	3.76	2.88	1.24	-0.24	-1.60	-2.85
194	FECL3	14.65	12.34	10.23	8.30	6.51	4.84	3.28	0.42	-2.13	-4.45	-6.57
195	FECO3	-10.44	-10.69	-11.05	-11.47	-11.94	-12.44	-12.97	-14.06	-15.17	-16.28	-17.37
196	FEO	14.00	12.36	10.99	9.84	8.84	7.99	7.24	6.00	5.03	4.24	3.60
197	FE2O3HEM	0.14	-1.93	-3.64	-5.06	-6.26	-7.27	-8.15	-9.57	-10.65	-11.50	-12.17
198	FE2O3MGH	6.40	6.40	6.40	6.40	6.40	6.40	6.40	6.40	6.40	6.40	6.40
199	FE3O4	9.94	6.57	3.79	1.45	-0.52	-2.21	-3.67	-6.04	-7.89	-9.34	-10.52
200	FEOH13AM	-38.67	-37.20	-36.10	-35.29	-34.70	-34.29	-34.02	-33.78	-33.83	-34.07	-34.45
201	FES2 PYR	-110.75	-103.30	-97.52	-93.03	-89.52	-86.80	-84.70	-81.90	-80.52	-80.02	-80.20
202	FESTROLT	-49.48	-49.90	-50.78	-52.00	-53.47	-55.12	-56.91	-60.73	-64.76	-68.86	-73.03
203	FESMAKIN	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
204	FORSTERI	32.65	29.28	26.47	24.10	22.07	20.32	18.80	16.28	14.30	12.70	11.38
205	FLUORITE	-9.21	-9.05	-9.01	-9.07	-9.21	-9.39	-9.62	-10.15	-10.75	-11.39	-12.08
206	GOETHITE	-0.09	-1.07	-1.86	-2.52	-3.06	-3.52	-3.90	-4.51	-4.95	-5.27	-5.51
207	GIBBS AM	-33.38	-32.41	-31.70	-31.29	-31.00	-30.85	-30.80	-30.92	-31.27	-31.75	-32.33
208	GIBBS C	-33.82	-32.76	-32.01	-31.49	-31.14	-30.94	-30.84	-30.90	-31.18	-31.61	-32.15
209	GREENALI	23.80	23.80	23.80	23.80	23.80	23.80	23.80	23.80	23.80	23.80	23.80
210	GREIGITE	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70	-19.70
211	GYPSUM	-4.92	-4.86	-4.88	-4.98	-5.13	-5.33	-5.55	-6.07	-6.65	-7.27	-7.92
212	HALITE	1.48	1.58	1.61	1.60	1.56	1.50	1.41	1.26	0.96	0.69	0.43
213	HALLOYSI	14.27	11.30	8.88	6.88	5.21	3.81	2.63	0.72	-0.70	-1.78	-2.61
214	HEULANDI	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
215	HGO	2.85	2.48	2.15	1.85	1.58	1.34	1.12	0.72	0.37	0.06	-0.22
216	HUNTITE	-31.12	-32.22	-33.71	-35.47	-37.42	-39.50	-41.67	-46.16	-50.71	-55.23	-59.68
217	HYDRMAGN	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20	-30.20
218	ILLITE	13.52	10.34	7.75	5.61	3.82	2.31	1.03	-1.03	-2.59	-3.79	-4.74
219	KAOLINIT	10.26	7.63	5.49	3.74	2.29	1.07	0.04	-1.58	-2.78	-3.66	-4.36
220	KENYAITE	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00	-25.00
221	KYANITE	16.09	12.66	9.83	7.46	5.46	3.74	2.26	-0.16	-2.03	-3.52	-4.71
222	K2O	90.73	83.91	78.16	73.23	68.98	65.26	61.98	56.48	52.05	48.39	45.33
223	LARNITE	42.54	38.76	35.58	32.87	30.53	28.49	26.70	23.69	21.27	19.28	17.61
224	LAUMNTIT	15.07	11.85	9.24	7.09	5.30	3.80	2.54	0.53	-0.96	-2.08	-2.94
225	LEUCITE	11.54	9.85	8.47	7.31	6.34	5.52	4.81	3.69	2.84	2.19	1.69
226	LEONITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
227	MAGADITE	-14.34	-14.34	-14.34	-14.34	-14.34	-14.34	-14.34	-14.30	-14.34	-14.34	-14.34
228	MAGNESIT	-7.71	-8.04	-8.46	-8.94	-9.45	-10.00	-10.56	-11.70	-12.85	-13.99	-15.11
229	MALACHIT	-34.02	-33.18	-32.72	-32.54	-32.57	-32.57	-33.06	-33.94	-35.04	-36.27	-37.59
230	MARIALIT	4.05	1.71	-0.45	-2.25	-3.63	-5.15	-6.37	-8.04	-9.57	-11.28	-13.80
231	MEIONITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
232	MERWINIT	75.51	68.49	62.59	57.57	53.25	49.50	46.20	40.70	36.29	32.68	29.67
233	MGCL2	24.57	22.15	20.00	18.09	16.34	14.76	13.30	10.70	8.44	6.44	4.65

