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WATEQF - A FORTRAN IV VERSION OF WATEQ, A COMPUTER PROGRAM FOR CALCULATING CHEMICAL EQUILIBRIUM OF NATURAL WATERS

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WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written in 1973 by A. H. Truesdell and B. F. Jones in Programming Language/one (PL/1). With but a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to the PL/1 version. This report notes the differences between WATEQF and WATEQ, demonstrates how to set up the input data to execute WATEQF, provides a test case for comparison, and makes available a listing of WATEQF.

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Requests, at cost, for the card deck listed in Attachment B should be directed to: Ralph N. Eicher, Chief, Office of Teleprocessing, MS 805, National Center, U.S. Geological Survey, Reston, Virginia 22092.

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ABSTRACT

WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written in 1973 by A. H. Truesdell and B. F. Jones in Programming Language/one (PL/1). With but a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to the PL/1 version. This report notes the differences between WATEQF and WATEQ, demonstrates how to set up the input data to execute WATEQF, provides a test case for comparison, and makes available a listing of WATEQF.

INTRODUCTION

WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written by Truesdell and Jones (1973) in Programming Language/one (PL/1). With but a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to the PL/1 version. For discussion of the program theory and original source of most of the thermochemical data, see Truesdell and Jones (1974). It is the purpose of this report to note the differences between WATEQF and WATEQ, demonstrate how to set up the input data to execute WATEQF, provide a test case for comparison (Attachment A), and make available a listing of WATEQF (Attachment B). This report also provides a list of all equilibrium reactions that are considered (Attachment C).

DIFFERENCES BETWEEN WATEQF AND WATEQ

1. In addition to the 100 aqueous species used in the WATEQ aqueous model, WATEQF includes 14 species of manganese and computes saturation data for 21 manganese minerals. See Table 1 for the thermochemical data used.

2. All reference to maximum and minimum estimates of log K used by WATEQ have been omitted in WATEQF.

3. In addition to calculating pe from dissolved oxygen and Eh, pe can also be set by the dissolved oxygen relation of Sato (1960) and by the $SO_4^{=}$ / $S^{=}$ ratio.

4. The carbon-bearing species are computed from either titration alkalinity, carbonate alkalinity, or total carbon in solution.

5. An option has been added that allows calculation of activity coefficients of charged ion pairs from either the Debye-Hückle equation or the Davies equation.

6. Thermodynamic data used in the program can be changed through the use of optional input cards.

7. Various print options are provided to limit the amount of printed output.

8. WATEQF now consists of a main program and 5 subroutines, PREP, SET, MODEL, PRINT, and SAT. PREP reads the water data, converts the units of concentration to molality, and calculates all temperature dependent data at the temperature of the water

sample. SET initalizes values of individual species for the iterative Mass Action - Mass Balance loop. MODEL calculates activity coefficients and solves Mass Action and Mass Balance equations for the species considered. PRINT prints the results calculated from the aqueous model, and SAT calculates and prints the thermodynamic saturation state of the water with respect to the various minerals considered by the program.

9. The method of convergence on Mass Balance for anions has been changed to a more accurate and rapid convergence method, essentially identical to the method used by Truesdell and Jones (1974) for Mass Balance on cations.

10. The aqueous model will not be solved on analyses if pH is outside the interval 3.0 - 11.0, or if there is greater than 30 percent error in charge balance. This procedure is useful in screening data for punching and/or errors in the analysis. The procedure can be ignored, however, with the appropriate option specified in the input.

11. There are several changes in the aqueous model over those of Truesdell and Jones (1973) as shown in Table 1 and Attachment B, although none results in major differences between the calculations of WATEQ and WATEQF for most natural waters. The choice of speciation, thermodynamic data, and activity coefficients used by WATEQF are in a continuous process of revision, as better data become available. The responsibility for final selection of constants used in WATEQF rests with the user.

INPUT

The data matrix of species considered and thermochemical constants is read initially, either from disk or cards. The format of the data matrix is summarized as follows:

Variables	Format
(NSPEC(I), Z(I), GFW(I), DHA(I), I=1,115)	(5X, A8, 2X, I2, 3X, F10.4, 1X, F4.1)
(NREACT(I), DH(I), LOGKTO(I), I=1,193)	(5X, A8, 2X, 2F10.4)

Following input of the data matrix, data cards for one or more water analyses are read. Each water analysis requires 5 cards (4 data cards followed by a blank card). WATEQF can receive additional data on option cards that fit into the data stream between card 4 and the blank card (5).

The required input for each water analysis is summarized as follows:

Card	Variables	Format	Comments
1	TITL	20A4	Title
2	TEMP, PH, EHM, EHMC, EMFZ, DENS, DOX, FLAG, CORALK, PECALC, IGO, (PRT(I), I=1,4) IDAVES, ISPEC, IMIN	(5(F6.0,1X), 2F5.0, 1X, 9I1, 2I3)	See description below
3	CUNITS(I) (I=1,2,3,4, 5,6)	(6E12.5,8X)	Ca,Mg,Na,K,Cl,SO_4 (in order)
4	CUNITS(I) (I=7,35,8,45, 88,62)	(6E12.5,8X)	HCO_3^-,SiO_2,Fe,PO_4, SR, F (in order)
----------Optional input appears here-----			
5	Blank card		Required to note end of data for a particular analysis

DESCRIPTION OF INPUT VARIABLES

NSPEC(I)	Names of the species
Z(I)	Charge of the species
GFW(I)	Gram formula wt. of ith species
DHA(I)	Debye-Hückel $\mathring{a}$ parameter for ith species
NREACT(I)	Name of ith reaction
DH(I)	ΔH_r^o for ith reaction (Kcal/mole)
LOGKTO(I)	Log K for the ith reaction at 25°C
TITL	General description, identifying information, etc.
TEMP	Temperature in degrees C.
pH	Negative log of the activity of hydrogen ion.
EHM	"True" Eh of solution to which no temperature correction will be made (volts)

EHMC — Electical potential (volts) of the Eh cell with a calomel reference electrode.

EMFZ — Electrical potential (volts) of the Eh cell with calomel reference in Zobell's solution.

DENS — Solution density (g/cm^3). If not known, read 1.0.

DOX — Dissolved oxygen content (mg/l).

FLAG — Signal for units of input concentrations (CUNITS). 1=meq/l, 2=mg/l, 3=ppm, 4=molality.

CORALK — Carbon signal. Set to zero (or blank) if the alkalinity has not been corrected for silica, boron, etc. CORALK=1 if this correction has been made. Normally, one would report alkalinity as HCO_3 (and CO_3 if detected) and set CORALK to zero. To input total carbon rather than alkalinity, set CORALK to 2. Total CO_2 can then be input as HCO_3^-, or, if desired, as the individual species of HCO_3^-, $CO_3^=$ and $H_2CO_3^*$. $H_2CO_3^*$ and $CO_3^=$ are read on an optional "CONC" card. ($H_2CO_3^*$ denotes $H_2CO_3^o + CO_{2aq}$).

PECALC — Signal for pe calculation. If PECALC = 0, pe is set to 100 and oxidation-reduction is ignored. =1 computes pe from Eh, =2 computes pe from dissolved oxygen, =3 computes pe from dissolved oxygen using the Sato (1960) relation, =4 computes pe from $SO_4^= / S^=$.

IGO — =0 or blank, if desired to have the data checked for possible input error or analytical error. pH must be greater than 3 and less than 11 and the analysis must have less than 30% error in charge balance. =1 if this check is not desired.

PRT(I), I=1,4 — Signals which when set to some non-zero value (say 1) omit print of: I=1, thermochemical data table; I=2, mass balance convergence iterations; I=3, ion ratios; I=4, mineral saturation calculations. To obtain the above printout, leave the appropriate value of PRT(I) blank or zero.

IDAVES — Signal used to indicate desired method of calculation of activity coefficients, γ_i, of charged ion pairs. If 1, the Davies equation,

$$\log \gamma_i = \frac{-A\, z_i^2 \sqrt{I}}{1 + \sqrt{I}} - 0.3I$$

is used. If zero, or blank, the Debye-Hückel equation,

$$\log \gamma_i = \frac{-A\, Z_i^2\, \sqrt{I}}{1 + Ba_i\, \sqrt{I}}$$

is used. A and B are constants that depend on the dielectric constant, density and temperature of the solvent, Z_i is the charge on the ion, I is ionic strength ($I = 1/2\ \Sigma_i\ m_i\ Z_i^2$, where m_i is the molality of the ith ion), and a_i is the "ion size" parameter. As a general rule, the Davies equation is probably accurate to ionic strengths less than 0.5 and the Debye-Hückel equation is more accurate at ionic strength less than 0.1 (Stumm and Morgan, 1970). Activity coefficients of Ca^+, Mg^{++}, Na^+, K^+, Cl^-, $SO_4^=$, $CO_3^=$, and HCO_3^- are always calculated from the extended Debye- Hückel equations of Truesdell and Jones (1974).

ISPEC — Number of species desired in output (if less than total number possible for the given water analysis). Leave ISPEC blank or zero to obtain output for all possible species for the defined system. If ISPEC is greater than zero, ISPEC values of KSPEC (species index numbers) must be read (Type 1 optional input; see below).

IMIN — Number of minerals for which saturation data are required (if less than the total possible). Leave IMIN blank (or zero) to obtain saturation data on all possible minerals for the defined system. If IMIN is greater than zero, IMIN values of KMIN (mineral reaction index numbers) must be read (Type 1 optional input; see below).

Total concentration (units of FLAG) of Calcium (1), Magnesium (2), Sodium (3), Potassium (4), Chloride (5), Sulfate (6), Carbon, as HCO_3^-, (7),Silica, as SiO_2, (35) Iron (8), Phosphate, as PO_4^{3-} (45), Strontium (88), and Fluoride (62), where the numbers in parentheses are the appropriate species index numbers in the program. To enter other species, use Type 2 optional input cards (see below).

DESCRIPTION OF OPTIONAL INPUT

Additional input is optional and must appear between cards 4 and 5. Two types of optional input cards are used, Type 1 and Type 2. If used, Type 1 optional input cards must precede Type 2 optional input cards.

Type 1 Optional Input

These cards are used to limit the number of species or minerals in the output. Omit these cards to obtain the complete calculated results for the given water analysis. To specify individual species for which output is desired, read ISPEC values of KSPEC(I),

Variable	Format
(KSPEC(I), I=1, ISPEC)	(16I5)

where KSPEC(I) is the index number of the ith species for which output is desired. Species index numbers are listed in the data tables of Attachment A. To specify individual minerals for which saturation data is desired, read IMIN values of KMIN(I),

Variable	Format
(KMIN(I), I=1, IMIN)	(16I5)

where KMIN(I) is the index number of the ith mineral reaction for which saturation output is desired. Mineral index numbers are listed in the data tables of Attachment A. If values of both KSPEC(I) and KMIN(I) are entered, KSPEC(I) must be read before KMIN(I).

Type 2 Optional Input

Type 2 optional input cards are used to (1) enter the total concentrations of species not included on cards 3 and 4 ("CONC" card(s)); (2) change the convergence tests on mass balance for anion species ("EROR" card); (3) change ΔH^o_r ("DELH" card(s)); (4) change log K at 25°C ("TABL" card(s)); or, (5) change existing analytical expressions for logK(T), or enter new analytical expressions for reactions previously defined by the Van't Hoff equation ("LOGK" card(s)). It is possible to use none, 1,2,3, 4, or all 5 cases of type 2 optional input in a single data set, providing the sequencing is 1., "CONC", 2., "EROR", 3., "DELH", 4., "TABL", 5., "LOGK". The form of type 2 optional input cards is

Variable	Format
(WORD,(INT(I),VAL(I), I=1,5))	(A4,1X,5(I3,E12.5))

where WORD is "CONC", "EROR", "DELH", "TABL", or "LOGK". The meaning of INT(I) and VAL(I) is described below for each value of WORD.

"CONC" enters concentration (units of FLAG) of constituents not on card 3 and 4. INT(I) = 17 (H_2S), 18 (CO_3), 39 (NH_4), 51 (Al), 81(Li), 85 (NO_3), 86 (H_2CO_3), 87 (B), 90 (Ba), 98 (Br), and 101 (Mn). VAL (I) is the concentration of the INT(I) constituent.

"EROR" overrides pre-set mass balance convergence constraints on anions. Pre-set values of EROR1-EROR5 are 0.001 (0.1 percent error in mass balance). EROR1-EROR5 are entered on the "EROR" card as VAL (1) - VAL (5). In the order 1=carbon, 2=sulfate, 3=fluoride, 4=phosphate, 5=chloride. Values of INT(I) are not used.

"DELH" overrides values of the standard delta enthalpy of reaction (25 degrees C) used in computing the temperature dependence of equilibrium constants from the Van't Hoff equation. INT(I) is the index number of the ith reaction (see Attachment A) for which DH(I) is to be changed and VAL(I) is the appropriate new value of DH(INT(I)).

"TABL" overrides values of LOGKTO(INT(I)) (log K of reaction at 25 degrees C used in computing the temperature dependence of equilibrium constants from the Van't Hoff equation). INT(I) is the index number of the ith reaction (see Attachment B) for which LOGKTO is to be changed and VAL(I) is the appropriate new value of LOGKTO(I).

"LOGK" overrides existing analytical expressions for log K as a function of T (degree K), or enters as many as 35 new, previously undefined analytical expressions for log K (T degrees K).The form of the analytical expression must be

$$\text{Log KT(INT(I))} = A + BT + C/T + DT^2 + E/T^2,$$

where T is temperature in degree K and A,B,C,D, and E are fit parameters (may be zero or blank). INT(1) is the index number of reaction (see Attachment A) and INT(2)-INT(5) are ignored. VAL(1)=A, VAL(2)=B, VAL(3)=C, VAL(4)=D, VAL(5)=E.

Values of A,B,C,D, and E for analytical expressions pre-set in the program are listed in the data tables of Attachment A. Note that the analytical expression for reaction (26) is further modified in the program (see card B1600 of Attachment B). If any of the cards, "EROR", "DELH", "TABL", "LOGK", are used in a particular water data set, calculations for that data set and all subsequent data sets will use the new input values. The last card in each water analysis data set must be blank, whether option cards are used or not.

OXIDATION-REDUCTION OPTIONS

There are several possible options that result from choosing appropriate values of EHM, EHMC, DOX, EMFZ, and PECALC. To specify Eh directly, the desired value should be read as EHM (in volts). This value of Eh will not be corrected for temperature. If the redox potential with Calomel reference was measured in the field and it is desired to correct that measurement for temperature, the measured value should be read as EHMC (in volts). EHM must then be greater than 9.0. Any value of EHMC less than 9.0 is then considered real and a temperature-corrected Eh (EHM) is computed. If no Eh was measured, EHMC and EHM should be greater than 9.0. If the Eh-Calomel of a standard Zobell's solution was measured in the field, read the value as EMFZ (in volts) and EHMC will be corrected. If EMFZ is greater than 9.0, EHMC will be corrected for temperature only (provided EHMC is less than 9.0).

Oxidation-reduction equations used in calculating the distribution of species are written in terms of pe. pe can be computed from Eh, dissolved oxygen, or $SO_4^{=}$ / $S^{=}$. If PECALC = 1, pe is calculated from Eh. If PECALC = 2, pe is computed from dissolved oxygen. If PECALC = 3, pe is computed from dissolved oxygen using the relation of Sato (1960). If PECALC = 4, pe is computed from $SO_4^{=}$ / $S^{=}$ (provided $SO_4^{=}$ and total H_2S are entered). If PECALC = 0, redox relations are ignored. If pe is to be computed from dissolved oxygen, a real value of DOX must be read, and to calculate pe from Eh requires either a real value of EHM or EHMC to be read.

Six possible examples of redox options are tabulated and discussed below:

	EHM	EHMC	EMFZ	DOX	PECALC
1)	< 9	> 9	> 9	blank	1
2)	< 9	> 9	> 9	> 0.0	2
3)	> 9	< 9	> 9	blank	1
4)	> 9	< 9	> 9	> 0.0	2
5)	> 9	< 9	< 9	blank	1
6)	blank or >9	blank or >9	blank or >9	blank	0

1) Eh is to be used without correction and pe is to be computed from Eh.

2) Same as 1) but pe is computed from dissolved oxygen.

3) Eh was measured in the field and it is desired to correct that measurement for temperature. The Eh of standard Zobell's solution was not measured. pe is to be computed from Eh.

4) Same as 3) but pe is to be computed from dissolved oxygen.

5) Eh was measured in the field as well as the Eh of standard Zobell's solution. pe is to be computed from Eh.

6) No information on oxidation-reduction is available, and redox relations are to be ignored. (pe is set to 100)

Other possible options should be obvious from these examples.

OUTPUT

The output of WATEQF consists of a table of data constants used in the calculations (printed once). The output for each water analysis lists the title card and tabulates most of the input data. At the end of each iteration through the equilibria equations, the difference between the computed and analytical anion species is tabulated so that convergence progress can be followed. When convergence on the aqueous model has been obtained, various parameters that describe the solution are printed. Some of these are ionic strength, activity of water, comparison of computed and analytical charge balance, pH, pe, temperature, P_{CO_2}, P_{O_2}, total dissolved solids, and others. The concentration of each aqueous species (value greater than zero) is printed as ppm, molality, and activity, and log values, as well as ionic activity coefficients and their logs. Mole ratios and log activity ratios are computed and tabulated. The activity product of 101 minerals and their saturation index, ΔG_r and logK are printed. Saturation output for minerals in which the activity of an ith species in the reaction is zero are omitted from the tabulation. Parts of the output can be deleted with appropriate values of PRT(I), as described above, and by use of the ISPEC and IMIN options.