234	MGFE2O4	[illegible]	18.80	15.[illegible]	12.10	9.49	[illegible]	5.31	2.[illegible]	-0.35	-2.34	-3.94
235	MGOPERIC	24.04	21.68	19.71	18.04	16.61	15.36	14.28	12.48	11.05	9.89	8.94
236	MICROCLN	2.12	1.29	0.64	0.11	-0.33	-0.68	-0.98	-1.45	-1.79	-2.04	-2.24
237	MIRABILT	-2.41	-1.13	-0.04	0.92	1.76	2.51	3.18	4.33	5.28	6.10	6.80
238	MNCL2	9.92	8.80	7.75	6.76	5.82	4.93	4.08	2.51	1.06	-0.27	-1.51
239	MNCO3	-10.47	-10.52	-10.71	-10.99	-11.35	-11.76	-12.21	-13.17	-14.19	-15.22	-16.26
240	MNO	19.92	17.96	16.32	14.93	13.73	12.69	11.77	10.25	9.04	8.05	7.23
241	MNO2	-84.77	-78.84	-73.81	-69.49	-65.73	-62.43	-59.52	-54.59	-50.59	-47.26	-44.46
242	MNS	0.01	-0.35	-0.71	-1.07	-1.42	-1.77	-2.10	-2.76	-3.37	-3.96	-4.51
243	MONTICEL	33.59	30.39	27.71	25.44	23.49	21.80	20.32	17.87	15.91	14.32	13.00
244	MONT CA	9.14	6.14	3.70	1.68	-0.01	-1.44	-2.65	-4.60	-6.07	-7.20	-8.10
245	MONT K	8.67	5.86	3.57	1.69	0.12	-1.21	-2.33	-4.12	-5.47	-6.51	-7.32
246	MONT MG	9.08	6.04	3.57	1.51	-0.02	-1.64	-2.87	-4.83	-6.32	-7.47	-8.36
247	MONT NA	9.01	6.12	3.77	1.83	0.22	-1.14	-2.29	-4.13	-5.51	-6.57	-7.39
248	MONTCANA	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
249	MONTSEAW	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
250	MORDENIT	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
251	MUSCOVIT	13.37	9.65	6.64	4.15	2.07	0.32	-1.16	-3.53	-5.31	-6.67	-7.73
252	NA2O	72.82	67.20	62.48	58.46	55.00	51.99	49.35	44.94	41.41	38.54	36.15
253	NA2SO4	-0.24	-0.21	-0.27	-0.40	-0.58	-0.79	-1.04	-1.59	-2.18	-2.81	-3.45
254	NAHCOLIT	6.04	5.77	5.51	5.26	5.02	4.79	4.57	4.14	3.74	3.36	2.99
255	NATRON	-2.52	-1.44	-0.53	0.24	0.91	1.49	1.99	2.83	3.49	4.02	4.45
256	NATRTHRM	0.06	-0.01	-0.21	-0.48	-0.80	-1.17	-1.56	-2.39	-3.26	-4.14	-5.02
257	NEPHELIN	16.97	14.67	12.77	11.19	9.85	8.70	7.71	6.10	4.84	3.83	3.01
258	NESQUHON	-4.47	-4.58	-4.78	-5.03	-5.33	-5.65	-6.00	-6.73	-7.49	-8.25	-9.01
259	NICOLITE	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
260	O2 GAS	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
261	PBCL2	-5.45	-4.98	-4.70	-4.58	-4.57	-4.64	-4.78	-5.20	-5.74	-6.35	-7.00
262	PBCO3	-13.94	-13.45	-13.21	-13.15	-13.22	-13.39	-13.64	-14.30	-15.11	-16.01	-16.95
263	PBOLITHR	13.83	12.74	11.81	11.01	10.30	9.68	9.12	8.17	7.38	6.72	6.15
264	PBOMASIC	13.99	12.88	11.93	11.11	10.40	9.76	9.20	8.23	7.44	6.77	6.19
265	PBS	-15.98	-14.67	-13.65	-12.84	-12.19	-11.68	-11.28	-10.70	-10.36	-10.18	-10.12
266	PBSO4	-7.98	-7.76	-7.69	-7.74	-7.88	-8.08	-8.32	-8.92	-9.59	-10.31	-11.06
267	PHILLIPS	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90	-6.90
268	PHLOGPTE	25.02	20.81	17.25	14.18	11.50	9.15	7.06	3.49	0.55	-1.93	-4.06
269	PLAG(AN)	29.30	24.69	20.06	17.40	14.53	12.06	9.79	6.34	3.47	1.12	-0.70
270	PREHNITE	37.67	32.41	28.04	24.36	21.22	18.52	16.17	12.31	9.27	6.83	4.84
271	PYROPHYL	3.40	1.32	-0.36	-1.74	-2.88	-3.83	-4.64	-5.91	-6.85	-7.56	-8.10
272	QUARTZ	-4.38	-3.98	-3.64	-3.34	-3.06	-2.81	-2.60	-2.26	-1.92	-1.57	-1.11
273	SANADNHI	2.45	1.51	0.76	0.15	-0.35	-0.77	-1.12	-1.68	-2.09	-2.40	-2.64
274	SEPIOLIT	20.80	18.78	17.10	15.75	14.67	13.65	12.77	11.50	10.52	9.61	9.15
275	SILICAAM	-3.31	-3.02	-2.76	-2.55	-2.36	-2.20	-2.06	-1.82	-1.63	-1.48	-1.36
276	SILICGEL	-2.94	-2.71	-2.52	-2.36	-2.20	-2.06	-1.93	-1.74	-1.53	-1.30	-0.95
277	SILLIMAN	16.46	12.95	10.05	7.62	5.55	3.79	2.26	-0.23	-2.16	-3.69	-4.92
278	SPINEL	38.58	32.83	28.06	24.04	20.62	17.68	15.13	10.95	7.68	5.07	2.95
279	SRCO3	-12.08	-11.03	-11.77	-11.85	-12.04	-12.31	-12.64	-13.41	-14.29	-15.22	-16.18
280	STRENGIT	-27.21	-27.20	-27.41	-27.76	-28.22	-28.76	-29.36	-30.66	-32.03	-33.43	-34.84
281	SYLVITE	0.46	0.78	1.01	1.15	1.23	1.27	1.28	1.20	1.06	0.87	0.65
282	TALC	21.42	19.01	17.07	15.47	14.13	13.00	12.04	10.51	9.34	8.44	7.72
283	TREMOLIT	63.09	56.52	51.10	46.59	42.78	39.53	36.75	32.26	28.85	26.21	24.14
284	TRONA	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18	-2.18
285	WAIRAKIT	21.66	17.46	13.99	11.09	8.63	6.52	4.71	1.74	-0.56	-2.39	-3.86
286	WITHERIT	-13.83	-13.27	-12.95	-12.83	-12.84	-12.97	-13.17	-13.76	-14.51	-15.34	-16.23
287	WALLASTO	14.31	13.03	11.97	11.06	10.28	9.60	9.00	7.99	7.18	6.51	5.95
288	ZNCO3	-9.51	-9.72	-10.04	-10.44	-10.88	-11.37	-11.88	-12.95	-14.03	-15.16	-16.25
289	ZNO	13.18	11.70	10.47	9.43	8.54	7.77	7.10	6.00	5.13	4.42	3.85
290	ZNS	-12.44	-11.82	-11.35	-10.99	-10.72	-10.52	-10.38	-10.21	-10.16	-10.19	-10.27
291	ZNSO4	5.94	4.62	3.41	2.29	1.25	0.28	-0.64	-2.33	-3.85	-5.24	-6.52
292	ZOISITE	46.96	39.83	33.90	28.89	24.62	20.94	17.73	12.45	8.29	4.94	2.20
293	VIVIANIT	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00	-36.00

294		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
295		999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99	999.99
296	FE2TOFE3	21.35	22.42	23.50	24.58	25.67	26.77	27.86	30.08	32.30	34.54	36.80
297	CU+TOCU2	7.48	8.30	9.13	9.99	10.85	11.74	12.64	14.47	16.36	18.29	20.26
298	HG22HG2	50.34	51.21	52.12	53.05	54.00	54.98	55.98	58.04	60.18	62.38	64.64
299	MN2TOMN3	37.89	38.72	39.56	40.41	41.27	42.14	43.02	44.81	46.62	48.46	50.33

APPENDIX 29. LIST OF AQUEOUS SPECIES TOGETHER WITH THEIR CHARGE, DISTANCE OF NEAREST APPROACH (a°), AND GRAM FORMULA WEIGHT