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Table 1: Revised Thermochemical Data[1/,2/]

I	NREACT	Source	ΔH_r^o	LogK 25°C	Analytical Expression for log K(T°K)
10	SIDERITE	1		-10.55	
13	CALCITE	2[3/]			13.543 - 0.0401T - 3000./T
25	KMGOH	3			0.684 + 0.0051T
31	KNAHPO	4	0.0	0.29	
33	KKHPO	4	0.0	0.29	
36	KH2CO3	5[4/]			-14.8435 + 0.032786T + 3404.71/T
63	FLUOR	6		-10.50	
69	KHCO3	7[4/]			-6.4980 + 0.02379T + 2902.39/T
74	KMGCO3	8			0.991 + 0.00667T
75	KMGHCO3	9			$2.319 - .011056T + 2.29812 \times 10^{-5} T^2$
78	KCAHCO3	2			-2.95 + .0133T
79	KCACO3	10			-27.393 + 4114/T + .05617T
80	KCAF+	11	4.12	0.94	
149	BLANK	12			
158	KMN 3+	13	25.760	-25.507	
159	KMNCL+	14	0.0	0.607	
160	KMNCL2	14	0.0	0.041	
161	KMNCL3-	14	0.0	-0.305	
162	KMNOH+	14	0.0	3.449	
163	KMN(OH)3	14	0.0	7.782	
164	KMNF+	14	0.0	0.850	
165	KMNSO4	15	3.700	1.708	
166	KMNNO3,2	14	-0.396	0.059	
167	KMNHCO3+	16	0.0	1.716	

UNITED STATES GOVERNMENT

Memorandum

TO : The Record

DATE: April 21, 1977

FROM : L. Niel Plummer

SUBJECT: Summary of Errors, changes and revision of WATEQF

1. Reaction 91 log K_{25} = +40.64 , ΔH_r° = -65.44. ΔH_r° is wrong in write up. Program is correct, however.

2. Table errors on ΔH_r° and log K_{25} for reaction 90. Correct ΔH_r° = 4.9104. Correct log K_{25} = 1.9869. Analytical expression which is currently used in the program is correct.

3. Summation of mass balance on anions now preceeds anion loop. Listing shows summation within anion loop. Printed mass balance in sea water test case in WRI 76-13 are eroneous owing to improper location of summation.

4. CaF^+ was enormously summed into CO_{2TOT}. See card E320.

5. If Fe or Mn are specified without redox information, the program will now set PE to zero, print a message stating that such has occurred, and continue calculation. Previously, the program would fail on iteration. With this change, the program will not fail but, of course, one should always supply desired redox information whenever iron and/or manganese are specified.

6. A new option for units of input concentration has been added. Millimoles per liter (1000 x M) may be input. For this case, FLAG is set to zero.

7. In correcting titration alkalinity for non-carbonate alkalinity, a new option (CORALK = 3) has been added which considers all possible non-carbonate alkalinity species. This is similar to CORALK = 0 which considers only the major non-carbonate alkalinity species.

8. The values of EPM are now correctly calculated from PPM rather than molality.

9. Prints have been added to show:

   a) FLAG, CORALK, PECALC, IDAVES options

   b) charge balance in Meq/kg H_2O

   c) total alkalinity in Meq/kg H_2O

   d) carbonate alkalinity in Meq/kg H_2O

10. It is now possible to override an existing analytical expression with a Van't Hoff relation for the temperature dependence of equilibrium constants. This is done internally whenever an optional DELH or TABL card is used for a pre-existing analytical expression.

11. The minimum number of iterations required to solve the aqueous model within the mass balance limits has been changed from 5 to 2.

12. Corrections to WRI 76-13

   a) Page 54, line 69 should read: $CO_3^{2-} + H^+ = HCO_3^-$

   b) Page 57, line 127 should read: $Li^+ + SO_4^{2-} = LiSO_4^-$

13. Other changes have been made to improve the efficiency of the program which may be found by comparison of a current listing with that in WRI 76-13.

Niel Plummer

L. Niel Plummer
Hydrologist

UNITED STATES GOVERNMENT

Memorandum

TO : Users of WATEQF - A FORTRAN IV version of WATEQ: A Computer Program for Calculating Chemical Equilibria of Natural Waters

DATE: May 17, 1977

FROM : L. Niel Plummer, WRN, NR

SUBJECT: Change of resident disk for WATEQF and TABLES, and program revision.

Due to a recent upgrading of on-line disk facilities in the Northeastern Region, it has been necessary to move the program WATEQF and data TABLES from the on-line disk CCD907 to CCD808. To use WATEQF off a Reston disk after May 17, 1977, your control language should be changed to indicate the new location of the program and data file (CCD808).

The following control cards will now execute the program:

```
/*RELAY  PUNCH RE2
//...(JOB CARD)...
/*ROUTE  PRINT REMOTEXX
//EXEC PGM=WATEQF,REGION=110K
//STEPLIB DD UNIT=3330,VOL=SER=CCD808,DISP=SHR,DSN=BFJONES.PGMLIB
//FT05F001 DD DDNAME=SYSIN
//FT06F001 DD SYSOUT=A
//FT07F001 DD SYSOUT=B
//FT09F001 DD UNIT=3330,VOL=SER=CCD808,DISP=SHR,
// DSN=BFJONES.TABLES.WATEQF
//SYSIN DD *
   Insert Water Analyses Here
//
$$$
```

In addition a revision of WATEQF has recently been completed. The more important changes are summarized on the attached memo dated April 21, 1977. You may obtain current listings or card decks of WATEQF by using one of the attached utility routines.

If you have any questions or problems, feel free to contact me.

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Hydrologist

Attachment

I	NREACT	Source	ΔH_r^o	LogK 25°C	Analytical Expression for log K(T°K)
168	KMNO4-	14	176.620	-127.824	
169	KMNO4--	14	150.020	-118.440	
170	BLANK	12			
171	KHMNO2--	17	0.0	-34.440	
172	MANGANO	18	-24.025	17.938	
173	PYROLUST	18	-29.180	15.861	
174	BIRNSITE	19	0.0	18.091	
175	NUSTITE	19	0.0	17.504	
176	BIXBYITE	18	-15.245	-0.611	
177	HAUSMITE	18	-80.140	61.540	
178	MNOH2	19	4.100	-12.912	
179	MNOH3	17	20.090	-35.644	
180	MANGANIT	19	0.0	-0.238	
181	RHODOCHR	18	-2.079	-10.539	
182	BLANK	12			
183	MNCL2	18	-17.622	8.760	
184	MNCL2,1W	14	-7.175	5.522	
185	MNCL2,2W	14	1.710	3.974	
186	MNCL2,4W	14	17.380	2.710	
187	TEPHRITE	18	-40.060	23.122	
188	RHODONIT	18	-21.885	9.522	
189	MNS GRN	17	-5.790	3.800	
190	MNSO4	14	-15.480	2.669	
191	MN2SO4,3	17	-39.060	-5.711	
192	MN3PO4,2	17	2.120	-23.827	
193	MNHPO4	14	0.0	-12.947	

Data sources for Table 1

1. Langmuir (1969).
2. Jacobson and Langmuir (1974).
3. McGee and Hostetler (1975).
4. Estimated using the pH and composition of NBS buffers (6.86 and 7.41), and charge balance.
5. Harned and Davis (1943).
6. E. A. Jenne (1975), oral communication to B. F. Jones.
7. Harned and Scholes (1941).
8. Siebert (1974).
9. Fit to the data of Siebert (1974).
10. Reardon and Langmuir (1974).
11. Nordstrom and Jenne (1976).
12. Not presently used
13. ΔG_f^o, ΔH_f^o Mn^{++}, Wagman, et. al, (1969). ΔG_f^o, ΔH_f^o Mn^{3+}, Latimer (1952).
14. Wagman, et. al. (1969).
15. ΔG_f^o, Hem (1963), ΔH_f^o Wagman, et. al, (1969).
16. Hem (1963).
17. Latimer (1952).
18. Robie and Waldbaum (1968).
19. Garrels and Christ (1965).

Footnotes to Table 1

1/ No attempt has been made for internal consistency of thermodynamic data in WATEQF. Responsibility for selection of thermodynamic data rests with the user. The revised thermodynamic data of Table 1 do not reflect the forth coming revision of U.S. Geological Survey Bulletin 1259 which may have profound effects on the thermodynamic data for Aluminium.

2/ The ion pairs $Na_2CO_3^o$ and $Na_2SO_4^o$ are no longer used in WATEQF. The CaF^+ ion pair has been added to the model.

3/ This analytical expression for the calcite equilibrium constant assumes that the ion pair $CaHCO_3^+$ is present in the aqueous model. If $CaHCO_3^+$ is deleted from the model via an optional LOGK card (by setting log $K_{CaHCO_3^+}$ to, for example, to -30.), log $K_{calcite}$ should by changed to 13.870 - 0.04035T - 305.9./T, as recommended by Jacobson and Langmuir (1974).

4/ Reactions 36 and 63 have been changed from dissociation (in WATEQ) to association in WATEQF. For the most part, all ion pair reactions are written as association in WATEQF, that is, most ion pair equilibria show the pair as a product. All mineral equilibria are written with the solid as reactant. See Attachment C for details of all reactions in WATEQF.

List of data cards for test case

```
   SEA WATER OF P.K.BREWER FROM CHEMICAL OCEANOGRAPHY (1975)
  25.0  8.20     .400     9.9     9.9  1.03 0.0  201      1
 412.          1290.          10770.          380.          19360.          2709.
 140.34        4.27           0.002           0.190         8.0             1.3
CONC  51 .002          81  0.180        85  0.20          87  4.440         90  0.002
CONC  90  0.002        98 67.           101 0.0002

//
```

DATA

I	NREACT	DH	LOGKTO
1	KFE +3	9.7000	-13.0130
2	KFEH+2	20.1150	-15.4730
3	KFECH+	13.2180	-9.3190
4	KFECH3	32.9950	-29.4580
5	KFESO4	15.9200	-8.8860
6	KFECL	18.1520	-11.6000
7	KFECL2	0.0	-10.9190
8	KFECL3	0.0	-11.9250
9	KFESO	0.5600	2.2000
10	SIDERITE	-5.3280	-10.5500
11	MAGNESIT	-6.1690	-8.2400
12	DOLOMITE	-8.2900	-17.0200
13	CALCITE	-3.1900	-8.4100*
14	KH3SIO4	8.9350	-9.9290*
15	KH2SIO4	29.7170	-21.6170*
16	KHPO4	-3.5300	12.3460
17	KH2PO4	-4.5200	19.5530
18	ANHYDRIT	-3.7690	-4.5480
19	GYPSUM	0.2610	-4.7590
20	BRUCITE	0.8500	-11.4100
21	CHRYSOTL	27.5850	-51.8000
22	ARAGONIT	-2.9590	-8.2150
23	KMGF	4.6740	1.8200
24	KCASO4	1.5000	2.3090
25	KMGOH	2.0900	2.2100*
26	KH3BO3	3.2240	-9.2400*
27	KNH3	12.4770	-9.2440*
28	FORSTRIT	4.8700	-28.1100
29	DIOPSIDE	21.1000	-36.2200
30	CLENSTIT	6.6750	-16.8700
31	KNAHPO	0.0	0.2900
32	TREMOLIT	90.2150	-140.3000
33	KKHPO4	0.0	0.2900
34	KMGHPO4	3.3000	2.8700
35	KCAHPO4	3.3000	2.7390
36	KH2CO3	-2.2430	6.3510*
37	SEPIOLIT	26.5320	-40.1000
38	TALC	45.0650	-62.2900
39	HYDMAG	-25.5200	-37.8200
40	ADULAR	30.8200	-20.5700
41	ALBITE	25.8960	-18.0000
42	ANORTH	17.5300	-19.3300
43	ANALCM	18.2060	-12.7000
44	KMICA	67.8600	-49.0900
45	PHLOG	0.0	-63.5300
46	ILLITE	54.6840	-40.3100
47	KAOLIN	49.1500	-36.9100
48	HALLOY	44.6800	-32.8200
49	BEIDEL	60.3550	-45.2600

I	NSPEC	Z	DHA	GFW
1	CA	2	6.0	40.0800
2	MG	2	6.5	24.3120
3	NA	1	4.0	22.9898
4	K	1	3.0	39.1020
5	CL	-1	3.0	35.4530
6	SO4	-2	4.0	96.0616
7	HCO3	-1	5.4	61.0173
8	FE	2	6.0	55.8470
9	FE	3	9.0	55.8470
10	FEOH	2	5.0	72.8544
11	FEOH	1	5.0	72.8549
12	FE(OH)3	-1	5.0	106.8690
13	FEHPO4	1	5.4	151.8200
14	H2S AQ	0	0.0	34.0799
15	FESO4	1	5.0	151.9086
16	FECL	2	5.0	91.3000
17	ANAL H2S	0	0.0	34.0799
18	CO3	-2	5.4	60.0094
19	MGOH	1	6.5	41.3194
20	MGF	1	4.5	43.3104
21	MGCO3 AQ	0	0.0	84.3214
22	MGHCO3	1	4.0	85.3293
23	MGSO4 AQ	0	0.0	120.3736
24	H4SIO4AQ	0	0.0	96.1155
25	H3SIO4	-1	4.0	95.1075
26	H2SIO4	-2	5.4	94.0995
27	OH	-1	3.5	17.0074
28	FECL2	1	5.0	126.7530
29	CAOH	1	6.0	57.0874
30	CAHCO3	1	6.0	101.0973
31	CACO3 AQ	0	0.0	100.0890
32	CASO4 AQ	0	0.0	136.1416
33	FECL3	0	0.0	162.2060
34	FESO4	0	0.0	151.9086
35	SIO2 TOT	0	0.0	60.0848
36	H3BO3 AQ	0	0.0	61.8331
37	H2BO3	-1	2.5	60.8251
38	NH3 AQ	0	0.0	17.0306
39	NH4	1	2.5	18.0386
40	MGPO4	-1	5.4	119.2834
41	MGH2PO4	1	5.4	121.2993
42	NACO3	-1	5.4	82.9992
43	NAHCO3	0	0.0	83.9909
44	NASO4	-1	5.4	119.0514
45	PO4	-3	5.0	94.9714
46	KSO4	-1	5.4	135.1636
47	HPO4	-2	5.0	95.9794
48	H2PO4	-1	5.4	96.9873
49	CAF+	1	5.0	59.0784

50	CHLCR	54.7600	-90.6100
51	ALUNIT	29.8200	-85.3200
52	GIBCRS	14.4700	-32.7700
53	BOEHM	11.9050	-33.4100
54	PYRCPH	0.0	-42.4300
55	PHILIP	0.0	-19.8600
56	ERICN	0.0	0.0
57	CLINOP	0.0	0.0
58	MORCEN	0.0	0.0
59	NAHCOL	3.7200	-0.5480
60	TRONA	-18.0000	-0.7950
61	NATRON	15.7450	-1.3110
62	THRNAT	-2.8020	0.1250
63	FLUCR	1.5300	-10.5000
64	MONTCA	58.3730	-45.0000
65	HALITE	0.9180	1.5820
66	THENAR	-0.5720	-0.1790
67	MIRABI	18.9870	-1.1130
68	MACKIT	0.0	-4.6310
69	KHCO3	-3.6040	10.3300*
70	KNACO3	8.9110	1.2680
71	KNAHCO3	0.0	-0.2500
72	KNASO4	1.1000	0.7200
73	KKSO4	3.0820	0.8470*
74	KMGCO3	2.7100	2.9800*
75	KMGHCO3	1.0770	1.0660*
76	KMGSO4	1.2700	2.2380
77	KCACH	1.1900	1.4000
78	KCAHCO3	5.4100	1.0150*
79	KCACO3	4.0230	3.1530*
80	KCAF+	4.1200	0.9400
81	KALOH	1.9900	8.9980
82	KALOH2	0.0	18.2350
83	KALOH4	-9.3200	33.9380
84	KALF	0.0	7.0100
85	KALF2	20.0000	12.7500
86	KALF3	2.5000	17.0200
87	KALF4	0.0	19.7200
88	KALSO4	2.2900	3.2000
89	KASC42	3.0700	5.1000
90	KHSO4	~~4.8190~~	~~2.0540*~~
91	KH2SC	~~-45.4400~~	40.6440
92	KH2S	5.2990	-6.9420*
93	KHS	12.1000	-12.9180
94	KOXY	34.1570	-20.7800
95	KCH4	-57.4350	30.7410
96	HYXAPT	17.2250	-59.3500
97	FLUAPT	19.6950	-66.7900
98	CHALC	4.6150	-3.5230
99	MAGADI	0.0	-14.3000
100	CRISTO	5.5000	-3.5860
101	SILGEL	4.4400	-3.0170
102	QUARTZ	6.2200	-4.0050
103	KFECH2	0.0	-20.1730
104	KFECH3	0.0	-26.5710
105	KFECH4	0.0	-34.8940
106	KFECH2	28.5650	-20.5700
107	VIVIAN	0.0	-36.0000
108	MAGNET	-40.6600	-9.5650
109	HEMATI	-30.8450	-4.0070
110	MAGHEM	0.0	6.3700

50	NAHPO4	-1	5.4	118.9692
51	AL	3	9.0	26.9815
52	ALOH	2	5.4	43.9889
53	AL(OH)2	1	5.4	60.9962
54	AL(OH)4	-1	4.5	95.0110
55	ALF	2	5.4	45.9799
56	ALF2	1	5.4	64.9783
57	ALF3	0	0.0	83.9767
58	ALF4	-1	4.5	102.9751
59	ALSO4	1	4.5	123.0431
60	AL(SO4)2	-1	4.5	219.1047
61	KHPO4	-1	5.4	135.0814
62	F	-1	3.5	18.9984
63	HSO4	-1	4.5	97.0696
64	H	1	9.0	1.0080
65	FEH2PO4	1	5.4	152.8340
66	H2S CALC	0	0.0	34.0799
67	HS	-1	3.5	33.0720
68	S	-2	5.0	32.0640
69	BLANK	0	0.0	1.0000
70	PO2	0	0.0	31.9988
71	PCH4	0	0.0	16.0430
72	AH2O	0	0.0	18.0153
73	MGHPO4	0	0.0	120.2914
74	CAHPO4	0	0.0	136.0594
75	CAPO4	-1	5.4	135.0514
76	CAH2PO4	1	5.4	137.0673
77	FE(OH)2	1	5.4	89.8616
78	FE(OH)3	0	0.0	106.8689
79	FE(OH)4	-1	5.4	123.8762
80	FE(OH)2	0	0.0	89.8616
81	LI	1	6.0	6.9390
82	LIOH	0	0.0	23.9464
83	LISO4	-1	5.0	103.0006
84	NH4CALC	1	2.5	18.0386
85	NO3	-1	3.0	62.0049
86	H2CO3	0	0.0	62.0253
87	B TOT	0	0.0	10.8100
88	SR	2	5.0	87.6200
89	SROH	1	5.0	104.6274
90	BA	2	5.0	137.3400
91	BAOH	1	5.0	154.3474
92	NH4SO4	-1	5.0	114.1002
93	HCL	0	0.0	36.4610
94	NACL	0	0.0	58.4428
95	KCL	0	0.0	74.5550
96	H2SO4	0	0.0	98.0775
97	BLANK	0	0.0	1.0000
98	BR	-1	4.0	79.9090
99	FEH2PO4	2	5.4	152.8340
100	FEHPO4	0	0.0	151.8200
101	MN	2	6.0	54.9400
102	MN	3	9.0	54.9400
103	MNCL	1	5.0	90.3970
104	MNCL2	0	0.0	125.8540
105	MNCL3	-1	5.0	161.3110
106	MNOH	1	5.0	71.8480
107	MN(OH)3	-1	5.0	105.9640
108	MNF	1	5.0	73.9400
109	MNSO4	0	0.0	151.0060
110	MN(NO3)2	0	0.0	178.9560

111	GOETH	25.5550	-41.2000
112	GREENA	0.0	-63.1900
113	FECH3A	0.0	4.8850
114	ANNITE	62.4800	-84.2400
115	PYRITE	11.3000	-18.4800
116	MONTBF	0.0	-34.9700
117	MONTAB	0.0	-29.7800
118	HUNTITE	-25.7600	-30.5100
119	GREGITE	0.0	-17.9700
120	FESPPT	0.0	-3.9150
121	KFEH2P	0.0	2.7000
122	KCAPO4	3.1000	6.4590
123	KCAH2P	3.4000	1.4080
124	KMGPO4	3.1000	6.5890
125	KMGH2P	3.4000	1.5130
126	KLICH	4.8320	0.2000
127	KLISO4	0.0	0.6400
128	KNH4R	-187.0550	119.0770
129	LAUMON	39.6100	-31.9600
130	KSRCH	1.1500	0.8200
131	KBACH	1.7500	0.6400
132	KNH4SO	0.0	1.1100
133	KHCL	18.6300	-6.1000
134	KNACL	0.0	-1.6020
135	KKCL	0.0	-1.5850
136	KH2SO4	0.0	-1.0000
137	KO2 SATO	0.0	-11.3850
138	KCO2	-5.0000	-1.4520
139	KFEHPO	0.0	3.6000
140	KFEHP+	0.0	-7.6130
141	ALCH3A	12.9900	-31.6100
142	PREHNT	10.3900	-11.5200
143	STRCNT	2.3610	-11.4100
144	CELEST	-1.0540	-5.9740
145	BARITE	6.1410	-9.7560
146	WITHERIT	6.9500	-13.3200
147	STRENGIT	-2.0300	-26.4000
148	LEON	90.0700	-69.5700
149	BLANK	0.0	0.0
150	NESQUE	-4.5510	-5.2110
151	ARTIN	0.4980	-18.4000
152	K O2AQ	33.4570	-21.4950
153	KW	13.3450	-13.9980
154	SEP PT	0.0	-37.2120
155	DIASP	-15.4050	-35.0600
156	WAIRKT	26.1400	-26.6200
157	KFEHP2	0.0	-7.5830
158	KMN 3+	25.7600	-25.5070
159	KMNCL+	0.0	0.6070
160	KMNCL2	0.0	0.0410
161	KMNCL3-	0.0	-0.3050
162	KMNCH+	0.0	3.4490
163	KMN(OH)3	0.0	7.7820
164	KMNF+	0.0	0.8500
165	KMNSO4	3.7000	1.7080
166	KMNO3,2	-0.3960	0.0590
167	KMNHCO3+	0.0	1.7160
168	KMNC4-	176.6200	-127.8240
169	KMNC4--	150.0200	-118.4400
170	BLANK	0.0	0.0
171	KMNO2--	0.0	-34.4400

111	MNHCO3	1	5.0	115.9590
112	MNO4	-1	3.0	118.9400
113	MNO4	-2	5.0	118.9400
114	BLANK	0	0.0	1.0000
115	MMNO2	-1	5.0	87.9480

172	MANGANO	-24.0250	17.9380
173	PYRCLUST	-29.1800	15.8610
174	BIRNSITE	0.0	18.0910
175	NUSTITE	0.0	17.5040
176	BIXBYITE	-15.2450	-0.6110
177	HAUSMITE	-80.1400	61.5400
178	MNOH2	4.1000	-12.9120
179	MNOH3	20.0900	-35.6440
180	MANGANIT	0.0	-0.2380
181	RHODOCHR	-2.0790	-10.5390
182	BLANK	0.0	0.0
183	MNCL2	-17.6220	8.7600
184	MNCL2,1W	-7.1750	5.5220
185	MNCL2,2W	1.7100	3.9740
186	MNCL2,4W	17.3800	2.7100
187	TEPHRITE	-40.0600	23.1220
188	RHODONIT	-21.8850	9.5220
189	MNS GRN	-5.7900	3.8000
190	MNSO4	-15.4800	2.6690
191	MN2SO4,3	-39.0600	-5.7110
192	MN3PO4,2	2.1200	-23.8270
193	MNHPO4	0.0	-12.9470

"*" DENOTES THAT AN ANALYTICAL EXPRESSION FOR KT HAS BEEN USED

SUMMARY OF ANALYTICAL EXPRESSIONS OF THE FORM LOG K = A+B*T+C/T+D*T**2+E/T**2

I	NREACT	A	B	C	D	E
13	CALCITE	13.5430	-0.0401	-3000.0000	0.0	0.0
14	KH3SIO4	6.3680	-0.0163	-3405.8999	0.0	0.0
15	KH2SIO4	39.4780	-0.0659	-12355.0977	0.0	0.0
25	KMGOH	0.6840	0.0051	0.0	0.0	0.0
26	KH3BO3	28.6059	0.0121	1573.2100	0.0	0.0
27	KNH3	0.6322	-0.0012	-2835.7598	0.0	0.0
36	KH2CO3	-14.8435	0.0328	3404.7100	0.0	0.0
69	KHCO3	-6.4980	0.0238	2902.3899	0.0	0.0
73	KKSO4	3.1060	0.0	-673.5999	0.0	0.0
74	KMGCO3	0.9910	0.0067	0.0	0.0	0.0
75	KMGHCO3	2.3190	-0.0111	0.0	2.2981E-05	0.0
78	KCAHCO3	-2.9500	0.0133	0.0	0.0	0.0
79	KCACO3	-27.3930	0.0562	4114.0000	0.0	0.0
90	KHSO4	-5.3505	0.0183	557.2461	0.0	0.0
92	KH2S	11.1700	-0.0239	-3279.0000	0.0	0.0

SEA WATER OF P.K.BREWER FROM CHEMICAL OCEANOGRAPHY (1975)

INITIAL SOLUTION

TEMPERATURE = 25.00 DEGREES C PH = 8.200 ANALYTICAL EPMCAT = 608.205 ANALYTICAL EPMAN = 608.826

***** OXIDATION - REDUCTION *****

DISSOLVED OXYGEN = 0.0 MG/L
EH MEASURED WITH CALOMEL = 9.9000 VOLTS
MEASURED EH OF ZOBELL SOLUTION = 9.9000 VOLTS
CORRECTED EH = 0.4000 VOLTS
PE COMPUTED FROM CORRECTED EH = 6.761

*** TOTAL CONCENTRATIONS OF INPUT SPECIES ***

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL MG/LITRE
CA	2	1.033261E-02	-1.9858	4.119998E 02
MG	2	5.333470E-02	-1.2730	1.290000E 03
NA	1	4.708921E-01	-0.3271	1.077000E 04
K	1	9.768441E-03	-2.0102	3.799998E 02
CL	-1	5.489001E-01	-0.2605	1.936000E 04
SO4	-2	2.834654E-02	-1.5475	2.709000E 03
HCO3	-1	2.311902E-03	-2.6360	1.403400E 02
SIO2 TOT	0	7.143382E-05	-4.1461	4.269999E 00
FE	2	3.599738E-08	-7.4437	2.000000E-03
PO4	-3	2.010951E-06	-5.6966	1.899999E-01
SR	2	9.177571E-05	-4.0373	7.999999E 00
F	-1	6.878075E-05	-4.1625	1.299998E 00
AL	3	7.450825E-08	-7.1278	2.000000E-03
LI	1	2.607451E-05	-4.5838	1.799999E-01
NO3	-1	3.242236E-06	-5.4892	1.999999E-01
B TOT	0	4.128553E-04	-3.3842	4.439999E 00
BA	2	1.463773E-08	-7.8345	2.000000E-03
BR	-1	8.427915E-04	-3.0743	6.699998E 01
MN	2	3.659167E-09	-8.4366	2.000000E-04

*** CONVERGENCE ITERATIONS ***

ITERATION	S1-ANALCO3	S2-SO4TOT	S3-FTOT	S4-PTOT	S5-CLTOT
1	-4.656613E-10	-3.725290E-09	0.0	-2.728484E-12	0.0
2	3.259629E-09	-1.117587E-08	-1.455192E-11	-1.818989E-12	5.960464E-08
3	2.328306E-09	-1.490116E-08	0.0	-2.728484E-12	1.192093E-07
4	1.862645E-09	-7.450581E-09	0.0	-3.637979E-12	3.576279E-07
5	1.862645E-09	-3.725290E-09	-2.910383E-11	-2.728484E-12	1.192093E-07

****DESCRIPTION OF SOLUTION ****

	ANALYTICAL	COMPUTED		
EPMCAT	608.205	583.262	PH	ACTIVITY H2O = 0.9812
EPMAN	608.826	583.904	8.200	PCO2 = 3.460119E-04
				LOG PCO2 = -3.4609
			TEMPERATURE	PO2 = 5.107577E-24
EH = 0.4000	PE = 6.761		25.00 DEG C	PCH4 = 0.0
PE CALC S =	1.000000E 02			CO2 TOT = 2.006540E-03
PE CALC DOX=	1.000000E 02		IONIC STRENGTH	DENSITY = 1.0300
PE SATO DOX=	1.000000E 02		6.534811E-01	TDS = 35146.9MG/L

IN COMPUTING THE DISTRIBUTION OF SPECIES, PE = 6.761 EQUIVALENT EH = 0.400VOLTS

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA	2	3.61332E 02	9.33376E-03	-2.0299	2.33587E-03	-2.6316	2.50260E-01	-0.6016
2	MG	2	1.13155E 03	4.81874E-02	-1.3171	1.38831E-02	-1.8575	2.88107E-01	-0.5404
3	NA	1	1.01719E 04	4.58082E-01	-0.3391	3.23410E-01	-0.4902	7.06008E-01	-0.1512
4	K	1	3.57777E 02	9.47310E-03	-2.0235	5.91987E-03	-2.2277	6.24914E-01	-0.2042
64	H	1	1.63225E-05	1.67651E-08	-7.7756	6.30969E-09	-8.2000	3.76358E-01	-0.4244
5	CL	-1	1.87132E 04	5.46479E-01	-0.2624	3.41503E-01	-0.4666	6.24914E-01	-0.2042
6	SO4	-2	1.14131E 03	1.23008E-02	-1.9101	2.26131E-03	-2.6456	1.83835E-01	-0.7356
7	HCO3	-1	7.28181E 01	1.23556E-03	-2.9081	8.36081E-04	-3.0778	6.76680E-01	-0.1696
18	CO3	-2	1.71511E 00	2.95904E-05	-4.5288	6.20417E-06	-5.2073	2.09669E-01	-0.6785
86	H2CO3	0	6.08126E-01	1.01509E-05	-4.9935	1.18385E-05	-4.9267	1.16626E 00	0.0668
27	OH	-1	6.81892E-02	4.15104E-06	-5.3818	1.56228E-06	-5.8062	3.76358E-01	-0.4244
62	F	-1	6.51394E-01	3.54981E-05	-4.4498	1.33600E-05	-4.8742	3.76358E-01	-0.4244
98	BR	-1	6.50485E 01	8.42792E-04	-3.0743	3.17191E-04	-3.4987	3.76358E-01	-0.4244
19	MGOH	1	3.75954E-01	9.42018E-06	-5.0259	3.54536E-06	-5.4503	3.76358E-01	-0.4244
23	MGSO4 AQ	0	5.43189E 02	4.67195E-03	-2.3305	5.43058E-03	-2.2652	1.16238E 00	0.0653
22	MGHCO3	1	2.95603E 01	3.58665E-04	-3.4453	1.34987E-04	-3.8697	3.76358E-01	-0.4244
21	MGCO3 AQ	0	5.75978E 00	7.07206E-05	-4.1505	8.22043E-05	-4.0851	1.16238E 00	0.0653
20	MGF	1	1.36208E 00	3.25604E-05	-4.4873	1.22544E-05	-4.9117	3.76358E-01	-0.4244
29	CAOH	1	1.34299E-02	2.43563E-07	-6.6134	9.16671E-08	-7.0378	3.76358E-01	-0.4244
32	CASO4 AQ	0	1.21723E 02	9.25679E-04	-3.0335	1.07599E-03	-2.9682	1.16238E 00	0.0653
30	CAHCO3	1	5.25149E 00	5.37801E-05	-4.2694	2.02406E-05	-4.6938	3.76358E-01	-0.4244