* LIST OF AQUEOUS SPECIES *

I	PAGE1	Z	DHA	GFW
0	CA +2	2	6.0	40.08000
1	MG +2	2	6.5	24.31200
2	NA +1	1	4.0	22.98980
3	K +1	1	3.0	39.10200
4	CL -1	-1	3.0	35.45300
5	SO4 -2	-2	4.0	96.06160
6	HCO3 -1	-1	5.4	61.01732
7	H +1	1	9.0	1.00797
8	OH -1	-1	3.5	17.00737
9	AH2O	0	0.0	18.01500
10	H4SIO4	0	0.0	96.11548
11	SIO2 AQ	0	0.0	60.08480
12	AG +1	1	2.5	107.87000
13	AL +3	3	9.0	26.98150
14	BA +2	2	5.0	137.34000
15	CU +1	1	2.5	63.54000
16	CU +2	2	6.0	63.54000
17	FE +2	2	6.0	55.84700
18	FE +3	3	9.0	55.84700
19	HG2 +2	2	4.0	401.18000
20	HG +2	2	5.0	200.59000
21	LI +1	1	6.0	6.93900
22	MN +2	2	6.0	54.93800
23	MN +3	3	9.0	54.93800
24	PB +2	2	4.5	207.19000
25	SR +2	2	5.0	87.62000
26	ZN +2	2	6.0	65.37000
27	AS(OH)4-	-1	4.0	142.95110
28	PO4 -3	-3	5.0	94.97140
29	F -1	-1	3.5	18.99840
30	H3BO3 AQ	0	0.0	61.83311
31	NH3 AQ	0	0.0	17.03061
32	H2S AQ	0	0.0	34.07994
33	ALF +2	2	5.4	45.97990
34	ALF2 +1	1	5.4	64.97830
35	ALF3	0	0.0	83.97670
36	ALF4 -1	-1	4.5	102.97510
37	AL(OH)+2	2	5.4	43.98887
38	AL(OH)2+	1	5.4	60.99624
39	AL(OH)4-	-1	4.5	95.01098
40	AL(SO4)+	1	4.5	123.04310
41	ALSO4)2-	-1	4.5	219.10470
42	AGCL	0	0.0	143.32300
43	AGCL2 -1	-1	4.0	178.77600
44	AGCL3 -2	-2	5.0	214.22900
45	AGCL4 -3	-3	6.0	249.68200
46	AG(SO4)-	-1	4.0	203.93160
47	AGSO42-3	-3	6.0	299.99320
48	AS(OH)3	0	0.0	125.94370
49	ASOH)8-3	-3	6.0	210.98060
50	BACO3 AQ	0	0.0	197.34940
51	BAHCO3)+	1	4.0	198.35730
52	BA(OH)+1	1	5.0	154.34740
53	BASO4 AQ	0	0.0	233.40160
54	CACO3 AQ	0	0.0	100.08940
55	CAHCO3)+	1	6.0	101.09730
56	CA(OH)+1	1	6.0	57.08737
57	CAPO4 -1	-1	5.4	135.05140
58	CAHPO4	0	0.0	136.05940
59	CAH2PO4+	1	5.4	137.06730
60	CASO4 AQ	0	0.0	136.14160
61	CUCL	0	0.0	98.99300
62	CUCL2 -1	-1	4.0	134.44600
63	CUCL3 -2	-2	5.0	169.89900
64	CUCL +1	1	4.0	98.99300
65	CUCL2	0	0.0	134.44600
66	CUCL3 -1	-1	4.0	169.89900
67	CUCL4 -2	-2	5.0	205.35200
68	CU(OH)+1	1	4.0	80.54737
69	CUSO4	0	0.0	159.60160
70	FECL +1	1	4.0	91.30000
71	FECL2	0	0.0	126.75300
72	FECL3 -1	-1	4.0	162.20600
73	FECL4 -2	-2	5.0	197.65900
74	FE(OH)+1	1	5.0	72.85437
75	FE(OH)2	0	0.0	89.86174
76	FEOOH -1	-1	5.0	88.85377
77	FESO4	0	0.0	151.90860
78	FECL +2	2	5.0	91.30000
79	FECL2 +1	1	5.0	126.75300
80	FECL3	0	0.0	162.20600
81	FECL4 -1	-1	4.0	197.65900
82	FESO4 +1	1	5.0	151.90860
83	FESO4)2-	-1	4.0	247.97020
84	FE(OH)+2	2	5.0	72.85437
85	FE(OH)2+	1	5.4	89.86174
86	FE(OH)3	0	0.0	106.86910
87	FE(OH)4-	-1	5.4	123.87650
88	H4(BO4)-	-1	2.6	78.84014
89	H2SIO4-2	-2	5.4	94.09954
90	H3SIO4)-	-1	4.0	95.10751
91	HAS(OH)4	0	0.0	143.95910
92	HASOH8-2	-2	5.0	211.98860
93	H2ASOH8-	-1	4.0	212.99650
94	H3ASNOH8	0	0.0	214.00450
95	HF AQ	0	0.0	20.00640
96	H2CO3	0	0.0	62.02530
97	CO3 -2	-2	5.4	60.00935
98	HPO4 -2	-2	5.0	95.97937
99	H2PO4 -1	-1	5.4	96.98734
100	HS -1	-1	3.5	33.07197
101	S -2	-2	5.0	32.06400
102	HSO4 -1	-1	4.5	97.06957
103	HNO3 AQ	0	0.0	63.01290
104	HGCL +1	1	4.0	236.04300
105	HGCL2	0	0.0	271.49600
106	HGCL3 -1	-1	4.0	306.94900
107	HGCL4 -2	-2	5.0	342.40200
108	HGSO4	0	0.0	296.65160
109	HGSH2S)2	0	0.0	300.81400
110	HG(HS)3-	-1	4.0	299.80600
111	HGSHS2-2	-2	5.0	298.79800
112	KCL	0	0.0	74.55500
113	HGS2 -2	-2	5.0	264.71800
114	KHSO4	0	0.0	136.17160
115	KSO4 -1	-1	5.4	135.16360
116	KHPO4 -1	-1	5.4	135.08140
117	LI(OH)	0	0.0	23.94637
118	LI(SO4)-	-1	5.0	103.00060
119	MGCO3 AQ	0	0.0	84.32135
120	MGHCO3)+	1	4.0	85.32932
121	MGF +1	1	4.5	43.31040
122	MG(OH)+1	1	6.5	41.31937
123	MGSO4 AQ	0	0.0	120.37360
124	MG(PO4)-	-1	5.4	119.28340
125	MGHPO4	0	0.0	120.29140
126	MGH2PO4+	1	5.4	121.29930
127	MNCL +1	1	4.0	90.39100
128	MNCL2	0	0.0	125.84400
129	MNCL3 -1	-1	4.0	161.29700
130	MNCL4 -2	-2	5.0	196.75000
131	MNHCO3+1	1	4.0	115.95530
132	MNSO4 AQ	0	0.0	150.99960
133	MNCL +2	2	5.0	90.39100
134	MNCL2 +1	1	4.0	125.84400
135	NO3 -1	-1	3.0	62.00490
136	NACL	0	0.0	58.44290
137	NACO3 -1	-1	5.4	82.99915
138	NAHCO3	0	0.0	84.00712
139	NA2CO3AQ	0	0.0	105.98900
140	NA2SO4AQ	0	0.0	142.04120
141	NASO4 -1	-1	5.4	119.05140
142	NAHPO4-1	-1	5.4	118.96920
143	NH4 +1	1	2.5	18.03858
144	NH4OH	0	0.0	35.04593
145	NH4PO4-2	-2	5.0	113.01000
146	NH4SO4)-	-1	5.0	114.10020
147	PBCL +1	1	4.0	242.64300
148	PBCL2	0	0.0	278.09600
149	PBCL3 -1	-1	4.0	313.54900
150	PBCL4 -2	-2	5.0	349.00200
151	PBSO4 AQ	0	0.0	303.25160
152	PBSO42-2	-2	5.0	399.31320
153	SR(OH)-1	-1	5.0	104.62740
154	SRCO3 AQ	0	0.0	147.62940
155	SRHCO3)+	1	4.0	148.63730
156	SRSO4 AQ	0	0.0	183.68160
157	ZNCL +1	1	4.0	100.82300
158	ZNCL2	0	0.0	136.27600
159	ZNCL3 -1	-1	4.0	171.72900
160	ZNCL4 -2	-2	5.0	207.18200
161	ZNSO4 AQ	0	0.0	161.43160

APPENDIX 2C. ACTIVITY COEFFICIENT OF $CO_{2(aq)}$ AS A FUNCTION OF TEMPERATURE AND AN EQUIVALENT NaCl SOLUTION

** GAMMA CO2 AS A FUNCTION OF TEMP. & EQ. NACL **

EMNACL	0C	25C	50C	100C	150C	200C	250C	270C	300C	350C
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
1	1.30	1.27	1.24	1.20	1.19	1.23	1.34	1.42	1.50	1.58
2	1.65	1.57	1.50	1.44	1.40	1.47	1.67	1.83	2.00	2.20
3	2.10	1.93	1.80	1.74	1.70	1.74	1.86	2.03	2.29	2.59