31	CACO3 AQ	0	1.71277E 00	1.77171E-05	-4.7516	2.05940E-05	-4.6863	1.16238E 00	0.0653
45	CAF+	1	4.12101E-02	7.22193E-07	-6.1413	2.71803E-07	-6.5657	3.76358E-01	-0.4244
44	NASO4	-1	1.17265E 03	1.01979E-02	-1.9915	3.83808E-03	-2.4159	3.76358E-01	-0.4244
43	NAHCO3	0	1.06122E 01	1.30814E-04	-3.8833	1.52055E-04	-3.8180	1.16238E 00	0.0653
42	NACO3	-1	7.92191E 00	9.88177E-05	-4.0052	3.71908E-05	-4.4296	3.76358E-01	-0.4244
94	NACL	0	1.34107E 02	2.37575E-03	-2.6242	2.76152E-03	-2.5589	1.16238E 00	0.0653
46	KSO4	-1	3.26339E 01	2.49967E-04	-3.6021	9.40769E-05	-4.0265	3.76358E-01	-0.4244
95	KCL	0	3.25655E 00	4.52230E-05	-4.3446	5.25663E-05	-4.2793	1.16238E 00	0.0653
63	HSO4	-1	3.45010E-04	3.67983E-09	-8.4342	1.38493E-09	-8.8586	3.76358E-01	-0.4244
96	H2SO4	0	7.33701E-16	7.74512E-21	-20.1110	9.00277E-21	-20.0456	1.16238E 00	0.0653
92	HCL	0	5.18568E-11	1.47250E-15	-14.8319	1.71160E-15	-14.7666	1.16238E 00	0.0653
24	H4SIO4AQ	0	6.26948E 00	6.75330E-05	-4.1705	7.84990E-05	-4.1051	1.16238E 00	0.0653
25	H3SIO4	-1	3.57776E-01	3.89470E-06	-5.4095	1.46580E-06	-5.8339	3.76358E-01	-0.4244
26	H2SIO4	-2	5.57482E-04	6.13369E-09	-8.2123	4.76717E-10	-9.3217	7.77211E-02	-1.1095
8	FE	2	1.49539E-07	2.77226E-12	-11.5572	2.15463E-13	-12.6666	7.77211E-02	-1.1095
9	FE	3	1.16061E-12	2.15161E-17	-16.6672	1.20651E-19	-18.9185	5.60746E-03	-2.2512
10	FEOH	2	5.89008E-08	8.37036E-13	-12.0773	6.50553E-14	-13.1867	7.77211E-02	-1.1095
11	FEOH	1	3.00543E-09	4.27097E-14	-13.3695	1.60741E-14	-13.7939	3.76358E-01	-0.4244
12	FE(OH)3	-1	7.74126E-13	7.49961E-18	-17.1250	2.82254E-18	-17.5493	3.76358E-01	-0.4244
77	FE(OH)2	1	4.65519E-05	5.36341E-10	-9.2706	2.01856E-10	-9.6950	3.76358E-01	-0.4244
78	FE(OH)3	0	1.11484E-03	1.08004E-08	-7.9666	1.25542E-08	-7.9012	1.16238E 00	0.0653
79	FE(OH)4	-1	2.95018E-03	2.46569E-08	-7.6081	9.27983E-09	-8.0325	3.76358E-01	-0.4244
80	FE(OH)2	0	1.04722E-12	1.20654E-17	-16.9185	1.40246E-17	-16.8531	1.16238E 00	0.0653
13	FEHPO4	1	6.51352E-16	4.44187E-21	-20.3524	1.67173E-21	-20.7768	3.76358E-01	-0.4244
100	FEHPO4	0	5.96912E-12	4.07061E-17	-16.3903	4.73160E-17	-16.3250	1.16238E 00	0.0653
65	FEH2PO4	1	2.37437E-13	1.60845E-18	-17.7936	6.05352E-19	-18.2180	3.76358E-01	-0.4244
99	FEH2PO4	2	3.45755E-16	2.34222E-21	-20.6304	1.82040E-22	-21.7398	7.77211E-02	-1.1095
15	FESO4	1	1.42494E-12	9.71164E-18	-17.0127	3.65506E-18	-17.4371	3.76358E-01	-0.4244
16	FECL	2	1.20998E-12	1.37210E-17	-16.8626	1.06641E-18	-17.9721	7.77211E-02	-1.1095
28	FECL2	1	5.68416E-13	4.64287E-18	-17.3332	1.74738E-18	-17.7576	3.76358E-01	-0.4244
33	FECL3	0	7.93385E-15	5.06402E-20	-19.2955	5.88632E-20	-19.2301	1.16238E 00	0.0653
34	FESO4	0	9.74738E-09	6.64330E-14	-13.1776	7.72204E-14	-13.1123	1.16238E 00	0.0653
101	MN	2	1.47595E-04	2.78139E-09	-8.5557	2.16173E-10	-9.6652	7.77211E-02	-1.1095
102	MN	3	3.67296E-22	6.92160E-27	-26.1598	3.88126E-29	-28.4110	5.60746E-03	-2.2512
106	MNOH	1	1.74956E-07	2.52111E-12	-11.5984	9.48841E-13	-12.0228	3.76358E-01	-0.4244
107	MN(OH)3	-1	1.35350E-14	1.32244E-19	-18.8786	4.97712E-20	-19.3030	3.76358E-01	-0.4244
111	MNHCO3	1	2.79687E-06	2.49716E-11	-10.6025	9.39827E-12	-11.0269	3.76358E-01	-0.4244
109	MNSO4	0	3.13132E-06	2.14690E-11	-10.6682	2.49551E-11	-10.6028	1.16238E 00	0.0653
110	MN(NO3)2	0	5.48291E-17	3.17208E-22	-21.4987	3.68716E-22	-21.4333	1.16238E 00	0.0653
103	MNCL	1	6.92897E-05	7.93584E-10	-9.1004	2.98672E-10	-9.5248	3.76358E-01	-0.4244
104	MNCL2	0	2.89797E-06	2.38399E-11	-10.6227	2.77111E-11	-10.5573	1.16238E 00	0.0653
105	MNCL3	-1	1.76643E-06	1.13373E-11	-10.9455	4.26690E-12	-11.3699	3.76358E-01	-0.4244
108	MNF	1	3.87977E-09	5.43257E-14	-13.2650	2.04459E-14	-13.6894	3.76358E-01	-0.4244
112	MNO4	-1	2.33488E-33	2.03243E-38	-37.6920	7.64921E-39	-38.1164	3.76358E-01	-0.4244
113	MNO4	-2	4.74426E-30	4.12971E-35	-34.3841	3.20965E-36	-35.4935	7.77211E-02	-1.1095
115	HMNO2	-1	6.78987E-15	7.99308E-20	-19.0973	3.00826E-20	-19.5217	3.76358E-01	-0.4244
51	AL	3	2.52320E-12	9.68200E-17	-16.0140	5.42915E-19	-18.2653	5.60746E-03	-2.2512
52	ALOH	2	4.61546E-10	1.08630E-14	-13.9641	8.44285E-16	-15.0735	7.77211E-02	-1.1095
53	AL(OH)2	1	3.56341E-07	6.04841E-12	-11.2184	2.27637E-12	-11.6428	3.76358E-01	-0.4244
54	AL(OH)4	-1	6.83698E-03	7.45022E-08	-7.1278	2.80395E-08	-7.5522	3.76358E-01	-0.4244
55	ALF	2	4.24116E-11	9.54983E-16	-15.0200	7.42223E-17	-16.1295	7.77211E-02	-1.1095
56	ALF2	1	9.09599E-11	1.44931E-15	-14.8388	5.45458E-16	-15.2632	3.76358E-01	-0.4244
57	ALF3	0	9.47798E-12	1.16852E-16	-15.9324	1.35826E-16	-15.8670	1.16238E 00	0.0653
58	ALF4	-1	2.40585E-13	2.41888E-18	-17.6164	9.10365E-19	-18.0408	3.76358E-01	-0.4244
59	ALSO4	1	6.14425E-13	5.16999E-18	-17.2865	1.94577E-18	-17.7109	3.76358E-01	-0.4244
60	AL(SO4)2	-1	1.96644E-13	9.29194E-19	-18.0319	3.49710E-19	-18.4563	3.76358E-01	-0.4244
45	PO4	-3	6.44737E-05	7.02859E-10	-9.1531	3.94126E-12	-11.4044	5.60746E-03	-2.2512
47	HPO4	-2	6.57957E-02	7.09739E-07	-6.1489	5.51616E-08	-7.2584	7.77211E-02	-1.1095
48	H2PO4	-1	1.39531E-03	1.48948E-08	-7.8270	5.60579E-09	-8.2514	3.76358E-01	-0.4244
40	MGPO4	-1	6.50158E-02	5.64310E-07	-6.2485	2.12383E-07	-6.6729	3.76358E-01	-0.4244
73	MGHPO4	0	5.67454E-02	4.88399E-07	-6.3112	5.67705E-07	-6.2459	1.16238E 00	0.0653

41 MGH2PO4	1	7.89406E-04	6.73784E-09	-8.1715	2.53584E-09	-8.5959	3.76358E-01	-0.4244
75 CAPO4	-1	9.18123E-03	7.03850E-08	-7.1525	2.64900E-08	-7.5769	3.76358E-01	-0.4244
74 CAHPO4	0	7.98704E-03	6.07765E-08	-7.2163	7.06454E-08	-7.1509	1.16238E 00	0.0653
76 CAH2PO4	1	1.17853E-04	8.90192E-10	-9.0505	3.35031E-10	-9.4749	3.76358E-01	-0.4244
61 KHPO4	-1	2.20732E-04	1.69180E-09	-8.7716	6.36721E-10	-9.1960	3.76358E-01	-0.4244
50 NAHPO4	-1	1.06205E-02	9.24248E-08	-7.0342	3.47848E-08	-7.4586	3.76358E-01	-0.4244
36 H3BO3 AQ	0	1.92491E 01	3.22305E-04	-3.4917	3.74641E-04	-3.4264	1.16238E 00	0.0653
37 H2BO3	-1	5.31978E 00	9.05502E-05	-4.0431	3.40793E-05	-4.4675	3.76358E-01	-0.4244
85 NO3	-1	1.94175E-01	3.24224E-06	-5.4892	1.22024E-06	-5.9136	3.76358E-01	-0.4244
81 LI	1	1.73048E-01	2.58195E-05	-4.5881	9.71737E-06	-5.0125	3.76358E-01	-0.4244
82 LIOH	0	4.78771E-07	2.06998E-11	-10.6840	2.40610E-11	-10.6187	1.16238E 00	0.0653
83 LISO4	-1	2.53553E-02	2.54864E-07	-6.5937	9.59200E-08	-7.0181	3.76358E-01	-0.4244
88 SR	2	7.76697E 00	9.17755E-05	-4.0373	7.13289E-06	-5.1467	7.77211E-02	-1.1095
89 SROH	1	1.97695E-05	1.95627E-10	-9.7086	7.36259E-11	-10.1330	3.76358E-01	-0.4244
90 BA	2	1.94174E-03	1.46377E-08	-7.8345	1.13766E-09	-8.9440	7.77211E-02	-1.1095
91 BAOH	1	3.07324E-09	2.06146E-14	-13.6858	7.75848E-15	-14.1102	3.76358E-01	-0.4244

MOLE RATIOS FROM ANALYTICAL MOLALITY		MOLE RATIOS FROM COMPUTED MOLALITY		LOG ACTIVITY RATIOS	
CL/CA	= 5.3123E 01	CL/CA	= 5.8549E 01	LOG CA/H2	= 13.7684
CL/MG	= 1.0292E 01	CL/MG	= 1.1341E 01	LOG MG/H2	= 14.5425
CL/NA	= 1.1657E 00	CL/NA	= 1.1930E 00	LOG NA/H1	= 7.7098
CL/K	= 5.6191E 01	CL/K	= 5.7687E 01	LOG K/H1	= 5.9723
CL/AL	= 7.3670E 06	CL/AL	= 5.6443E 15	LOG AL/H3	= 6.3347
CL/FE	= 1.5248E 07	CL/FE	= 1.9712E 11	LOG FE/H2	= 3.7334
CL/SO4	= 1.9364E 01	CL/SO4	= 4.4426E 01	LOG CA/MG	= -0.7740
CL/HCO3	= 2.3742E 02	CL/HCO3	= 4.4229E 02	LOG NA/K	= 1.7374
CA/MG	= 1.9373E-01	CA/MG	= 1.9370E-01		
NA/K	= 4.8205E 01	NA/K	= 4.8356E 01		

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT	DELGR
40	ADLLAR	9.3462E-23	2.6916E-21	-22.0294	-20.5700	3.4723E-02	-1.45938	-1.99101
41	ALBITE	5.1061E-21	1.0000E-18	-20.2919	-18.0000	5.1061E-03	-2.29191	-3.12681
141	ALCH3A	2.0703E-36	2.4549E-32	-35.6840	-31.6100	8.4336E-05	-4.07399	-5.55806
51	ALLNIT			-97.1522	-85.3200		-11.83218	-16.14241
43	ANALCM	6.1443E-17	1.9953E-13	-16.2115	-12.7000	3.0794E-04	-3.51153	-4.79071
18	ANHYDRIT	5.2822E-06	2.8314E-05	-5.2772	-4.5480	1.8656E-01	-0.72919	-0.99482
114	ANNITE			-94.8502	-84.2400		-10.61021	-14.47531
42	ANCRTH	1.3173E-26	4.6776E-20	-25.8803	-19.3300	2.8162E-07	-6.55033	-8.93649
22	ARAGONIT	1.4492E-08	6.0954E-09	-7.8389	-8.2150	2.3776E 00	0.37613	0.51315
151	ARTIN	7.8052E-23	3.9812E-19	-22.1076	-18.4000	1.9605E-04	-3.70763	-5.05824
145	BARITE	2.5727E-12	1.7539E-10	-11.5896	-9.7560	1.4668E-02	-1.83362	-2.50158
53	BCEHM	2.1100E-36	3.8906E-34	-35.6757	-33.4100	5.4234E-03	-2.26573	-3.09109
20	BRUCITE	3.3885E-14	3.8905E-12	-13.4700	-11.4100	8.7096E-03	-2.06000	-2.81042
13	CALCITE	1.4492E-08	3.3503E-09	-7.8389	-8.4749	4.3257E 00	0.63605	0.86776
144	CELEST	1.6130E-08	1.0617E-06	-7.7924	-5.9740	1.5192E-02	-1.81837	-2.48077
98	CHALC	8.1536E-05	2.9992E-04	-4.0887	-3.5230	2.7186E-01	-0.56565	-0.77171
50	CHLOR			-83.0749	-90.6100		7.53506	10.27994
21	CHRYSOTL	2.6362E-49	1.5850E-52	-48.5790	-51.8000	1.6632E 03	3.22095	4.39427
30	CLENSTIT	2.8159E-18	1.3490E-17	-17.5504	-16.8700	2.0874E-01	-0.68039	-0.92824
57	CLINOP	5.6364E-29	1.0000E 00	-28.2490	0.0	5.6364E-29	-28.24899	-38.53955
100	CRISTO	8.1536E-05	2.5942E-04	-4.0887	-3.5860	3.1430E-01	-0.50265	-0.68576

29	DICPSIDE	1.3341E-36	6.0259E-37	-35.8748	-36.2200	2.2139E 00	0.34516	0.47089
12	DOLOMITE	1.2483E-15	9.5503E-18	-14.9037	-17.0200	1.3070E 02	2.11629	2.88721
56	ERION	4.3553E-23	1.0000E 00	-22.3610	0.0	4.3553E-23	-22.36098	-30.50664
113	FECH3A	4.5375E 05	7.6736E 04	5.6568	4.8850	5.9131E 00	0.77182	1.05297
97	FLLAPT	6.2952E-58	1.6219E-67	-57.2010	-66.7900	3.8814E 09	9.58899	13.08208
63	FLLOR	4.1694E-13	3.1623E-11	-12.3799	-10.5000	1.3184E-02	-1.87994	-2.56476
28	FORSTRIT	9.7244E-32	7.7629E-29	-31.0121	-28.1100	1.2527E-03	-2.90216	-3.95936
52	GIBCRS	2.0703E-36	1.6983E-33	-35.6840	-32.7700	1.2190E-03	-2.91398	-3.97549
111	GOETH	4.6891E-37	6.3098E-42	-36.3289	-41.2000	7.4315E 04	4.87107	6.64551
112	GREENA			-81.0064	-63.1900		-17.81639	-24.30655
19	GYPSUM	5.0854E-06	1.7418E-05	-5.2937	-4.7590	2.9196E-01	-0.53467	-0.72944
65	HALITE	1.1045E-01	3.8194E 01	-0.9569	1.5820	2.8917E-03	-2.53885	-3.46371
48	HALLOY	2.2028E-40	1.5136E-33	-39.6570	-32.8200	1.4553E-07	-6.83704	-9.32764
109	HEMATI	2.1795E 11	9.8401E-05	11.3384	-4.0070	2.2149E 15	15.34536	20.93536
118	HUNTITE	9.2612E-30	3.0904E-31	-29.0333	-30.5100	2.9968E 01	1.47665	2.01457
39	HYDMAG	2.0456E-35	1.5136E-38	-34.6892	-37.8200	1.3514E 03	3.13080	4.27128
96	HYXAPT	7.3613E-59	4.4671E-60	-58.1331	-59.3500	1.6479E 01	1.21693	1.66024
46	ILLITE	5.1673E-44	4.8980E-41	-43.2867	-40.3100	1.0550E-03	-2.97675	-4.06112
47	KACLIN	2.2028E-40	1.2303E-37	-39.6570	-36.9100	1.7904E-03	-2.74704	-3.74774
44	KMICA	3.1562E-54	8.1287E-50	-53.5009	-49.0900	3.8828E-05	-4.41086	-6.01765
129	LALMON	8.1175E-35	1.0965E-32	-34.0906	-31.9600	7.4029E-03	-2.13060	-2.90673
148	LECN	6.7152E-69	2.6917E-70	-68.1730	-69.5700	2.4948E 01	1.39703	1.90594
99	MAGADI	2.0445E-23	5.0119E-15	-22.6894	-14.3000	4.0793E-09	-8.38942	-11.44552
110	MAGHEM	2.1795E 11	2.3442E 06	11.3384	6.3700	9.2973E 04	4.96836	6.77823
11	MAGNESIT	8.6134E-08	5.7545E-09	-7.0648	-8.2400	1.4968E 01	1.17516	1.60325
108	MAGNET	1.9469E-05	2.7227E-10	-4.7106	-9.5650	7.1507E 04	4.85435	6.62269
64	MONTCA	3.9531E-50	1.0000E-45	-49.4031	-45.0000	3.9530E-05	-4.40308	-6.00703
116	MONTBF	1.3391E-33	1.0716E-35	-32.8732	-34.9700	1.2497E 02	2.09680	2.86062
117	MONTAB	1.8044E-28	1.6596E-30	-27.7437	-29.7800	1.0872E 02	2.03631	2.77810
58	MORDEN	6.3015E-27	1.0000E 00	-26.2006	0.0	6.3015E-27	-26.20055	-35.74489
67	MIRABI	1.9564E-04	7.7090E-02	-3.7085	-1.1130	2.5378E-03	-2.59555	-3.54106
59	NAHCOL	2.7040E-04	2.8314E-01	-3.5680	-0.5480	9.5500E-04	-3.02000	-4.12012
61	NATRON	5.3675E-07	4.8865E-02	-6.2702	-1.3110	1.0984E-05	-4.95923	-6.76578
150	NESQUE	8.1367E-08	6.1518E-06	-7.0896	-5.2110	1.3227E-02	-1.87855	-2.56287
55	PHILIP	6.7781E-22	1.3804E-20	-21.1689	-19.8600	4.9101E-02	-1.30891	-1.78572
45	PHLOG	3.7770E-63	2.9513E-64	-62.4229	-63.5300	1.2798E 01	1.10713	1.51043
142	PREHNT	6.0673E-17	3.0200E-12	-16.2170	-11.5200	2.0091E-05	-4.69701	-6.40804
54	PYROPH	1.4926E-48	3.7155E-43	-47.8261	-42.4300	4.0173E-06	-5.39607	-7.36175
102	QUARTZ	8.1536E-05	9.8856E-05	-4.0887	-4.0050	8.2480E-01	-0.08365	-0.11413
37	SEPIOLIT	6.0495E-40	7.9436E-41	-39.2183	-40.1000	7.6155E 00	0.88170	1.20288
10	SIDERITE	1.3368E-18	2.8184E-11	-17.8739	-10.5500	4.7431E-08	-7.32393	-9.99190
101	SILGEL	8.1536E-05	9.6162E-04	-4.0887	-3.0170	8.4791E-02	-1.07165	-1.46203
147	STRENGIT	4.5784E-31	3.9812E-27	-30.3393	-26.4000	1.1500E-04	-3.93930	-5.37431
143	STRONT	4.4254E-11	3.8905E-12	-10.3541	-11.4100	1.1375E 01	1.05594	1.44060
38	TALC	1.7862E-57	5.1289E-63	-56.7481	-62.2900	3.4826E 05	5.54190	7.56071
66	THENAR	2.3652E-04	6.6222E-01	-3.6261	-0.1790	3.5717E-04	-3.44713	-4.70285
62	THENAT	6.3672E-07	1.3335E 00	-6.1961	0.1250	4.7748E-07	-6.32105	-8.62369
32	TREMOLIT			-128.4978	-140.3000		11.80220	16.10150
60	TRONA	1.6893E-10	1.6032E-01	-9.7723	-0.7950	1.0537E-09	-8.97728	-12.24753
107	VIVIAN	1.3350E-61	1.0000E-36	-60.8745	-36.0000	1.3349E-25	-24.87453	-33.93584
146	WITHERIT	7.0584E-15	4.7863E-14	-14.1513	-13.3200	1.4747E-01	-0.83130	-1.13413
154	SEP PT	6.0495E-40	6.1379E-38	-39.2183	-37.2120	9.8558E-03	-2.00631	-2.73716
155	DIASP	2.1100E-36	8.7099E-36	-35.6757	-35.0600	2.4226E-01	-0.61572	-0.84002
156	WAIRKT	8.4317E-35	2.3989E-27	-34.0741	-26.6200	3.5148E-08	-7.45410	-10.16948
172	MANGANO	5.3278E 06	8.6692E 17	6.7266	17.9380	6.1457E-12	-11.21143	-15.29553
173	PYROLUST	1.3603E 11	7.2609E 15	11.1336	15.8610	1.8734E-05	-4.72736	-6.44944
174	BIRNSITE	1.3603E 11	1.2330E 18	11.1336	18.0910	1.1032E-07	-6.95735	-9.49177
175	NUSTITE	1.3603E 11	3.1915E 17	11.1336	17.5040	4.2623E-07	-6.37036	-8.69096
176	BIXBYITE	2.2555E-08	2.4491E-01	-7.6468	-0.6110	9.2094E-08	-7.03576	-9.59875
177	HALSMITE	1.2409E 50	3.4672E 61	50.0938	61.5400	3.5790E-12	-11.44624	-15.61588
178	MNCH2	5.2763E-22	1.2246E-13	-21.2777	-12.9120	4.3085E-09	-8.36568	-11.41313

179	MNCH3	1.4800E-46	2.2659E-36	-45.8297	-35.6440	6.5202E-11	-10.18574	-13.89621
180	MANGANIT	1.4876E-04	5.7810E-01	-3.8275	-0.2380	2.5733E-04	-3.58951	-4.89710
181	RHODOCHR	1.3412E-15	2.8907E-11	-14.8725	-10.5390	4.6396E-05	-4.33352	-5.91213
183	MNCL2	2.5211E-11	5.7544E 08	-10.5984	8.7600	4.3812E-20	-19.35840	-26.41028
184	MNCL2,1W	2.4738E-11	3.3266E 05	-10.6067	5.5220	7.4363E-17	-16.12863	-22.00397
185	MNCL2,2W	2.4272E-11	9.4189E 03	-10.6149	3.9740	2.5770E-15	-14.58889	-19.90332
186	MNCL2,4W	2.3369E-11	5.1286E 02	-10.6314	2.7100	4.5565E-14	-13.34136	-18.20135
187	TEPHRITE	2.3145E 09	1.3243E 23	9.3645	23.1220	1.7477E-14	-13.75754	-18.76913
188	RHODONIT	9.3909E-08	3.3265E 09	-7.0273	9.5220	2.8230E-17	-16.54929	-22.57787
190	MNSO4	4.8884E-13	4.6666E 02	-12.3108	2.6690	1.0475E-15	-14.97983	-20.43669
191	MN2SO4,3	1.7420E-65	1.9454E-06	-64.7590	-5.7110	8.9548E-60	-59.04794	-80.55797
192	MN3PO4,2	1.5692E-52	1.4894E-24	-51.8043	-23.8270	1.0536E-28	-27.97731	-38.16890
193	MNHPO4	1.1925E-17	1.1298E-13	-16.9236	-12.9470	1.0555E-04	-3.97655	-5.42514
107	VIVIAN	1.3350E-61	1.0000E-36	-60.8745	-36.0000	1.3349E-25	-24.87453	-33.93584