APPENDIX 2D. VALUES OF DEVIATION FUNCTION B AS A FUNCTION OF TEMPERATURES OF APPENDIX 2C

BDOT=	0.038	0.041	0.043	0.046	0.047	0.047	0.034	0.015	0.000	0.000

APPENDIX 3. PRINTOUT OF RESULTS OBTAINED FOR A TEST SAMPLE

SEA WATER ANALYSIS (GOLDBERG,1963) TEST FOR SOLMNEQ JUNE,1972 DATE=02/22/73

DATA IN MG/L

ANAL MEQ/L CAT= 597.6715 ANAL MEQ/L AN= 594.5725

PH	EH	T	ION STRENGTH	PCO2 ATM	CO2 TOT	PPM CO2 TOT
8.10	9.0000	25.00	0.63942	0.0007184	1.424604E-03	71.498804

CALC MEQ/L CAT	CALC MEQ/L AN	AH2O	CO3CALC	PH2O ATM	DENSITY	TDS MG/L
564.386	563.441	0.9817	2.9309E-05	0.0313	1.0300	34517.49

	ION		ANAL PPM	CALC PPM	ANAL MG/L	CALC MG/L	ANAL MOLAL	CALC MOLAL	ALFA	GAMMA	P ION
0	CA +2	2	388.3495	352.9767	400.0000	363.5660	1.0025E-02	9.1122E-03	2.2477E-03	0.246669	2.6483
1	MG +2	2	1310.6796	1196.6608	1350.0000	1232.5606	5.5780E-02	5.0923E-02	1.3485E-02	0.264778	1.8702
2	NA +1	1	10194.1748	9703.7263	10500.0000	9994.8381	4.5990E-01	4.3672E-01	2.9328E-01	0.671538	0.5327
3	K +1	1	368.9320	363.6363	380.0000	374.5454	9.7623E-03	9.6221E-03	6.0406E-03	0.627779	2.2189
4	CL -1	-1	18446.6019	18103.3153	19000.0000	18646.4148	5.3833E-01	5.2833E-01	3.3168E-01	0.627779	0.4793
5	SO4 -2	-2	2621.3592	1187.0110	2700.0000	1222.6213	2.8235E-02	1.2785E-02	2.1694E-03	0.169681	2.6637
6	HCO3 -1	-1	137.8641	92.9859	142.0000	95.7754	2.3378E-03	1.5768E-03	1.1353E-03	0.720042	2.9449
7	H +1	1		0.0000		0.0000		9.8894E-09	7.9433E-09	0.803212	8.1000
8	OH -1	-1		0.0312		0.0322		1.8990E-06	1.2359E-06	0.650789	5.9080
9	AH2O	0								1.172642	
10	H4SIO4	0		9.4522		9.7357		1.0175E-04	1.1932E-04	1.172642	3.9233
11	SIO2 AQ	0	6.2136	6.2136	6.4000	6.4000	1.0700E-04	1.0700E-04		1.172642	
12	AG +1	1	0.0003	0.0000	0.0003	0.0000	2.7937E-09	2.8715E-14	1.7290E-14	0.602136	13.7622
13	AL +3	3	0.0097	0.0000	0.0100	0.0000	3.7231E-07	2.3627E-15	2.0284E-16	0.085850	15.6928
14	BA +2	2	0.0291	0.0267	0.0300	0.0275	2.1943E-07	2.0147E-07	4.2104E-08	0.208978	7.3757
15	CU +1	1	0.0029	0.0000	0.0030	0.0000	4.7429E-08	2.0528E-12	1.2360E-12	0.602136	11.9080
16	CU +2	2		0.0000		0.0000		3.2019E-19	7.8981E-20	0.246669	19.1025
17	FE +2	2	0.0971	0.0721	0.1000	0.0742	1.7987E-06	1.3355E-06	3.2943E-07	0.246669	6.4822
18	FE +3	3		0.0000		0.0000		1.0952E-23	9.4025E-25	0.085850	24.0268
19	HG2 +2	2								0.169681	
20	HG +2	2	0.0029	0.0000	0.0030	0.0000	1.5024E-08	5.5924E-52	1.1687E-52	0.208978	51.9323
21	LI +1	1	0.1650	0.1650	0.1700	0.1700	2.4610E-05	2.4610E-05	1.8147E-05	0.737379	4.7412
22	MN +2	2	0.0019	0.0017	0.0020	0.0018	3.6570E-08	3.2330E-08	7.9748E-09	0.246669	8.0983
23	MN +3	3		0.0000		0.0000		2.9748E-37	2.5539E-38	0.085850	37.5928
24	PB +2	2	0.0029	0.0004	0.0030	0.0005	1.4545E-08	2.2052E-09	4.1788E-10	0.189492	9.3790
25	SR +2	2	7.7670	7.2687	8.0000	7.4868	9.1718E-05	8.5834E-05	1.7937E-05	0.208978	4.7462
26	ZN +2	2	0.0097	0.0061	0.0100	0.0063	1.5367E-07	9.6359E-08	2.3708E-08	0.246669	7.6240
27	AS(OH)4-	-1	0.0055	0.0003	0.0057	0.0003	4.0055E-08	2.2069E-09	1.4820E-09	0.671538	8.8291
28	PO4 -3	-3	0.2039	0.0000	0.2100	0.0000	2.2212E-06	1.9263E-10	5.2746E-12	0.027382	11.2778
29	F -1	-1	1.2621	0.6694	1.3000	0.7100	6.8737E-05	3.7543E-05	2.4433E-05	0.650789	4.6120
30	H3BO3 AQ	0	25.5340	22.3890	26.3000	23.0606	4.2727E-04	3.7464E-04	4.3932E-04	1.172642	3.3572
31	NH3 AQ	0	0.6214	0.6214	0.6400	0.6400	3.7750E-05	3.7750E-05		1.172642	
32	H2S AQ	0	0.0971	0.0040	0.1000	0.0041	2.9476E-06	1.2174E-07	1.4275E-07	1.172642	6.8454
33	ALF +2	2		0.0000		0.0000		2.0622E-13	4.6251E-14	0.224277	13.3349
34	ALF2 +1	1		0.0000		0.0000		6.6947E-13	4.8205E-13	0.720042	12.3169
35	ALF3	0		0.0000		0.0000		1.1269E-13	1.3215E-13	1.172642	12.8789
36	ALF4 -1	-1		0.0000		0.0000		1.1491E-15	7.9255E-16	0.690335	15.1010
37	AL(OH)+2	2		0.0000		0.0000		1.9876E-12	4.4578E-13	0.224277	12.3509
38	AL(OH)2+	1		0.0002		0.0003		4.2046E-09	3.0275E-09	0.720042	8.5189
39	AL(OH)4-	-1		0.0338		0.0348		3.6810E-07	2.5411E-07	0.690335	6.5950
40	AL(SO4)+	1		0.0000		0.0000		6.6747E-16	4.6078E-16	0.690335	15.3365
41	ALSO4)2-	-1		0.0000		0.0000		1.0984E-16	7.5829E-17	0.690335	16.1202
42	AGCL	0		0.0000		0.0000		9.9852E-12	1.1709E-11	1.172642	10.9315
43	AGCL2 -1	-1		0.0001		0.0001		4.9223E-10	3.3055E-10	0.671538	9.4808
44	AGCL3 -2	-2		0.0001		0.0001		5.8864E-10	1.2301E-10	0.208978	9.9100
45	AGCL4 -3	-3		0.0004		0.0004		1.7029E-09	6.7712E-11	0.039764	10.1693