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C     **** PROGRAM WATEQF **** A FORTRAN IV VERSION OF WATEQ                    A  10
C                                                                               A  20
C     REVISED FROM PL1 VERSION OF TRUESDELL AND JONES.                          A  30
C     NIEL PLUMMER, SUMMER 1972.                                                A  40
C     LATEST REVISION AUGUST, 1976.                                             A  50
C                                                                               A  60
C                                                                               A  70
C     **** DESCRIPTION OF INPUT - 5 CARDS ARE REQUIRED ****                     A  80
C     CARD 1    TITLE, JOB DESCRIPTION.  (20A4)                                 A  90
C     CARD 2     TEMP,PH,EHM,EHMC,EHMZ,DENS,DOX,FLAG,CORALK,PECALC,IGO,         A 100
C                (PRT(I),I=1,4),IDAVES,ISPEC,IMIN                               A 110
C                (5(F6.0,1X),2F5.0,1X,9I1,2I3)                                  A 120
C       TEMP....TEMPERATURE IN DEGREES C                                        A 130
C       PH......NEGATIVE LOG ACTIVITY H+                                        A 140
C       EHM.....PREFERRED EH ...SEE OPTIONS                                     A 150
C       EHMC....MEASURED EH ... SEE OPTIONS                                     A 160
C       EHMZ....MEASURED EH OF ZOBELL SOLUTION                                  A 170
C       DENS....DENSITY OF SOLUTION   (G/CC)                                    A 180
C       DOX.....DISSOLVED OXYGEN (MG/L)                                         A 190
C       FLAG....SIGNAL FOR UNITS OF INPUT CONCENTRATION.                        A 200
C         1=MEQ/L, 2=MG/L, 3=PPM, 4=MOLALITY, 0 = MASS UNITS (GRAMS/KG)         A 210
C       CORALK..=0 IF ALKALINITY HAS NOT BEEN CORRECTED FOR BORON ETC.          A 220
C         =1 IF THE CORRECTION HAS BEEN MADE.  =2 IF TOTAL CO2 IS INPUT         A 230
C         RATHER THAN ALKALINITY, =3 CORRECTS FOR ALL POSSIBLE NON-CARBONATE ALKALINITY A 240
C       PECALC..=0 WILL SET PE TO 100,  =1 COMPUTES PE FROM EH,                 A 250
C         =2 COMPUTES PE FROM DOX(THEORETICAL).  = 3 COMPUTES PE FROM          A 260
C         THE SATO RELATION,  = 4 COMPUTES PE FROM S-- - SO4--.                A 270
C       IGO..=0,OR BLANK, IF DESIRED TO HAVE DATA CHECKED FOR INPUT             A 280
C         ERROR. PH MUST BE GREATER THAN 3 AND LESS THAN 11, AND THE           A 290
C         ANALYSIS MUST HAVE LESS THAN 30% ERROR IN CHARGE BALANCE.  =1        A 300
C         IF THIS CHECK IS NOT TO BE MADE.                                     A 310
C       (PRT(I),I=1,4), CAN BE SET TO 1 TO DELETE PRINT OF                     A 320
C          THERMOCHEMICAL DATA,MASS BALANCE CONVERGENCE ITERATIONS,            A 330
C         RATIOS OF IONS, AND MINERAL SATURATION, RESPECTIVELY.  PRT(I)        A 340
C         SHOULD BE SET TO ZERO OR BLANK TO OBTAIN THE RESPECTIVE PRINT.       A 350
C       IDAVES..=1, ACTIVITY COEFFICIENTS OF CHARGED ION PAIRS ARE             A 360
C         CALCULATED FROM THE DAVIES EQUATION.  =0 (OR BLANK), ACTIVITY        A 370
C         COEFFICIENTS OF CHARGED ION PAIRS ARE CALCULATED FROM THE            A 380
C         DEBYE-HUCKEL EQUATION.  IDAVES HAS NO EFFECT ON GAMMA(1)-            A 390
C         GAMMA(7), AND GAMMA(18).                                             A 400
C       ISPEC.. = NUMBER OF SPECIES DESIRED IN OUTPUT(IF LESS THAN TOTAL       A 410
C         POSSIBLE). TO OBTAIN OUTPUT OF MOLALITY, ACTIVITY, ETC. OF           A 420
C         ALL POSSIBLE SPECIES FOR THE DEFINED SYSTEM, LEAVE ISPEC             A 430
C         BLANK (OR ZERO).  IF ISPEC GT. ZERO, ISPEC VALUES OF KSPEC           A 440
C         (SPECIES INDEX NUMBER) MUST BE READ (SEE BELOW).  IF ISPEC =         A 450
C         BLANK (ZERO), OMIT KSPEC CARD(S).                                    A 460
C       IMIN.. = NUMBER OF MINERALS FOR WHICH SATURATION OUTPUT IS             A 470
C         DESIRED (IF LESS THAN TOTAL POSSIBLE).  TO OBTAIN SATURATION         A 480
C         DATA ON ALL POSSIBLE MINERALS FOR THE DEFINED SYSTEM, LEAVE          A 490
C         IMIN BLANK (OR ZERO).  IF IMIN GT. ZERO, IMIN VALUES OF KMIN         A 500
C         (MINERAL INDEX NUMBER) MUST BE READ (SEE BELOW).  IF IMIN =          A 510
C         BLANK (OR ZERO), OMIT KMIN CARDS(S).                                 A 520
C     CARD 3     CA MG NA K CL SO4    (6(E12.5),8X)                           A 530
C     CARD 4     HCO3 SIO2 FE PO4 SR F     (6(E12.5),8X)                      A 540
C             ... OPTIONAL CARDS OF TYPE 1 APPEAR HERE ...                      A 550
C             ... OPTIONAL CARDS OF TYPE 2 APPEAR HERE ..                       A 560
C     CARD 5     BLANK CARD      (DENOTES END OF DATA FOR A PARTICULAR          A 570
C         WATER ANALYSIS.)                                                      A 580
C                                                                               A 590
C     ....DESCRIPTION OF OPTIONAL INPUT....                                     A 600
C         ALL OPTIONAL INPUT MUST APPEAR BETWEEN CARDS 4 AND 5.                 A 610
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C        TYPE 1 CARDS MUST PRECEED TYPE 2 CARDS.                          A  620
C                                                                         A  630
C     ****************************                                        A  640
C     TYPE 1 OPTIONAL INPUT CARDS                                         A  650
C     ****************************                                        A  660
C     (KSPEC(I),I=1,ISPEC)  (16I5)  KSPEC(I) IS THE INDEX NUMBER OF THE  A  670
C         ITH SELECTED SPECIES FOR WHICH OUTPUT IS DESIRED.  OMIT CARD    A  680
C         IF ISPEC = BLANK (OR ZERO).                                     A  690
C     (KMIN(I),I=1,IMIN)  (16I5)  KMIN(I) IS THE INDEX NUMBER OF THE      A  700
C         ITH SELECTED MINERAL FOR WHICH SATURATION OUTPUT IS DESIRED.    A  710
C         OMIT CARD IF IMIN = BLANK (OR ZERO).                            A  720
C     NOTE THAT IF BOTH KSPEC AND KMIN ARE READ, KSPEC(I) MUST BE READ    A  730
C     BEFORE KMIN(I).                                                     A  740
C                                                                         A  750
C     ****************************                                        A  760
C     TYPE 2 OPTIONAL INPUT CARDS                                         A  770
C     ****************************                                        A  780
C     WORD,(INT(I),VAL(I),I=1,5)  (A4,1X,5(I3,E12.5))                     A  790
C     WORD = 'CONC', 'EROR', 'DELH', 'TABL', OR'LOGK'.                    A  800
C                                                                         A  810
C       'CONC',,ENTERS CONCENTRATION (UNITS OF FLAG) OF CONSTITUENTS      A  820
C       NOT ON CARDS 3 AND 4.  INT(I) = 17(H2S),18(CO3),39(NH4),51(AL),   A  830
C       81(LI),85(NO3),86(H2CO3),87(B),90(BA),98(BR),AND 101(MN).         A  840
C       VAL(I) IS THE CONCENTRATION OF THE INT(I) CONSTITUENT.            A  850
C                                                                         A  860
C       'EROR',,OVERRIDES PRE-SET MASS BALANCE CONVERGENCE CONSTRAINTS    A  870
C       ON ANIONS.  PER-SET VALUES OF EROR1-EROR5 ARE 0.001(0.1% ERROR    A  880
C       IN MASS BALANCE).  EROR1-EROR5 ARE ENTERED ON THE 'EROR' CARD     A  890
C       AS VAL(1)-VAL(5), IN THE ORDER 1=CARBON, 2=SULFATE, 3=FLUORIDE,   A  900
C       4=PHOSPHATE, 5=CHLORIDE.  VALUES OF INT(I) ARE NOT USED.          A  910
C                                                                         A  920
C       'DELH',,OVERRIDES VALUES OF THE STANDARD DELTA ENTHALPY OF        A  930
C       REACTION (25 DEG. C) USED IN COMPUTING THE TEMPERATURE            A  940
C       DEPENDENCE OF EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION.  A  950
C       INT(I) IS THE INDEX NUMBER OF THE ITH REACTION FOR WHICH DH(I)    A  960
C       IS TO BE CHANGED AND VAL(I) IS THE APPPRIATE NEW VALUE OF         A  970
C       DH(INT(I)).                                                       A  980
C                                                                         A  990
C       'TABL',,OVERRIDES VALUES OF LOGKTO(INT(I)) (LOG K OF REACTION AT  A 1000
C       25 DEG. C USED IN COMPUTING THE TEMPERATURE DEPENDENCE OF         A 1010
C       EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION).  INT(I) IS    A 1020
C       THE INDEX NUMBER OF THE ITH REACTION FOR WHICH LOGKTO IS TO BE    A 1030
C       CHANGED AND VAL(I) IS THE APPROPRIATE NEW VALUE OF LOGKTO(I).     A 1040
C                                                                         A 1050
C       'LOGK',,OVERRIDES EXISTING ANALYTICAL EXPRESSIONS FOR LOG K AS A  A 1060
C       FUNCTION OF T(DEG.K), OR ENTERS NEW, PREVIOUSLY UNDEFINED         A 1070
C       ANALYTICAL EXPRESSIONS FOR LOG K(T DEG.K).  THE FORM OF THE       A 1080
C       ANALYTICAL EXPRESSION MUST BE                                     A 1090
C             LOG KT(INT(I))=A+B*T+C/T+D*T**2+E/T**2                      A 1100
C       WHERE T IS TEMPERATURE IN DEG. K, AND A,B,C,D, AND E ARE FIT      A 1110
C       PARAMETERS (MAY BE ZERO OR BLANK).  INT(1) IS THE INDEX NUMBER    A 1120
C       OF REACTION AND INT(2)-INT(5) ARE IGNORED.  VAL(1)=A,VAL(2)=B,    A 1130
C       VAL(3)=C,VAL(4)=D,VAL(5)=E.                                       A 1140
C                                                                         A 1150
C                                                                         A 1160
C     IF ANY OF THE CARDS, 'EROR','DELH','TABL','LOGK', ARE USED IN A     A 1170
C     PARTICULAR WATER DATA SET, CALCULATIONS FOR THAT DATA SET AND ALL    A 1180
C     SUBSEQUENT DATA SETS WILL USE THE NEW INPUT VALUES.  THE ORDER OF    A 1190
C     TYPE 2 OPTIONAL INPUT CARDS IS 'CONC','EROR','DELH','TABL',AND      A 1200
C     'LOGK', IF ALL 5 ARE USED.  THE LAST CARD IN EACH WATER ANALYSIS    A 1210
C     DATA SET MUST BE BLANK, WHETHER OPTION CARDS ARE USED OR NOT.       A 1220
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C                                                                       A 1230
      INTEGER D,E,DD,RBIT,CORALK,Z(120),PRT(4)                          A 1240
      INTEGER PECALC,PECK                                               A 1250
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT A 1260
     1OT,MGTOT,LITOT,NH4TOT,KW                                          A 1270
      REAL *8NSPEC(120),NREACT(200)                                     A 1280
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P A 1290
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA A 1300
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120), A 1310
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI( A 1320
     4120),ITER,RBIT,C1SAVE,CCRALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT A 1330
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT A 1340
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC, A 1350
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                         A 1360
      D=115                                                             A 1370
      E=193                                                             A 1380
      IPRT=0                                                            A 1390
      NEQU=15                                                           A 1400
      READ (9,50) (NSPEC(I),Z(I),GFW(I),DHA(I),I=1,D)                   A 1410
      READ (9,60) (NREACT(I),DH(I),LOGKTO(I),I=1,E)                     A 1420
   10 CONTINUE                                                          A 1430
      READ (5,70,END=40) TITL                                           A 1440
      ICK=0                                                             A 1450
      CALL PREP                                                         A 1460
      IF (ICK.EQ.1) GO TO 10                                            A 1470
      CALL SET                                                          A 1480
   20 CONTINUE                                                          A 1490
      CALL MODEL                                                        A 1500
      IF (ITER.EQ.25) GO TO 30                                          A 1510
      IF (RBIT.EQ.1) GO TO 20                                           A 1520
      IF (ITER.LT.5) GO TO 20                                           A 1530
      CALL PRINT                                                        A 1540
      IF (PRT(4).NE.0) GO TO 10                                         A 1550
      CALL SAT                                                          A 1560
      GO TO 10                                                          A 1570
   30 PRINT 80                                                          A 1580
      GO TO 10                                                          A 1590
   40 STOP                                                              A 1600
C                                                                       A 1610
   50 FORMAT (5X,A8,2X,I2,3X,F10.4,1X,F4.1)                             A 1620
   60 FORMAT (5X,A8,2X,2F10.4)                                          A 1630
   70 FORMAT (20A4)                                                     A 1640
   80 FORMAT (10X,'CONVERGENCE DID NOT OCCUR WITHIN 200 ITERATIONS, CALC A 1650
     1ULATION TERMINATED',///)                                          A 1660
      END                                                               A 1670-
      SUBROUTINE PREP                                                   B   10
      INTEGER D,E,DD,RBIT,CORALK,Z(120),WORD,CARD(6),FLAG,PRT(4),SIGN(2) B   20
      INTEGER PECALC,PECK                                               B   30
      DIMENSION INT(5), VAL(5), INPT(22), GRAMS(120), IEQU(50), COEF(5,2 B   40
     100), V(120)                                                       B   50
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT B   60
     1OT,MGTOT,LITOT,NH4TOT,KW                                          B   70
      REAL *8NSPEC(120),NREACT(200)                                     B   80
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P B   90
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA B  100
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120), B  110
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI( B  120
     4120),ITER,RBIT,C1SAVE,CCRALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT B  130
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT B  140
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC, B  150
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                         B  160
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      DATA CARD/'CONC','EROR','DELH','TABL','LOGK','    '/,SIGN/' ','*'/ B  170
      DATA IEQU/13,14,15,25,26,27,36,69,73,74,75,78,79,90,92,35*0/       B  180
      DATA COEF/60*0.0,13.543,-0.0401,-3000.,2*0.0,6.368,-0.016346,-3405 B  190
     1.9,2*0.0,39.478,-0.065927,-12355.1,47*0.0,0.684,0.0051295,3*0.0,28 B  200
     2.6059,0.012078,1573.21,2*0.0,0.6322,-0.001225,-2835.76,42*0.,-14.8 B  210
     3435,+0.032786,+3404.71,162*0.,-6.498,+0.02379,+2902.39,17*0.0,3.10 B  220
     46,0.0,-673.6,2*0.0,0.991,0.00667,3*0.0,2.319,-.011056,0.0,2.29812E B  230
     5-05,11*0.0,-2.95,0.0133,3*0.0,-27.393,0.05617,4114.0,52*0.0,-5.350 B  240
     65,0.0183412,557.2461,7*0.0,11.17,-0.02386,-3279.0,542*0.0/         B  250
      DATA INPT/1,2,3,4,5,6,7,35,8,45,88,62,17,18,39,51,81,85,87,90,98,1 B  260
     101/                                                                B  270
      C=2.302585092                                                      B  280
      F=23.0603                                                          B  290
      R=1.98719E-03                                                      B  300
      EROR1=.001                                                         B  310
      EROR2=.001                                                         B  320
      EROR3=.001                                                         B  330
      EROR4=.001                                                         B  340
      EROR5=.001                                                         B  350
      ICK=0                                                              B  360
      PEDO=100.0                                                         B  370
      PESATO=100.                                                        B  380
      PES=100.0                                                          B  390
      DO 10 I=1,D                                                        B  400
      CONITS(I)=0.0                                                      B  410
      ALFA(I)=0.0                                                        B  420
      MI(I)=0.0                                                          B  430
      XLMI(I)=0.0                                                        B  440
      IF (Z(I).EQ.0) V(I)=1.0                                            B  450
      IF (Z(I).EQ.0) GO TO 10                                            B  460
      IF (Z(I).LT.0) V(I)=-1.0*Z(I)                                      B  470
      IF (Z(I).GT.0) V(I)=1.0*Z(I)                                       B  480
10    CONTINUE                                                           B  490
      PECK=0                                                             B  500
      PRINT 560                                                          B  510
      READ 570, TEMP,PH,EHM,EHMC,EMFZ,DENS,DOX,FLAG,CORALK,PECALC,IGO,(P B  520
     1RT(I),I=1,4),IDAVES,ISPEC,IMIN                                     B  530
      IF (IPRT.EQ.1) PRT(1)=1                                            B  540
      IF (PRT(1).NE.0) GO TO 70                                          B  550
      PRINT 580                                                          B  560
      DO 30 I=1,D                                                        B  570
      ISIG=SIGN(1)                                                       B  580
      DO 20 J=1,NEQU                                                     B  590
      IF (I.EQ.IEQU(J)) ISIG=SIGN(2)                                     B  600
20    CONTINUE                                                           B  610
      PRINT 590, I,NREACT(I),DH(I),LOGKTO(I),ISIG,I,NSPEC(I),Z(I),DHA(I) B  620
     1,GFW(I)                                                            B  630
30    CONTINUE                                                           B  640
      DD=D+1                                                             B  650
      DO 50 I=DD,E                                                       B  660
      ISIG=SIGN(1)                                                       B  670
      DO 40 J=1,NEQU                                                     B  680
      IF (I.EQ.IEQU(J)) ISIG=SIGN(2)                                     B  690
40    CONTINUE                                                           B  700
      PRINT 600, I,NREACT(I),DH(I),LOGKTO(I),ISIG                        B  710
50    CONTINUE                                                           B  720
      PRINT 510                                                          B  730
      DO 60 I=1,NEQU                                                     B  740
      PRINT 520, IEQU(I),NREACT(IEQU(I)),COEF(1,IEQU(I)),COEF(2,IEQU(I)) B  750
     1,COEF(3,IEQU(I)),COEF(4,IEQU(I)),COEF(5,IEQU(I))                   B  760
60    CONTINUE                                                           B  770
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   70 CONTINUE                                                          B  780
      IPRT=1                                                            B  790
      PRINT 610, TITL                                                   B  800
      READ 620, (CUNITS(INPT(I)),I=1,12)                                B  810
      IF (ISPEC.GT.0) READ 530, (KSPEC(I),I=1,ISPEC)                    B  820
      IF (IMIN.GT.0) READ 530, (KMIN(I),I=1,IMIN)                       B  830
   80 READ 630, WORD,(INT(I),VAL(I),I=1,5)                              B  840
      IF (WORD.NE.CARD(1)) GO TO 100                                    B  850
      DO 90 I=1,5                                                       B  860
      IF (INT(I).EQ.0) GO TO 90                                         B  870
      CUNITS(INT(I))=VAL(I)                                             B  880
   90 CONTINUE                                                          B  890
      GO TO 80                                                          B  900
  100 CONTINUE                                                          B  910
      IF (WORD.NE.CARD(2)) GO TO 110                                    B  920
      EROR1=VAL(1)                                                      B  930
      EROR2=VAL(2)                                                      B  940
      EROR3=VAL(3)                                                      B  950
      EROR4=VAL(4)                                                      B  960
      EROR5=VAL(5)                                                      B  970
      READ 630, WORD,(INT(I),VAL(I),I=1,5)                              B  980
  110 IF (WORD.NE.CARD(3)) GO TO 130                                    B  990
      DO 120 I=1,5                                                      B 1000
      IF (INT(I).EQ.0) GO TO 120                                        B 1010
      DH(INT(I))=VAL(I)                                                 B 1020
      PRINT 640, INT(I),NREACT(INT(I)),VAL(I)                           B 1030
  120 CONTINUE                                                          B 1040
      READ 630, WORD,(INT(I),VAL(I),I=1,5)                              B 1050
      GO TO 110                                                         B 1060
  130 IF (WORD.NE.CARD(4)) GO TO 150                                    B 1070
      DO 140 I=1,5                                                      B 1080
      IF (INT(I).EQ.0) GO TO 140                                        B 1090
      LOGKTO(INT(I))=VAL(I)                                             B 1100
      PRINT 650, INT(I),NREACT(INT(I)),VAL(I)                           B 1110
  140 CONTINUE                                                          B 1120
      READ 630, WORD,(INT(I),VAL(I),I=1,5)                              B 1130
      GO TO 130                                                         B 1140
  150 CONTINUE                                                          B 1150
C                                                                       B 1160
C                                                                       B 1170
C     VANT HOFF EQUATION FOR EFFECT OF T ON K                           B 1180
C                                                                       B 1190
      T=TEMP+273.16                                                     B 1200
      C1=(298.16-T)/(298.16*T*C*R)                                      B 1210
      DO 170 I=1,E                                                      B 1220
      LOGKT(I)=LOGKTO(I)-DH(I)*C1                                       B 1230
      LCHEK(I)=0                                                        B 1240
      IF (LOGKT(I).LT.-77.0.OR.LOGKT(I).GT.75.0) LCHEK(I)=1             B 1250
      IF (LCHEK(I).EQ.1) GO TO 160                                      B 1260
      KT(I)=10.**LOGKT(I)                                               B 1270
  160 CONTINUE                                                          B 1280
  170 CONTINUE                                                          B 1290
      KW=KT(153)                                                        B 1300
C                                                                       B 1310
C                                                                       B 1320
C     ANALYTICAL EXPRESSIONS FOR EFFECT OF T ON K                       B 1330
  180 IF (WORD.NE.CARD(5)) GO TO 220                                    B 1340
      IF (INT(1).EQ.0) GO TO 210                                        B 1350
      DO 190 I=1,5                                                      B 1360
      COEF(I,INT(1))=VAL(I)                                             B 1370
  190 CONTINUE                                                          B 1380
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      IEQ=0                                                                  B 1390
      DO 200 I=1,NEQU                                                        B 1400
      IF (IEQU(I).EQ.INT(1)) IEQ=1                                           B 1410
  200 CONTINUE                                                               B 1420
      IF (IEQ.EQ.0) NEQU=NEQU+1                                              B 1430
      IF (IEQ.EQ.0) IEQU(NEQU)=INT(1)                                        B 1440
      PRINT 660, INT(1),NREACT(INT(1)),COEF(1,INT(1)),COEF(2,INT(1)),COE     B 1450
     1F(3,INT(1)),COEF(4,INT(1)),COEF(5,INT(1))                              B 1460
  210 CONTINUE                                                               B 1470
      READ 630, WORD,(INT(I),VAL(I),I=1,5)                                   B 1480
      GO TO 180                                                              B 1490
  220 CONTINUE                                                               B 1500
      IF (WORD.EQ.CARD(6)) GO TO 230                                         B 1510
      PRINT 540                                                              B 1520
      READ 630, WORD,(INT(I),VAL(I),I=1,5)                                   B 1530
      GO TO 220                                                              B 1540
  230 CONTINUE                                                               B 1550
      DO 240 I=1,NEQU                                                        B 1560
      LOGKT(IEQU(I))=COEF(1,IEQU(I))+COEF(2,IEQU(I))*T+COEF(3,IEQU(I))/T     B 1570
     1+COEF(4,IEQU(I))*T*T+COEF(5,IEQU(I))/(T*T)                             B 1580
  240 CONTINUE                                                               B 1590
      LOGKT(26)=LOGKT(26)+ALOG10(KW)-13.2258*ALOG10(T)                       B 1600
      DO 250 I=1,NEQU                                                        B 1610
      KT(IEQU(I))=1E1**(LOGKT(IEQU(I)))                                      B 1620
  250 CONTINUE                                                               B 1630
C                                                                            B 1640
C                                                                            B 1650
C     CALCULATION OF ANALYZED MOLALITY                                       B 1660
      IF (FLAG.NE.1) GO TO 270                                               B 1670
      DO 260 I=1,D                                                           B 1680
      CUNITS(I)=CUNITS(I)*GFW(I)/V(I)                                        B 1690
  260 CONTINUE                                                               B 1700
      FLAG=2                                                                 B 1710
  270 CONTINUE                                                               B 1720
      IF (FLAG.NE.2) GO TO 290                                               B 1730
      DO 280 I=1,D                                                           B 1740
      CUNITS(I)=CUNITS(I)/DENS                                               B 1750
  280 CONTINUE                                                               B 1760
      FLAG=3                                                                 B 1770
  290 CONTINUE                                                               B 1780
      IF (FLAG.NE.3) GO TO 320                                               B 1790
      C1=0.0                                                                 B 1800
      DO 300 I=1,D                                                           B 1810
      C1=C1+CUNITS(I)                                                        B 1820
  300 CONTINUE                                                               B 1830
      DO 310 I=1,D                                                           B 1840
      C1SAVE=C1                                                              B 1850
      MI(I)=(CUNITS(I)/(1.0E+03*GFW(I)))*(1.0/(1.0-1.0E-06*C1))              B 1860
      IF (MI(I).GT.0.0) XLMI(I)=ALOG10(MI(I))                                B 1870
      GRAMS(I)=CUNITS(I)*DENS                                                B 1880
  310 CONTINUE                                                               B 1890
      GO TO 350                                                              B 1900
  320 CONTINUE                                                               B 1910
      C1=0.0                                                                 B 1920
      IF (FLAG.NE.4) GO TO 480                                               B 1930
      DO 330 I=1,D                                                           B 1940
      MI(I)=CUNITS(I)                                                        B 1950
      C1=C1+MI(I)*GFW(I)*1000./DENS                                          B 1960
      IF (MI(I).GT.0.0) XLMI(I)=ALOG10(MI(I))                                B 1970
  330 CONTINUE                                                               B 1980
      C1SAVE=C1                                                              B 1990
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      DO 340 I=1,D                                                          B 2000
      GRAMS(I)=MI(I)*1000.*GFW(I)*DENS*(1.0-1.0E-06*C1SAVE)                 B 2010
  340 CONTINUE                                                              B 2020
  350 CONTINUE                                                              B 2030
      TDS=0.0                                                               B 2040
      DO 360 I=1,D                                                          B 2050
      ANALMI(I)=MI(I)                                                       B 2060
      TDS=TDS+GRAMS(I)                                                      B 2070
  360 CONTINUE                                                              B 2080
      EPMCAT=0.0                                                            B 2090
      EPMAN=0.0                                                             B 2100
C                                                                           B 2110
C                                                                           B 2120
C     CALCULATION OF CATION-ANION BALANCE                                   B 2130
      DO 380 I=1,D                                                          B 2140
      IF (Z(I).GT.0) GO TO 370                                              B 2150
      EPMAN=EPMAN-Z(I)*MI(I)                                                B 2160
      GO TO 380                                                             B 2170
  370 EPMCAT=EPMCAT+Z(I)*MI(I)                                              B 2180
  380 CONTINUE                                                              B 2190
      EPMCAT=EPMCAT*1000.                                                   B 2200
      EPMAN=EPMAN*1000.                                                     B 2210
C                                                                           B 2220
C                                                                           B 2230
C     CALCULATION OF EH FROM FIELD DATA                                     B 2240
      IF (EHM.LT.9.0) GO TO 420                                             B 2250
      IF (EMFZ.GT.9.0) GO TO 390                                            B 2260
      C1=0.429+2.4E-03*(25.0-TEMP)-EMFZ                                     B 2270
      GO TO 400                                                             B 2280
  390 C1=0.244+8.6E-04*(25.0-TEMP)                                          B 2290
  400 CONTINUE                                                              B 2300
      IF (EHMC.LT.9.0) GO TO 410                                            B 2310
      GO TO 420                                                             B 2320
  410 EHM=EHMC+C1                                                           B 2330
  420 CONTINUE                                                              B 2340
      PEEH=EHM/(C*R*T/F)                                                    B 2350
      IF (PECALC.EQ.0) PE=100.                                              B 2360
      IF (EHM.GE.9.0) PEEH=100.                                             B 2370
      PRINT 560                                                             B 2380
      PRINT 670                                                             B 2390
      PRINT 680, TEMP,PH,EPMCAT,EPMAN                                       B 2400
      PRINT 690, DOX,EHMC,EMFZ,EHM,PEEH                                     B 2410
      IF (PECALC.EQ.1) PE=PEEH                                              B 2420
      PRINT 560                                                             B 2430
      PRINT 700                                                             B 2440
      DO 430 I=1,22                                                         B 2450
      IF (MI(INPT(I)).LE.0.0) GO TO 430                                     B 2460
      PRINT 710, NSPEC(INPT(I)),Z(INPT(I)),MI(INPT(I)),XLMI(INPT(I)),GRA    B 2470
     1MS(INPT(I))                                                           B 2480
  430 CONTINUE                                                              B 2490
      PRINT 560                                                             B 2500
      PRINT 560                                                             B 2510
      IF (PRT(2).NE.0) GO TO 440                                            B 2520
      PRINT 560                                                             B 2530
      PRINT 720                                                             B 2540
  440 CONTINUE                                                              B 2550
      IF (IGO.EQ.1) GO TO 450                                               B 2560
      IF (PH.LT.3.0.OR.PH.GT.11.0) GO TO 490                                B 2570
      DUM=((EPMCAT-EPMAN)/(1.+EPMCAT+EPMAN))*100.                           B 2580
      IF (ABS(DUM).GT.30.) GO TO 490                                        B 2590
  450 CONTINUE                                                              B 2600
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C                                                                       R 2610
C                                                                       R 2620
C     TEMPERATURE EFFECTS ON DEBYE-HUCKEL SOLVENT CONSTANTS             R 2630
      S1=374.11-TEMP                                                    R 2640
      S2=S1**0.333333                                                   R 2650
      S3=SQRT((1.0+0.1342489*S2-3.946263E-03*S1)/(3.1975E0-.3151548E0*S2 R 2660
     1-1.203374E-3*S1+7.48908E-13*S1**4))                               R 2670
      IF (T.LT.373.16) GO TO 460                                        R 2680
      C1=5321E0/T+233.76E0-T*(T*(8.292E-7*T-1.417E-3)+.9297E0)          R 2690
      GO TO 470                                                         R 2700
  460 C1=87.74E0-TEMP*(TEMP*(1.41E-6*TEMP-9.398E-4)+.4008E0)            R 2710
  470 CONTINUE                                                          R 2720
      C1=SQRT(C1*T)                                                     R 2730
      A=18246.0E02*S3/C1**3                                             R 2740
      B=50.29*S3/C1                                                     R 2750
      GO TO 500                                                         R 2760
  480 PRINT 730                                                         R 2770
      ICK=1                                                             R 2780
      GO TO 500                                                         R 2790
  490 PRINT 550                                                         R 2800
      ICK=1                                                             R 2810
  500 CONTINUE                                                          R 2820
      RETURN                                                            R 2830
C                                                                       R 2840
C                                                                       R 2850
  510 FORMAT (//,15X,'"*" DENOTES THAT AN ANALYTICAL EXPRESSION FOR KT H R 2860
     1AS BEEN USED',////,20X,'SUMMARY OF ANALYTICAL EXPRESSIONS OF THE F R 2870
     2ORM  LOG K = A+B*T+C/T+D*T**2+E/T**2',///,23X,'I    NREACT          A R 2880
     3            B             C         D             E'/)             R 2890
  520 FORMAT (22X,I3,2X,A8,3(1X,F11.4),2(1X,1PE11.4))                   R 2900
  530 FORMAT (16I5)                                                     R 2910
  540 FORMAT (/,10X,'WARNING--- INPUT ERROR, SEARCHING FOR BLANK CARD')  R 2920
  550 FORMAT (/,10X,'WARNING---CHECK INPUT PH AND/OR CATION-ANION BALANC R 2930
     1E ...CALCULATION TERMINATED')                                     R 2940
  560 FORMAT (//)                                                       R 2950
  570 FORMAT (5(F6.0,1X),2F5.0,1X,9I1,2I3)                              R 2960
  580 FORMAT (//,60X,'----',/,60X,'DATA',/,60X,'----',//,18X,'I',2X,'NRE R 2970
     1ACT',9X,'DH',8X,'LOGKTO',37X,'I',2X,'NSPEC',6X,'Z',2X,'DHA',6X,'GF R 2980
     2W',/)                                                             R 2990
  590 FORMAT (1H ,15X,I3,2X,A8,2(2X,F10.4),A1,33X,I3,2X,A8,2X,I2,2X,F3.1 R 3000
     1,2X,F10.4)                                                        R 3010
  600 FORMAT (1H ,15X,I3,2X,A8,2(2X,F10.4),A1)                          R 3020
  610 FORMAT (1H1,(5X,20A4),//)                                         R 3030
  620 FORMAT (6(E12.5),8X)                                              R 3040
  630 FORMAT (A4,1X,5(I3,E12.5))                                        R 3050
  640 FORMAT (5X,'NEW DATA *** DELTA H FOR REACTION ',I3,1X,A8,' HAS BEE R 3060
     1N CHANGED TO ',F9.4)                                              R 3070
  650 FORMAT (5X,'NEW DATA *** LOGKTO  FOR REACTION ',I3,1X,A8,' HAS BEE R 3080
     1N CHANGED TO ',F9.4)                                              R 3090
  660 FORMAT (5X,'NEW DATA *** LOGKT   FOR REACTION ',I3,1X,A8,' = ',1PE R 3100
     111.4,'+',E11.4,'*T+',E11.4,'/T+',E11.4,'*T**2+',E11.4,'*T**2')    R 3110
  670 FORMAT (57X,'----------------',/,57X,'INITIAL SOLUTION',/,57X,'--- R 3120
     1----------',///)                                                  R 3130
  680 FORMAT (15X,'TEMPERATURE = ',F6.2,' DEGREES C    PH = ',F6.3,'    R 3140
     1ANALYTICAL EPMCAT = ',F8.3,'    ANALYTICAL EPMAN = ',F8.3,//)     R 3150
  690 FORMAT (5X,'***** OXIDATION - REDUCTION *****',///,11X,'DISSOLVED  R 3160
     1OXYGEN = ',F6.3,' MG/L',/,11X,'EH MEASURED WITH CALOMEL = ',F7.4,' R 3170
     2 VOLTS',/,11X,'MEASURED EH OF ZOBELL SOLUTION = ',F7.4,' VOLTS',/, R 3180
     311X,'CORRECTED EH = ',F7.4,' VOLTS',/,11X,'PE COMPUTED FROM CORREC R 3190
     4TED E  = ',F7.3,/)                                                R 3200
  700 FORMAT '40X,'*** TOTAL CONCENTRATIONS OF INPUT SPECIES ***',//,50X R 3210
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     1,'TOTAL',13X,'LOG TOTAL',12X,'TOTAL',/,33X,'SPECIES',8X,'MOLALITY'  R 3220
     2,12X,'MOLALITY',11X,'MG/LITRE',/,33X,'-------',8X,'--------',12X,'  R 3230
     3--------',11X,'--------',/)                                          R 3240
  710 FORMAT (1H ,32X,A8,I3,3X,1PE13.6,8X,0PF9.4,8X,1PE13.6)               R 3250
  720 FORMAT (50X,'*** CONVERGENCE ITERATIONS ***',//,16X,'ITERATION',4X   R 3260
     1,'S1-ANALCO3',6X,'S2-SO4TOT',8X,'S3-FTOT',9X,'S4-PTOT',9X,'S5-CLTO  R 3270
     2T',/)                                                                R 3280
  730 FORMAT (10X,'INPUT ERROR---UNITS OF CONCENTRATION ARE NOT KNOWN',/   R 3290
     1//)                                                                  R 3300
      END                                                                  R 3310-
      SUBROUTINE SET                                                       C   10
      INTEGER D,E,DD,RBIT,CORALK,Z(120),WORD,CARD(6),FLAG,PRT(4),SIGN(2)   C   20
      INTEGER PECALC,PECK                                                  C   30
      DIMENSION INT(5), VAL(5), INPT(22), GRAMS(120), IEQU(50), COEF(5,2   C   40
     100)                                                                  C   50
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT   C   60
     10T,MGTOT,LITOT,NH4TOT,KW                                            C   70
      REAL *8NSPEC(120),NREACT(200)                                        C   80
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P   C   90
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA   C  100
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120),   C  110
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI(   C  120
     4120),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT   C  130
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT   C  140
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC,   C  150
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                           C  160
C                                                                         C  170
C                                                                         C  180
C     INITIALIZE STARTING VALUES FOR ITERATIVE LOOP                       C  190
      AH2O=1.0                                                            C  200
      DO 10 I=1,D                                                         C  210
      GAMMA(I)=1.0                                                        C  220
   10 CONTINUE                                                            C  230
      CO2TIT=MI(7)+2.0*MI(18)                                             C  240
      ANALCO=CO2TIT                                                       C  250
      IF (CORALK.EQ.2) CO2TIT=MI(7)+MI(18)+MI(86)                         C  260
      SITOT=MI(35)                                                        C  270
      CATOT=MI(1)                                                         C  280
      MGTOT=MI(2)                                                         C  290
      NATOT=MI(3)                                                         C  300
      KTOT=MI(4)                                                          C  310
      SO4TOT=MI(6)                                                        C  320
      FETOT=MI(8)                                                         C  330
      PTOT=MI(45)                                                         C  340
      PIONIC=PTOT                                                         C  350
      ALTOT=MI(51)                                                        C  360
      FTOT=MI(62)                                                         C  370
      BTOT=MI(87)                                                         C  380
      LITOT=MI(81)                                                        C  390
      NH4TOT=MI(39)                                                       C  400
      SRTOT=MI(88)                                                        C  410
      BATOT=MI(90)                                                        C  420
      CLTOT=MI(5)                                                         C  430
      MNTOT=MI(101)                                                       C  440
      MI(35)=0.0                                                          C  450
      MI(87)=0.0                                                          C  460
      TENPH=10.**PH                                                       C  470
      ALFA(64)=10.**(-PH)                                                 C  480
C                                                                         C  490
C                                                                         C  500
C     CALCULATION OF ANION ACTIVITIES EXCEPT CO2 AND PO4 SPECIES          C  510
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      ALFA(5)=MI(5)*GAMMA(5)                                                C  520
      ALFA(6)=MI(6)*GAMMA(6)                                                C  530
      ALFA(62)=MI(62)*GAMMA(62)                                             C  540
      ALFA(85)=MI(85)*GAMMA(85)                                             C  550
      ALFA(98)=MI(98)*GAMMA(98)                                             C  560
      ALFA(27)=AH2O*KW*TENPH                                                C  570
      MI(27)=ALFA(27)/GAMMA(27)                                             C  580
      MI(64)=1E0/(TENPH*GAMMA(64))                                          C  590
      ALFA(63)=ALFA(6)*KT(90)/TENPH                                         C  600
      MI(63)=ALFA(63)/GAMMA(63)                                             C  610
C                                                                           C  620
C                                                                           C  630
C     CO2 SPECIES                                                           C  640
      IF (CORALK.EQ.2) GO TO 20                                             C  650
      C1=2.0*TENPH/(GAMMA(18)*KT(69))                                       C  660
      MI(7)=CO2TIT/(1.+GAMMA(7)*C1)                                         C  670
      C2=KT(36)/(TENPH*GAMMA(86))                                           C  680
      ALFA(7)=MI(7)*GAMMA(7)                                                C  690
      MI(18)=C1*ALFA(7)/2.                                                  C  700
      MI(86)=C2*ALFA(7)                                                     C  710
      ALFA(18)=MI(18)*GAMMA(18)                                             C  720
      ALFA(86)=MI(86)*GAMMA(86)                                             C  730
      GO TO 30                                                              C  740
   20 CONTINUE                                                              C  750
      MI(7)=CO2TIT/(1.0+GAMMA(7)*((KT(36)/(TENPH*GAMMA(86)))+TENPH/(KT(6    C  760
     19)*GAMMA(18))))                                                       C  770
      MI(18)=MI(7)*GAMMA(7)*TENPH/(GAMMA(18)*KT(69))                        C  780
      MI(86)=MI(7)*GAMMA(7)*KT(36)/(TENPH*GAMMA(86))                        C  790
      ALFA(7)=MI(7)*GAMMA(7)                                                C  800
      ALFA(18)=MI(18)*GAMMA(18)                                             C  810
      ALFA(86)=MI(86)*GAMMA(86)                                             C  820
   30 CONTINUE                                                              C  830
C                                                                           C  840
C                                                                           C  850
C     PHOSPHATE SPECIES                                                     C  860
      MI(45)=PTOT/(1.+(KT(17)*GAMMA(45)/(GAMMA(48)*TENPH**2))+(KT(16)*GA    C  870
     1MMA(45)/(TENPH*GAMMA(47))))                                           C  880
      ALFA(45)=MI(45)*GAMMA(45)                                             C  890
      ALFA(47)=KT(16)*ALFA(45)/TENPH                                        C  900
      MI(47)=ALFA(47)/GAMMA(47)                                             C  910
      ALFA(48)=KT(17)*ALFA(45)/(TENPH**2)                                   C  920
      MI(48)=ALFA(48)/GAMMA(48)                                             C  930
      ITER=0                                                                C  940
      RETURN                                                                C  950
      END                                                                   C  960-
      SUBROUTINE MODEL                                                      D   10
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST(8),LIST1(5),LIST2(18),LIST3    D   20
     1(6),PRT(4),PECALC,PECK                                                D   30
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT    D   40
     1OT,MGTOT,LITOT,NH4TOT,KW,MUHALF                                       D   50
      REAL *8NSPEC(120),NREACT(200)                                         D   60
      DIMENSION NPAIR(5), L1M(9), L1K(9), L1C(9), L1A(9), L1ALK(9), L2M(    D   70
     113), L2K(13), L2C(13), L3M(7), L3K(7), L3C(7), L4M(14), L4K(14), L    D   80
     24C(14), L4A(14), L5M(9), L5K(9), L5C(9)                               D   90
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P    D  100
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA    D  110
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120),    D  120
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI(    D  130
     4120),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT    D  140
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT    D  150
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC,    D  160
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     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                                D  170
      DATA LIST/17,35,66,70,71,72,84,87/                                       D  180
      DATA LIST1/42,43,44,50,94/                                               D  190
      DATA LIST2/8,9,10,11,12,13,15,16,28,33,34,65,77,78,79,80,100,99/         D  200
      DATA LIST3/82,83,88,89,90,91/                                            D, 210
      DATA L1M/7,21,22,30,31,42,43,86,111/,L1K/69,74,75,78,79,70,71,36,1       D  220
     167/,L1C/64,2,2,1,1,3,3,64,101/,L1A/18,18,7,7,18,18,7,7,7/,L1ALK/1.       D  230
     20,2.0,1.0,1.0,2.0,2.0,1.0,0.0,1.0/,L2M/15,23,32,34,44,46,59,60,63,       D  240
     383,92,96,109/,L2K/5,76,24,9,72,73,88,89,90,127,132,136,165/,L2C/8,       D  250