46	AG(SO4)-	-1	0.0000	0.0000	1.1405E-15	7.6586E-16	0.671538	15.1159
47	AGSO42-3	-3	0.0000	0.0000	2.0465E-38	8.1375E-40	0.039764	39.0899
48	AS(OH)3	0	0.0025	0.0026	2.0799E-08	2.4390E-08	1.172642	7.6128
49	ASOH)8-3	-3	0.0000	0.0000	7.0828E-67	2.8164E-68	0.039764	67.5503
50	BACO3 AQ	0	0.0000	0.0000	7.5907E-11	8.9012E-11	1.172642	10.0506
51	BAHCO3)+	1	0.0004	0.0004	1.9605E-09	1.3166E-09	0.671538	8.8806
52	BA(OH)+1	1	0.0000	0.0000	1.2207E-11	8.6356E-12	0.707436	11.0637
53	BASO4 AQ	0	0.0036	0.0037	1.5904E-08	1.8649E-08	1.172642	7.7293
54	CACO3 AQ	0	1.9646	2.0236	2.0309E-05	2.3816E-05	1.172642	4.6231
55	CAHCO3)+	1	6.1533	6.3379	6.2976E-05	4.6437E-05	0.737379	4.3331
56	CA(OH)+1	1	0.0035	0.0036	6.3976E-08	4.7174E-08	0.737379	7.3263
57	CAPO4 -1	-1	0.0063	0.0065	4.8592E-08	3.4988E-08	0.720042	7.4561
58	CAHPO4	0	0.0094	0.0097	7.1574E-08	8.3931E-08	1.172642	7.0761
59	CAH2PO4+	1	0.0001	0.0001	1.0152E-09	7.3101E-10	0.720042	9.1361
60	CASO4 AQ	0	109.1696	112.4446	8.2969E-04	9.7293E-04	1.172642	3.0119
61	CUCL	0	0.0000	0.0000	3.4961E-33	4.0997E-33	1.172642	32.3972
62	CUCL2 -1	-1	0.0023	0.0024	1.7636E-08	1.1843E-08	0.671538	7.9265
63	CUCL3 -2	-2	0.0049	0.0050	2.9791E-08	6.2256E-09	0.208978	8.2058
64	CUCL +1	1	0.0000	0.0000	4.0847E-20	2.7431E-20	0.671538	19.5616
65	CUCL2	0	0.0000	0.0000	1.4447E-21	1.6941E-21	1.172642	20.7710
66	CUCL3 -1	-1	0.0000	0.0000	2.1508E-23	1.4443E-23	0.671538	22.8403
67	CUCL4 -2	-2	0.0000	0.0000	1.1489E-25	2.4009E-26	0.208978	25.6196
68	CU(OH)+1	1	0.0000	0.0000	3.4074E-19	2.2882E-19	0.671538	18.6405
69	CUSO4	0	0.0000	0.0000	2.5983E-20	3.0469E-20	1.172642	19.5161
70	FECL +1	1	0.0000	0.0000	1.6271E-27	1.0926E-27	0.671538	26.9615
71	FECL2	0	0.0000	0.0000	3.0905E-28	3.6240E-28	1.172642	27.4408
72	FECL3 -1	-1	0.0000	0.0000	1.7893E-28	1.2020E-28	0.671538	27.9201
73	FECL4 -2	-2	0.0000	0.0000	1.9077E-28	3.9868E-29	0.208978	28.3994
74	FE(OH)+1	1	0.0203	0.0209	2.8843E-07	2.0404E-07	0.707436	6.6903
75	FE(OH)2	0	0.0009	0.0010	1.0778E-08	1.2658E-08	1.172642	7.8983
76	FEOOH -1	-1	0.0000	0.0000	1.8199E-13	1.2874E-13	0.707436	12.8903
77	FESO4	0	0.0241	0.0248	1.6403E-07	1.9235E-07	1.172642	6.7159
78	FECL +2	2	0.0000	0.0000	4.5067E-23	9.4180E-24	0.208978	23.0260
79	FECL2 +1	1	0.0000	0.0000	1.9724E-23	1.3953E-23	0.707436	22.8553
80	FECL3	0	0.0000	0.0000	3.9466E-25	4.6230E-25	1.172642	24.3346
81	FECL4 -1	-1	0.0000	0.0000	2.7481E-27	1.8455E-27	0.671538	26.7339
82	FESO4 +1	1	0.0000	0.0000	4.0728E-23	2.8813E-23	0.707436	22.5404
83	FES04)2-	-1	0.0000	0.0000	3.3026E-39	2.2178E-39	0.671538	38.6541
84	FE(OH)+2	2	0.0000	0.0000	3.5084E-18	7.3318E-19	0.208978	18.1348
85	FE(OH)2+	1	0.0000	0.0000	2.5108E-16	1.8079E-16	0.720042	15.7428
86	FE(OH)3	0	0.0000	0.0000	4.7861E-14	5.6124E-14	1.172642	13.2509
87	FE(OH)4-	-1	0.0000	0.0000	3.0462E-14	2.1934E-14	0.720042	13.6589
88	H4(BO4)-	-1	4.0101	4.1304	5.2627E-05	3.1971E-05	0.607496	4.4952
89	H2SIO4-2	-2	0.0004	0.0004	3.9439E-09	8.8452E-10	0.224277	9.0533
90	H3SIO4)-	-1	0.4820	0.4965	5.2437E-06	3.5213E-06	0.671538	5.4533
91	HAS(OH)4	0	0.0024	0.0024	1.7049E-08	1.9992E-08	1.172642	7.6991
92	HASOH8-2	-2	0.0000	0.0000	5.2432E-64	1.0957E-64	0.208978	63.9603
93	H2ASOH8-	-1	0.0000	0.0000	3.1090E-54	2.0878E-54	0.671538	53.6803
94	H3ASNOH8	0	0.0000	0.0000	6.0329E-42	7.0745E-42	1.172642	41.1503
95	HF AQ	0	0.0000	0.0000	2.5050E-10	2.9374E-10	1.172642	9.5320
96	H2CO3	0	1.0807	1.1132	1.8029E-05	2.1141E-05	1.172642	4.6749
97	CO3 -2	-2	1.7288	1.7807	2.9809E-05	6.6854E-06	0.224277	5.1749
98	HPO4 -2	-2	0.0407	0.0419	4.3862E-07	9.1661E-08	0.208978	7.0378
99	H2PO4 -1	-1	0.0015	0.0016	1.6399E-08	1.1808E-08	0.720042	7.9278
100	HS -1	-1	0.0903	0.0930	2.8259E-06	1.8390E-06	0.650789	5.7354
101	S -2	-2	0.0000	0.0000	1.1079E-14	2.3152E-15	0.208978	14.6354
102	HSO4 -1	-1	0.0002	0.0002	2.2248E-09	1.5358E-09	0.690335	8.8137
103	HNO3 AQ	0	0.0000	0.0000	5.6312E-15	6.6034E-15	1.172642	14.1802
104	HGCL +1	1	0.0000	0.0000	1.0265E-46	6.8931E-47	0.671538	46.1614
105	HGCL2	0	0.0000	0.0000	1.9951E-40	2.3295E-40	1.172642	39.6309

106	HGCL3 -1	-1		0.0000		0.0000		1.4216E-38	9.5465E-39	0.671538	38.0202
107	HGCL4 -2	-2		0.0000		0.0000		5.6294E-39	1.1764E-33	0.208978	38.9234
108	HGSO4	0		0.0000		0.0000		5.4310E-54	6.3686E-54	1.172642	53.1960
109	HGSH2S)2	0		0.0000		0.0000		2.0059E-28	2.3522E-28	1.172642	27.6285
110	HG(HS)3-	-1		0.0000		0.0000		1.7155E-26	1.1520E-26	0.671538	25.7385
111	HGSHS2-2	-2		0.0000		0.0000		6.9401E-25	1.4503E-25	0.208978	24.6385
112	KCL	0		1.2311		1.2681		1.7086E-05	2.0035E-05	1.172642	4.6982
113	HGS2 -2	-2		0.0038		0.0040		1.5024E-08	3.1396E-09	0.208978	8.5031
114	KHSO4	0		0.0000		0.0000		7.9114E-32	9.2773E-32	1.172642	31.0426
115	KSO4 -1	-1		16.0738		16.5561		1.2304E-04	8.8598E-05	0.720042	4.0526
116	KHPO4 -1	-1		0.0000		0.0000		7.6896E-30	5.5369E-30	0.720042	29.2567
117	LI(OH)	0		0.0000		0.0000		2.8948E-11	3.3945E-11	1.172642	10.4602
118	LI(SO4)-	-1		0.0000		0.0000		5.5650E-28	3.9369E-28	0.707436	27.4048
119	MGCO3 AQ	0		15.7373		16.2094		1.9311E-04	2.2644E-04	1.172642	3.6450
120	MGHCO3)+	1		14.9343		15.3823		1.8109E-04	1.2161E-04	0.671538	3.7150
121	MGF +1	1		1.3199		1.3595		3.1531E-05	2.1767E-05	0.690335	4.6622
122	MG(OH)+1	1		0.3530		0.3636		8.8394E-06	6.6344E-06	0.750555	5.1782
123	MGSO4 AQ	0		516.1073		531.5905		4.4362E-03	5.2021E-03	1.172642	2.2838
124	MG(PO4)-	-1		0.0336		0.0346		2.9152E-07	2.0900E-07	0.720042	6.6780
125	MGHPO4	0		0.1579		0.1626		1.3579E-06	1.5923E-06	1.172642	5.7980
126	MGH2PO4+	1		0.0007		0.0007		6.0906E-09	4.3855E-09	0.720042	8.3580
127	MNCL +1	1		0.0000		0.0000		3.9388E-29	2.6450E-29	0.671538	28.5776
128	MNCL2	0		0.0002		0.0002		1.3614E-09	1.5964E-09	1.172642	8.7969
129	MNCL3 -1	-1		0.0000		0.0000		2.5515E-10	1.7134E-10	0.671538	9.7661
130	MNCL4 -2	-2		0.0000		0.0000		4.6183E-30	9.6512E-31	0.208978	30.0154
131	MNHCO3+1	1		0.0000		0.0000		1.3483E-31	9.0541E-32	0.671538	31.0432
132	MNSO4 AQ	0		0.0004		0.0004		2.6236E-09	3.0765E-09	1.172642	8.5119
133	MNCL +2	2		0.0000		0.0000		4.0534E-58	8.4707E-59	0.208978	58.0721
134	MNCL2 +1	1		0.0000		0.0000		4.1837E-59	2.8095E-59	0.671538	58.5514
135	NO3 -1	-1	2.1359	2.1359	2.2000	2.2000	3.5642E-05	3.5642E-05	2.2375E-05	0.627779	4.6502
136	NACL	0		661.8432		681.6985		1.1717E-02	1.3740E-02	1.172642	1.8620
137	NACO3 -1	-1		4.0674		4.1894		5.0704E-05	3.6509E-05	0.720042	4.4376
138	NAHCO3	0		12.9643		13.3533		1.5968E-04	1.8724E-04	1.172642	3.7276
139	NA2CO3AQ	0		0.0105		0.0108		1.0245E-07	1.2014E-07	1.172642	6.9203
140	NA2SO4AQ	0		0.0000		0.0000		1.5912E-24	1.8659E-24	1.172642	23.7291
141	NASO4 -1	-1		1167.3284		1202.3483		1.0145E-02	7.3050E-03	0.720042	2.1364
142	NAHPO4-1	-1		0.0000		0.0000		3.7334E-28	2.6832E-28	0.720042	27.5705
143	NH4 +1	1		0.6355		0.6545		3.6449E-05	2.1947E-05	0.602136	4.6586
144	NH4OH	0		0.0441		0.0454		1.3007E-06	1.5253E-06	1.172642	5.8166
145	NH4PO4-2	-2		0.0000		0.0000		5.5395E-36	1.1576E-36	0.208978	35.9364
146	NH4SO4)-	-1		0.0000		0.0000		6.7304E-28	4.7613E-28	0.707436	27.3223
147	PBCL +1	1		0.0019		0.0020		8.2166E-09	5.5178E-09	0.671538	8.2582
148	PBCL2	0		0.0006		0.0007		2.4172E-09	2.8345E-09	1.172642	8.5475
149	PBCL3 -1	-1		0.0003		0.0003		1.1121E-09	7.4679E-10	0.671538	9.1268
150	PBCL4 -2	-2		0.0002		0.0002		5.9403E-10	1.2414E-10	0.208978	9.9061
151	PBSO4 AQ	0		0.0000		0.0000		7.7308E-33	9.0655E-33	1.172642	32.0426
152	PBSO42-2	-2		0.0000		0.0000		9.4109E-35	1.9667E-35	0.208978	34.7063
153	SR(OH)-1	-1		0.0000		0.0000		2.0703E-10	1.4646E-10	0.707436	9.8343
154	SRCO3 AQ	0		0.0103		0.0106		7.2397E-08	8.4896E-08	1.172642	7.0711
155	SRHCO3)+	1		0.0793		0.0817		5.5184E-07	3.7058E-07	0.671538	6.4311
156	SRSO4 AQ	0		0.9337		0.9617		5.2594E-06	6.1674E-06	1.172642	5.2099
157	ZNCL +1	1		0.0031		0.0032		3.1597E-08	2.1219E-08	0.671538	7.6733
158	ZNCL2	0		0.0012		0.0012		9.0838E-09	1.0652E-08	1.172642	7.9726
159	ZNCL3 -1	-1		0.0007		0.0007		4.3760E-09	2.9387E-09	0.671538	8.5319
160	ZNCL4 -2	-2		0.0004		0.0004		2.1815E-09	4.5589E-10	0.208978	9.3411
161	ZNSO4 AQ	0		0.0016		0.0016		1.0073E-08	1.1813E-08	1.172642	7.9277

MOLE RATIOS BASED ON ANALYTICAL MOLALITY

CL/CA	CL/MG	CL/NA	CL/K	CL/AL	CL/FE	CL/SO4	CL/HCO3	CA/MG	SQRT(CA)/NA
5.3699E+01	9.6513E+00	1.1734E+00	5.5146E+01	1.4460E+06	2.9930E+05	1.7067E+01	2.3028E+02	1.7973E-01	2.1824E-01

NH3/NA	LI/NA	K/NA	MG/CA	SR/CA	BA/CA	SO4/CL	HCO3/CL	F/CL	B/CL
8.2280E-05	5.3641E-05	2.1278E-02	5.5639E+00	3.1486E-03	2.1887E-05	5.2446E-02	4.3424E-03	1.2768E-04	7.9366E-0

LOG OF ACTIVITY RATIOS

CA/H2	MG/H2	NA/H	K/H	AL/H3	FE/H2	CA/MG	NA/K
13.5517	14.3298	7.5673	5.8811	8.6072	9.7178	-0.7781	1.6862

LOG(NA/K)+1/3LOG(SQRT(CA)/NA) = 1.452E+00 LOG(NA/K)+4/3LOG(SQRT(CA)/NA) = 7.906E-01

SUBSURFACE TEMPERATURE (OC) FROM CHEMICAL DATA

QTZ TEMP (CONDUCTIVE)= 24.6 QTZ TEMP (ADIABATIC)= 33.9
AM.SILICA TEMP= -80.6 LOG(NA/K) TEMP= 89.6
LOG(NA/K)+1/3LOG(SQRT(CA)/NA) TEMP= 173.2 LOG(NA/K)+4/3LOG(SQRT(CA)/NA) TEMP= 270.0

IF THE SPRING IS BOILING OR STEAM IS LOST DURING RODUCTION THEN SELECT QTZ TEMP ADIABATIC ELSE SELECT QTZ TEMP CONDUCTIVE
AM.SILICA TEMP SHOULD BE CONSIDERED IF SAMPLE IS SATURATED WITH AM.SILICA I.E. IF DELG OF MIN.NO.275 IS POSITIVE
NA/K TEMP IS USEFUL IF CONC. OF CA IS LOW (MORE DEGS) VS NA
USE --4/3LOG-- TEMP IF <100 ELSE USE--1/3- TEMP
READ FOURNIER & TRUESDELL 1973

SEA WATER ANALYSIS (GOLDBERG,1963) TEST FOR SOLMNEQ JUNE,1972

	PHASE	AP	KT	LOG AP	LOG KT	AP/KT	DELG	LOG AP/KT
138	ACMITE	1.0233E+00	9.9770E+59	0.0100	59.9990			
139	AG	6.0579E+03	3.3113E-01	3.7823	-0.4800	1.8294E+04	5.8150	4.2623
140	AG2S A	6.9215E-26	3.6308E-22	-25.1598	-21.4400	1.9063E-04	-5.0749	-3.7198
141	AGCL	5.7348E-15	1.8197E-10	-14.2415	-9.7400	3.1515E-05	-6.1413	-4.5015
142	ADULARIA	5.6296E+02	1.8197E+01	2.7505	1.2600	3.0937E+01	2.0334	1.4905
143	AKERMANI	3.9333E+33	5.4954E+45	33.5948	45.7400	7.1574E-13	-16.5695	-12.1452
144	ALBITE L	2.7333E+04	8.7096E+03	4.4367	3.9400	3.1382E+00	0.6776	0.4967
145	ALBITE H	2.7333E+04	1.0000E+05	4.4367	5.0000	2.7333E-01	-0.7685	-0.5633
146	ALUNITE			-90.0730	-85.5300		-6.1979	-4.5430
147	ANALCIME	2.1671E+08	2.2909E+09	8.3359	9.3600	9.4597E-02	-1.3972	-1.0241
148	ANDALUSI	1.9186E+13	3.6308E+12	13.2830	12.5600	5.2842E+00	0.9863	0.7230
149	ANHYDRIT	4.8762E-06	2.2387E-05	-5.3119	-4.6500	2.1781E-01	-0.9030	-0.6619
150	ANNITE	7.4409E+31	3.1623E+26	31.8716	26.5000	2.3530E+05	7.3284	5.3716
151	APATCHLR	2.7923E-48	7.0795E-67	-47.5540	-66.1500	3.9442E+18	25.3701	18.5960
152	APATFLUR	2.0569E-52		-51.6868	-71.5800		27.1400	19.8932
153	APATHYDX	1.0404E-53	6.9183E-62	-52.9828	-61.1600	1.5039E+08	11.1560	8.1772
154	ARAGONIT	1.5027E-08	4.7863E-09	-7.8231	-8.3200	3.1395E+00	0.6779	0.4969
155	BARITE	9.1341E-11	1.9953E-10	-10.0393	-9.7000	4.5779E-01	-0.4629	-0.3393
156	BIOTITE		9.9770E+59		59.9990			
157	BOEHMITE	3.9002E+08	3.8905E+08	8.5911	8.5900	1.0025E+00	0.0015	0.0011
158	BORNITE	7.7943E-75		-74.1082	-115.2900		56.1836	41.1818
159	BRUCITE	2.0595E-14	6.1660E-12	-13.6862	-11.2100	3.3402E-03	-3.3783	-2.4762
160	CALCITE	1.5027E-08	4.3652E-09	-7.8231	-8.3600	3.4424E+00	0.7324	0.5369
161	CACL2	2.4727E-04	3.0903E+11	-3.6068	11.4900	8.0014E-16	-20.5963	-15.0968
162	CAO LIME	3.4971E+13	4.2658E+32	13.5437	32.6300	8.1980E-20	-26.0391	-19.0863
163	CA(OH)2	3.4330E-15	4.3652E-06	-14.4643	-5.3600	7.8645E-10	-12.4209	-9.1043
164	CAS	5.2039E-01	7.9433E+11	-0.2837	11.9000	6.5513E-13	-16.6220	-12.1837
165	CELESTIT	3.8914E-08	3.9811E-07	-7.4099	-6.4000	9.7747E-02	-1.3778	-1.0099
166	CHALCEDN	1.2381E-04	2.8184E-04	-3.9072	-3.5500	4.3931E-01	-0.4874	-0.3572
167	CHLOR MG		1.0471E+59	77.0454	59.0200		24.5918	18.0254
168	CRYSOCOL	1.4662E-07	9.9770E+59	-6.8338	59.9990			
169	CRYSOTIL	1.3642E+35	1.6218E+32	35.1349	32.2100	8.4118E+02	3.9904	2.9249
170	CINNABAR	2.7058E-50	1.6596E-40	-49.5677	-39.7800	1.6304E-10	-13.3532	-9.7877
171	CINABMET	2.7058E-50	3.8019E-39	-49.5677	-38.4200	7.1169E-12	-15.2086	-11.1477
172	CLINENST	2.5976E+10	2.2909E+11	10.4146	11.3600	1.1339E-01	-1.2898	-0.9454
173	CLINPTIL	8.2783E+04	9.9770E+59	4.9179	59.9990			
174	CORUNDUM	1.5496E+17	3.9811E+17	17.1902	17.6000	3.8923E-01	-0.5591	-0.4098
175	CRISTOBA	1.2381E-04	4.3652E-04	-3.9072	-3.3600	2.8364E-01	-0.7466	-0.5472
176	CRISTOBB	1.2381E-04	1.5488E-03	-3.9072	-2.8100	7.9941E-02	-1.4969	-1.0972
177	CU	4.3306E+05	2.1878E+04	5.6366	4.3400	1.9795E+01	1.7689	1.2966
178	CU2O	2.3770E-08	3.2359E-02	-7.6240	-1.4900	7.3458E-07	-8.3685	-6.1340
179	CU2S	3.5372E-22	2.0893E-35	-21.4513	-34.6800	1.6930E+13	18.0476	13.2287
180	CU5FES6		9.9770E+59	-87.8071	59.9990			
181	CUFES2	1.3946E-21	9.1201E-45	-20.8555	-44.0400	1.5292E+23	31.6302	23.1845
182	CUFE2S3	1.0637E-25	9.9770E+59	-24.9732	59.9990			
183	CUO	1.2288E-03	6.9183E+07	-2.9105	7.8400	1.7762E-11	-14.6667	-10.7505
184	CUS	1.8286E-17	8.9125E-23	-16.7379	-22.0500	2.0517E+05	7.2472	5.3121
185	CUMMINGT	5.0375E+36	9.9770E+59	36.7022	59.9990			
186	DICKITE	2.2892E+09	3.7154E+08	9.3597	8.5700	6.1615E+00	1.0774	0.7897
187	DIOPSIDE	1.1247E+20	7.2444E+19	20.0511	19.8600	1.5526E+00	0.2606	0.1911
188	DOLOMITE	1.3546E-15	1.0000E-17	-14.8682	-17.0000	1.3546E+02	2.9084	2.1318
189	ENSTATIT	2.5976E+10	9.9770E+59	10.4146	59.9990			
190	ERIONITE	4.5179E+11	9.9770E+59	11.6549	59.9990			
191	FAYALITE	3.2525E+15	1.6596E+17	15.5122	17.2200	1.9598E-02	-2.3299	-1.7078
192	FEASS		9.9770E+59		59.9990			

193	FECL2	3.6240E-08	7.9433E+07	-7.4408	7.9000	4.5623E-16	-20.9292	-15.3409
194	FECL3	3.4307E-26	2.1878E+12	-25.4646	12.3400	1.5682E-38	-51.5762	-37.8046
195	FECO3	2.2023E-12	2.0417E-11	-11.6571	-10.6900	1.0787E-01	-1.3194	-0.9671
196	FEO	5.1254E+09	2.2909E+12	9.7097	12.3600	2.2373E-03	-3.6157	-2.6503
197	FE2O3HEM	3.3296E+00	1.1749E-02	0.5224	-1.9300	2.8339E+02	3.3458	2.4524
198	FE2O3MGH	3.3296E+00	2.5119E+06	0.5224	6.4000	1.3255E-06	-8.0187	-5.8776
199	FE3O4	1.7065E+10	3.7154E+06	10.2321	6.5700	4.5932E+03	4.9962	3.6621
200	FEOH3AM	1.7748E-42	6.3096E-38	-41.7509	-37.2000	2.8128E-05	-6.2087	-4.5509
201	FES2 PYR			-76.8084	-103.3000		36.1421	26.4716
202	FESTRULT	7.6269E-05	1.2589E-50	-4.1177	-49.9000	6.0582E+45	62.4601	45.7823
203	FESMAKIN	7.6269E-05	9.9770E+59	-4.1177	59.9990			
204	FORSTERI	5.4498E+24	1.9055E+29	24.7364	29.2800	2.8601E-05	-6.1988	-4.5436
205	FLUORITE	1.3418E-12	8.9125E-10	-11.8723	-9.0500	1.5055E-03	-3.8504	-2.8223
206	GOETHITE	1.8079E+00	8.5114E-02	0.2572	-1.0700	2.1241E+01	1.8106	1.3272
207	GIBBS AM	3.8287E-34	3.8905E-33	-33.4169	-32.4100	9.8414E-02	-1.3738	-1.0069
208	GIBBS C	3.8287E-34	1.7378E-33	-33.4169	-32.7600	2.2032E-01	-0.8963	-0.6569
209	GREENALI	1.9891E+21	6.3096E+23	21.2987	23.8000	3.1525E-03	-3.4125	-2.5013
210	GREIGITE	8.3676E-46	1.9953E-20	-45.0774	-19.7000	4.1937E-26	-34.6220	-25.3774
211	GYPSUM	4.6991E-06	1.3804E-05	-5.3280	-4.8600	3.4042E-01	-0.6385	-0.4680
212	HALITE	9.7273E-02	3.8019E+01	-1.0120	1.5800	2.5585E-03	-3.5362	-2.5920
213	HALLOYSI	2.2892E+09	1.9953E+11	9.3597	11.3000	1.1473E-02	-2.6471	-1.9403
214	HEULANDI	2.1633E+03	9.9770E+59	3.3351	59.9990			
215	HGO	1.8183E-36	3.0200E+02	-35.7403	2.4800	6.0210E-39	-52.1433	-38.2203
216	HUNTITE	1.1009E-29	6.0256E-33	-28.9583	-32.2200	1.8270E+03	4.4499	3.2617
217	HYDRMAGN	1.4274E-35	6.3096E-31	-34.8454	-30.2000	2.2623E-05	-6.3377	-4.6454
218	ILLITE	1.5563E+13	2.1878E+10	13.1921	10.3400	7.1137E+02	3.8911	2.8521
219	KAOLINIT	2.2892E+09	4.2658E+07	9.3597	7.6300	5.3664E+01	2.3598	1.7297
220	KENYAITE	3.4961E-36	1.0000E-25	-35.4564	-25.0000	3.4961E-11	-14.2655	-10.4564
221	KYANITE	1.9186E+13	4.5709E+12	13.2830	12.6600	4.1974E+00	0.8479	0.6230
222	K2O	5.6771E+11		11.7541	83.9100		-98.4410	-72.1559
223	LARNITE	1.5142E+23	5.7544E+38	23.1802	38.7600	2.6314E-16	-21.2553	-15.5798
224	LAUMNTIT	1.1827E+15	7.0795E+11	15.0729	11.8500	1.6706E+03	4.3969	3.2229
225	LEUCITE	4.5468E+06	7.0795E+09	6.6577	9.8500	6.4226E-04	-4.3552	-3.1923
226	LEONITE	2.1506E-12	9.9770E+59	-11.6674	59.9990			
227	MAGADITE	1.5015E-20	4.5709E-15	-19.8235	-14.3400	3.2849E-06	-7.4810	-5.4835
228	MAGNESIT	9.0149E-08	9.1201E-09	-7.0450	-8.0400	9.8846E+00	1.3574	0.9950
229	MALACHIT	6.3694E-56	6.6069E-34	-55.1959	-33.1800	9.6406E-23	-30.0359	-22.0159
230	MARIALIT	1.9862E+12	5.1286E+01	12.2980	1.7100	3.8729E+10	14.4451	10.5880
231	MEIONITE	8.6145E+60	9.9770E+59	60.9352	59.9990			
232	MERWINIT	1.3755E+47	3.0903E+68	47.1385	68.4900	4.4510E-22	-29.1295	-21.3515
233	MGCL2	1.4834E-03	1.4125E+22	-2.8287	22.1500	1.0502E-25	-34.0781	-24.9787
234	MGFE2O4	6.9854E+14	6.3096E+18	14.8442	18.8000	1.1071E-04	-5.3968	-3.9558
235	MGOPERIC	2.0980E+14	4.7863E+21	14.3218	21.6800	4.3833E-08	-10.0387	-7.3582
236	MICROCLN	5.6296E+02	1.9498E+01	2.7505	1.2900	2.8872E+01	1.9925	1.4605
237	MIRABILT	1.5509E-04	7.4131E-02	-3.8094	-1.1300	2.0921E-03	-3.6565	-2.6794
238	MNCL2	8.7730E-10	6.3096E+08	-9.0569	8.8000	1.3904E-18	-24.3610	-17.8569
239	MNCO3	5.3314E-14	3.0200E-11	-13.2732	-10.5200	1.7654E-03	-3.7561	-2.7532
240	MNO	1.2408E+08	9.1201E+17	8.0937	17.9600	1.3605E-10	-13.4604	-9.8663
241	MNO2	1.9798E-35		-34.7034	-78.8400		60.2148	44.1366
242	MNS	1.8463E-06	4.4668E-01	-5.7337	-0.3500	4.1334E-06	-7.3449	-5.3837
243	MONTICEL	9.0841E+23	2.4547E+30	23.9583	30.3900	3.7067E-07	-8.7747	-6.4317
244	MONT CA	8.7263E+07	1.3804E+06	7.9408	6.1400	6.3216E+01	2.4568	1.8008
245	MONT K	4.1539E+07	7.2444E+05	7.6185	5.8600	5.7340E+01	2.3990	1.7585
246	MONT MG	1.0924E+08	1.0965E+06	8.0384	6.0400	9.9626E+01	2.7263	1.9984
247	MONT NA	1.4959E+08	1.3183E+06	8.1749	6.1200	1.1347E+02	2.8035	2.0549
248	MONTCANA		9.9770E+59		59.9990			
249	MONTSEAN		9.9770E+59		59.9990			
250	MORDENIT	4.0309E-09	9.9770E+59	-8.3946	59.9990			
251	MUSCOVIT	8.5636E+19	4.4668E+09	19.9327	9.6500	1.9171E+10	14.0285	10.2827
252	NA2O	1.3382E+15	1.5849E+67	15.1265	67.2000	8.4435E-53	-71.0430	-52.0735