     42,1,8,3,4,51,51,64,81,39,64,101/,L3M/20,55,56,57,58,108,49/,L3K/23       D  260
     5,84,85,86,87,164,80/,L3C/2,51,51,51,51,101,1/,L4M/13,40,41,47,48,5       D  270
     60,61,65,73,74,75,76,99,100/,L4K/140,124,125,16,17,31,33,121,34,35,       D  280
     7122,123,157,139/,L4C/8,2,2,64,64,3,4,8,2,1,1,1,8,8/,L4A/47,45,48,4       D  290
     85,45,47,47,48,47,47,45,48,48,47/,L5M/16,28,33,93,94,95,103,104,105       D  300
     9/,L5K/6,7,8,133,134,135,159,160,161/,L5C/8,8,8,64,3,4,101,101,101/       D  310
     $,NPAIR/9,13,7,14,9/                                                      D  320
      ITER=ITER+1                                                              D  330
C                                                                              D  340
C                                                                              D  350
C     CALCULATION OF TOTAL MOLALITY AND AH2O                                   D  360
      J=1                                                                      D  370
      C1=0.0                                                                   D  380
      DO 20 I=1,D                                                              D  390
      IF (I.EQ.LIST(J)) GO TO 10                                               D  400
      C1=C1+MI(I)                                                              D  410
      GO TO 20                                                                 D  420
   10 J=J+1                                                                    D  430
   20 CONTINUE                                                                 D  440
      AH2O=1.0-0.017*C1                                                        D  450
      LH2O=ALOG10(AH2O)                                                        D  460
      IF (DOX.GT.0.0) PEDO=-(ALOG10(KT(152))+PH+0.5*LH2O-0.25*ALOG10(DOX       D  470
     1/32E3))                                                                  D  480
      IF (DOX.GT.0.0) PESATO=-(ALOG10(KT(137))+PH+0.5*LH2O-0.25*ALOG10(D       D  490
     1OX/32E3))                                                                D  500
      IF (PECALC.EQ.2) PE=PEDO                                                 D  510
      IF (PECALC.EQ.3) PE=PESATO                                               D  520
C                                                                              D  530
C                                                                              D  540
C     CALCULATION OF ACTIVITY COEFFICIENTS                                     D  550
      MU=0.0                                                                   D  560
      J=1                                                                      D  570
      DO 40 I=1,D                                                              D  580
      IF (I.EQ.LIST(J)) GO TO 30                                               D  590
      MU=MU+0.5*MI(I)*Z(I)*Z(I)                                                D  600
      GO TO 40                                                                 D  610
   30 J=J+1                                                                    D  620
   40 CONTINUE                                                                 D  630
      MUHALF=SQRT(MU)                                                          D  640
      C1=-A*4E0*MUHALF                                                         D  650
      GAMMA(1)=1E1**(C1/(1E0+B*5E0*MUHALF)+0.165*MU)                           D  660
      GAMMA(2)=1E1**(C1/(1E0+B*5.5*MUHALF)+0.2*MU)                             D  670
      GAMMA(3)=1E1**(-A*MUHALF/(1E0+B*4E0*MUHALF)+0.075*MU)                    D  680
      GAMMA(4)=1E1**(-A*MUHALF/(1E0+B*3.5*MUHALF)+0.015*MU)                    D  690
      GAMMA(5)=GAMMA(4)                                                        D  700
      GAMMA(6)=1E1**(C1/(1E0+B*5E0*MUHALF)-0.04*MU)                            D  710
      DO 60 I=8,D                                                              D  720
      IF (Z(I).EQ.0) GO TO 50                                                  D  730
      IF (IDAVES.EQ.1) GAMMA(I)=1E1**((-A*Z(I)**2*MUHALF)/(1.0+MUHALF)-0       D  740
     1.3*MU)                                                                   D  750
      IF (IDAVES.EQ.1) GO TO 60                                                D  760
      GAMMA(I)=1E1**(-A*MUHALF*Z(I)**2/(1E0+DHA(I)*B*MUHALF))                  D  770
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      GO TO 60                                                          D  780
   50 GAMMA(I)=10.**(0.1*MU)                                            D  790
   60 CONTINUE                                                          D  800
      GAMMA(7)=1E1**(-A*MUHALF*Z(7)**2/(1E0+DHA(7)*B*MUHALF))           D  810
      GAMMA(18)=1E1**(-A*MUHALF*Z(18)**2/(1E0+DHA(18)*B*MUHALF))        D  820
      GAMMA(86)=1E1**(ML*(170.01/T-.8798+.0013935*T)+MU*MU*(28.81/T-.210 D  830
     18+.0003641*T))                                                    D  840
C                                                                       D  850
C                                                                       D  860
C     SULFUR SPECIES AND PE CALCULATION FROM S                          D  870
      C1=KT(92)*TENPH/GAMMA(67)                                         D  880
      C2=KT(92)*KT(93)*TENPH**2/GAMMA(68)                               D  890
      MI(14)=MI(17)/(1E0+GAMMA(14)*(C1+C2))                             D  900
      ALFA(14)=MI(14)*GAMMA(14)                                         D  910
      ALFA(17)=MI(17)*GAMMA(17)                                         D  920
      MI(67)=ALFA(14)*C1                                                D  930
      MI(68)=ALFA(14)*C2                                                D  940
      ALFA(67)=MI(67)*GAMMA(67)                                         D  950
      ALFA(68)=MI(68)*GAMMA(68)                                         D  960
      C1=ALFA(6)*ALFA(14)                                               D  970
      IF (C1.GT.0.0) GO TO 70                                           D  980
      GO TO 80                                                          D  990
   70 PES=0.125*ALOG10(KT(91))+0.125*ALOG10(ALFA(6))-1.25*PH-0.125*ALOG1 D 1000
     10(ALFA(14))-0.5*LH20                                              D 1010
      IF (PECALC.EQ.4) PE=PES                                           D 1020
   80 CONTINUE                                                          D 1030
      IF (PECALC.EQ.0.0.OR.PE.GE.100.) GO TO 90                         D 1040
      TENMPE=10.**(-PE)                                                 D 1050
      GO TO 100                                                         D 1060
   90 TENMPE=10.**(-30)                                                 D 1070
  100 CONTINUE                                                          D 1080
C                                                                       D 1090
C                                                                       D 1100
C     SILICA SPECIES                                                    D 1110
      C1=KT(14)*TENPH/GAMMA(25)                                         D 1120
      C2=KT(15)*TENPH**2/GAMMA(26)                                      D 1130
      MI(24)=SITOT/(1.0+GAMMA(24)*(C1+C2))                              D 1140
      ALFA(24)=MI(24)*GAMMA(24)                                         D 1150
      MI(25)=ALFA(24)*C1                                                D 1160
      MI(26)=ALFA(24)*C2                                                D 1170
      ALFA(25)=MI(25)*GAMMA(25)                                         D 1180
      ALFA(26)=MI(26)*GAMMA(26)                                         D 1190
C                                                                       D 1200
C                                                                       D 1210
C     BORON SPECIES                                                     D 1220
      C1=GAMMA(36)*KT(26)*TENPH/GAMMA(37)                               D 1230
      MI(36)=BTOT/(1.0+C1)                                              D 1240
      MI(37)=C1*MI(36)                                                  D 1250
      ALFA(36)=MI(36)*GAMMA(36)                                         D 1260
      ALFA(37)=MI(37)*GAMMA(37)                                         D 1270
C                                                                       D 1280
C                                                                       D 1290
C     NITROGEN SPECIES                                                  D 1300
      C1=TENPH*KT(27)/GAMMA(38)                                         D 1310
      C2=ALFA(6)*KT(132)/GAMMA(92)                                      D 1320
      MI(39)=NH4TOT/(1E0+GAMMA(39)*(C1+C2))                             D 1330
      ALFA(39)=MI(39)*GAMMA(39)                                         D 1340
      MI(38)=ALFA(39)*C1                                                D 1350
      ALFA(38)=MI(38)*GAMMA(38)                                         D 1360
      MI(92)=ALFA(39)*C2                                                D 1370
      ALFA(92)=MI(92)*GAMMA(92)                                         D 1380
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C                                                                       D 1390
C                                                                       D 1400
C     MAGNESIUM SPECIES                                                 D 1410
      MI(19)=ALFA(27)*KT(25)/GAMMA(19)                                  D 1420
      MI(20)=ALFA(62)*KT(23)/GAMMA(20)                                  D 1430
      MI(21)=ALFA(18)*KT(74)/GAMMA(21)                                  D 1440
      MI(22)=ALFA(7)*KT(75)/GAMMA(22)                                   D 1450
      MI(23)=ALFA(6)*KT(76)/GAMMA(23)                                   D 1460
      MI(40)=ALFA(45)*KT(124)/GAMMA(40)                                 D 1470
      MI(41)=ALFA(48)*KT(125)/GAMMA(41)                                 D 1480
      MI(73)=ALFA(47)*KT(34)/GAMMA(73)                                  D 1490
      MI(2)=MGTOT/(1.0+GAMMA(2)*(MI(19)+MI(20)+MI(21)+MI(22)+MI(23)+MI(4 D 1500
     10)+MI(41)+MI(73)))                                                D 1510
      ALFA(2)=MI(2)*GAMMA(2)                                            D 1520
      C1=ALFA(2)                                                        D 1530
      DO 110 I=19,23                                                    D 1540
      MI(I)=C1*MI(I)                                                    D 1550
      ALFA(I)=MI(I)*GAMMA(I)                                            D 1560
  110 CONTINUE                                                          D 1570
      MI(40)=C1*MI(40)                                                  D 1580
      ALFA(40)=MI(40)*GAMMA(40)                                         D 1590
      MI(41)=C1*MI(41)                                                  D 1600
      ALFA(41)=MI(41)*GAMMA(41)                                         D 1610
      MI(73)=C1*MI(73)                                                  D 1620
      ALFA(73)=MI(73)*GAMMA(73)                                         D 1630
C                                                                       D 1640
C                                                                       D 1650
C     CALCIUM SPECIES                                                   D 1660
      MI(29)=ALFA(27)*KT(77)/GAMMA(29)                                  D 1670
      MI(30)=ALFA(7)*KT(78)/GAMMA(30)                                   D 1680
      MI(31)=ALFA(18)*KT(79)/GAMMA(31)                                  D 1690
      MI(32)=ALFA(6)*KT(24)/GAMMA(32)                                   D 1700
      MI(74)=ALFA(47)*KT(35)/GAMMA(74)                                  D 1710
      MI(76)=ALFA(48)*KT(123)/GAMMA(76)                                 D 1720
      MI(75)=ALFA(45)*KT(122)/GAMMA(75)                                 D 1730
      MI(49)=ALFA(62)*KT(80)/GAMMA(49)                                  D 1740
      MI(1)=CATOT/(1.0+GAMMA(1)*(MI(29)+MI(30)+MI(31)+MI(32)+MI(74)+MI(7 D 1750
     15)+MI(76)+MI(49)))                                                D 1760
      C1=MI(1)*GAMMA(1)                                                 D 1770
      ALFA(1)=C1                                                        D 1780
      DO 120 I=29,32                                                    D 1790
      MI(I)=C1*MI(I)                                                    D 1800
      ALFA(I)=MI(I)*GAMMA(I)                                            D 1810
  120 CONTINUE                                                          D 1820
      MI(74)=C1*MI(74)                                                  D 1830
      ALFA(74)=MI(74)*GAMMA(74)                                         D 1840
      MI(75)=C1*MI(75)                                                  D 1850
      ALFA(75)=MI(75)*GAMMA(75)                                         D 1860
      MI(76)=C1*MI(76)                                                  D 1870
      ALFA(76)=MI(76)*GAMMA(76)                                         D 1880
      MI(49)=C1*MI(49)                                                  D 1890
      ALFA(49)=MI(49)*GAMMA(49)                                         D 1900
C                                                                       D 1910
C                                                                       D 1920
C     SODIUM SPECIES                                                    D 1930
      MI(42)=ALFA(18)*KT(70)/GAMMA(42)                                  D 1940
      MI(43)=ALFA(7)*KT(71)/GAMMA(43)                                   D 1950
      MI(44)=ALFA(6)*KT(72)/GAMMA(44)                                   D 1960
      MI(50)=ALFA(47)*KT(31)/GAMMA(50)                                  D 1970
      MI(94)=ALFA(5)*KT(134)/GAMMA(94)                                  D 1980
      MI(3)=NATOT/(1.0+GAMMA(3)*(MI(42)+MI(43)+MI(44)+MI(50)+MI(94)))   D 1990
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      ALFA(3)=MI(3)*GAMMA(3)                                                    D 2000
      C1=ALFA(3)                                                                D 2010
      DO 130 I=1,5                                                              D 2020
      MI(LIST1(I))=C1*MI(LIST1(I))                                              D 2030
      ALFA(LIST1(I))=MI(LIST1(I))*GAMMA(LIST1(I))                               D 2040
  130 CONTINUE                                                                  D 2050
C                                                                               D 2060
C                                                                               D 2070
C     POTASSIUM SPECIES                                                         D 2080
      MI(46)=ALFA(6)*KT(73)/GAMMA(46)                                           D 2090
      MI(61)=ALFA(47)*KT(33)/GAMMA(61)                                          D 2100
      MI(95)=ALFA(5)*KT(135)/GAMMA(95)                                          D 2110
      MI(4)=KTOT/(1.0+GAMMA(4)*(MI(46)+MI(61)+MI(95)))                          D 2120
      ALFA(4)=MI(4)*GAMMA(4)                                                    D 2130
      C1=ALFA(4)                                                                D 2140
      MI(46)=C1*MI(46)                                                          D 2150
      ALFA(46)=MI(46)*GAMMA(46)                                                 D 2160
      MI(61)=C1*MI(61)                                                          D 2170
      ALFA(61)=MI(61)*GAMMA(61)                                                 D 2180
      MI(95)=C1*MI(95)                                                          D 2190
      ALFA(95)=MI(95)*GAMMA(95)                                                 D 2200
C                                                                               D 2210
C                                                                               D 2220
C     ALUMINIUM SPECIES                                                         D 2230
      MI(52)=ALFA(27)*KT(81)/GAMMA(52)                                          D 2240
      MI(53)=ALFA(27)**2*KT(82)/GAMMA(53)                                       D 2250
      MI(54)=ALFA(27)**4*KT(83)/GAMMA(54)                                       D 2260
      MI(55)=ALFA(62)*KT(84)/GAMMA(55)                                          D 2270
      MI(56)=ALFA(62)**2*KT(85)/GAMMA(56)                                       D 2280
      MI(57)=ALFA(62)**3*KT(86)/GAMMA(57)                                       D 2290
      MI(58)=ALFA(62)**4*KT(87)/GAMMA(58)                                       D 2300
      MI(59)=ALFA(6)*KT(88)/GAMMA(59)                                           D 2310
      MI(60)=ALFA(6)**2*KT(89)/GAMMA(60)                                        D 2320
      MI(51)=ALTOT/(1.0+GAMMA(51)*(MI(52)+MI(53)+MI(54)+MI(55)+MI(56)+MI        D 2330
     1(57)+MI(58)+MI(59)+MI(60)))                                               D 2340
      ALFA(51)=MI(51)*GAMMA(51)                                                 D 2350
      C1=ALFA(51)                                                               D 2360
      DO 140 I=52,60                                                            D 2370
      MI(I)=C1*MI(I)                                                            D 2380
      ALFA(I)=MI(I)*GAMMA(I)                                                    D 2390
  140 CONTINUE                                                                  D 2400
C                                                                               D 2410
C                                                                               D 2420
C     IRON SPECIES                                                              D 2430
      IF (ABS(PE).LT.20.0.AND.FETOT.GT.0.0) GO TO 150                           D 2440
      GO TO 170                                                                 D 2450
  150 MI(9)=KT(1)/(TENMPE*GAMMA(9))                                             D 2460
      MI(10)=KT(2)*AH2O*TENPH/(TENMPE*GAMMA(10))                                D 2470
      MI(11)=KT(3)*AH2O*TENPH/GAMMA(11)                                         D 2480
      MI(12)=KT(4)*AH2O**3*TENPH**3/GAMMA(12)                                   D 2490
      MI(13)=KT(140)*ALFA(47)/(GAMMA(13)*TENMPE)                                D 2500
      MI(15)=KT(5)*ALFA(6)/(TENMPE*GAMMA(15))                                   D 2510
      MI(16)=KT(6)*ALFA(5)/(TENMPE*GAMMA(16))                                   D 2520
      MI(28)=KT(7)*ALFA(5)**2/(TENMPE*GAMMA(28))                                D 2530
      MI(33)=KT(8)*ALFA(5)**3/(TENMPE*GAMMA(33))                                D 2540
      MI(34)=KT(9)*ALFA(6)/GAMMA(34)                                            D 2550
      MI(65)=KT(121)*ALFA(48)/GAMMA(65)                                         D 2560
      MI(77)=KT(103)*(AH2O*TENPH)**2/(TENMPE*GAMMA(77))                         D 2570
      MI(78)=KT(104)*(AH2O*TENPH)**3/(TENMPE*GAMMA(78))                         D 2580
      MI(79)=KT(105)*(AH2O*TENPH)**4/(TENMPE*GAMMA(79))                         D 2590
      MI(80)=KT(106)*(AH2O*TENPH)**2/GAMMA(80)                                  D 2600
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      MI(99)=KT(157)*ALFA(48)/(TENMPE*GAMMA(99))                        D 2610
      MI(100)=KT(139)*ALFA(47)/GAMMA(100)                               D 2620
      MI(8)=FETOT/(1.0+GAMMA(8)*(MI(9)+MI(10)+MI(11)+MI(12)+MI(13)+MI(15 D 2630
     1)+MI(16)+MI(28)+MI(33)+MI(34)+MI(65)+MI(77)+MI(78)+MI(79)+MI(80)+M D 2640
     2I(100)+MI(99)))                                                   D 2650
      ALFA(8)=MI(8)*GAMMA(8)                                            D 2660
      C1=ALFA(8)                                                        D 2670
      DO 160 I=2,18                                                     D 2680
      MI(LIST2(I))=C1*MI(LIST2(I))                                      D 2690
      ALFA(LIST2(I))=MI(LIST2(I))*GAMMA(LIST2(I))                       D 2700
  160 CONTINUE                                                          D 2710
      GO TO 190                                                         D 2720
  170 CONTINUE                                                          D 2730
      DO 180 I=2,18                                                     D 2740
      MI(LIST2(I))=0.0                                                  D 2750
  180 CONTINUE                                                          D 2760
      ALFA(8)=MI(8)*GAMMA(8)                                            D 2770
  190 CONTINUE                                                          D 2780
C                                                                       D 2790
C     MANGANESE SPECIES                                                 D 2800
C                                                                       D 2810
      IF (ABS(PE).LT.20.0.AND.MNTOT.GT.0.0) GO TO 200                   D 2820
      GO TO 240                                                         D 2830
  200 MI(102)=KT(158)/(GAMMA(102)*TENMPE)                               D 2840
      MI(103)=KT(159)*MI(5)*GAMMA(5)/GAMMA(103)                         D 2850
      MI(104)=KT(160)*MI(5)**2*GAMMA(5)**2/GAMMA(104)                   D 2860
      MI(105)=KT(161)*MI(5)**3*GAMMA(5)**3/GAMMA(105)                   D 2870
      MI(106)=KT(162)*MI(27)*GAMMA(27)/GAMMA(106)                       D 2880
      MI(107)=KT(163)*MI(27)**3*GAMMA(27)**3/GAMMA(107)                 D 2890
      MI(108)=KT(164)*MI(62)*GAMMA(62)/GAMMA(108)                       D 2900
      MI(109)=KT(165)*MI(6)*GAMMA(6)/GAMMA(109)                         D 2910
      MI(110)=KT(166)*MI(85)**2*GAMMA(85)**2/GAMMA(110)                 D 2920
      MI(111)=KT(167)*MI(7)*GAMMA(7)/GAMMA(111)                         D 2930
      XMI112=LOGKT(168)+4*LH2O-(ALOG10(GAMMA(112))-8*PH-5*PE)           D 2940
      IF (XMI112.LT.-50.) MI(112)=0.0                                   D 2950
      IF (XMI112.LT.-50.) GO TO 210                                     D 2960
      MI(112)=10.**XMI112                                               D 2970
  210 CONTINUE                                                          D 2980
      XMI113=LOGKT(169)+4*LH2O-(ALOG10(GAMMA(113))-8*PH-4*PE)           D 2990
      IF (XMI113.LT.-50.) MI(113)=0.0                                   D 3000
      IF (XMI113.LT.-50.) GO TO 220                                     D 3010
      MI(113)=10.**XMI113                                               D 3020
  220 CONTINUE                                                          D 3030
      MI(115)=KT(171)*AH2O**2/(GAMMA(115)*ALFA(64)**3)                  D 3040
      MI(101)=MNTOT/(1.0+GAMMA(101)*(MI(102)+MI(103)+MI(104)+MI(105)+MI( D 3050
     1106)+MI(107)+MI(108)+MI(109)+MI(110)+MI(111)+MI(112)+MI(113)+MI(11 D 3060
     25)))                                                              D 3070
      ALFA(101)=MI(101)*GAMMA(101)                                      D 3080
      C1=ALFA(101)                                                      D 3090
      DO 230 I=102,113                                                  D 3100
      MI(I)=C1*MI(I)                                                    D 3110
      ALFA(I)=MI(I)*GAMMA(I)                                            D 3120
  230 CONTINUE                                                          D 3130
      MI(115)=C1*MI(115)                                                D 3140
      ALFA(115)=MI(115)*GAMMA(115)                                      D 3150
      GO TO 260                                                         D 3160
  240 DO 250 I=101,113                                                  D 3170
      MI(I)=0.0                                                         D 3180
  250 CONTINUE                                                          D 3190
      MI(115)=0.0                                                       D 3200
  260 CONTINUE                                                          D 3210
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C                                                                       D 3220
C                                                                       D 3230
C     CALCULATION OF PO2 AND PCH4                                       D 3240
      IF (ABS(PE).LT.19.0) GO TO 270                                    D 3250
      GO TO 280                                                         D 3260
  270 C1=ALOG10(KT(94))+PH+PE+0.5*LH2O                                  D 3270
      ALFA(70)=10.**(4.0*C1)                                            D 3280
  280 CONTINUE                                                          D 3290
      IF (ABS(PE).LT.19.0.AND.ALFA(7).GT.0.0) GO TO 290                 D 3300
      GO TO 300                                                         D 3310
  290 XLALFA(71)=(ALOG10(KT(95))-8.0*PE-9.0*PH-3.0*LH2O+ALOG10(ALFA(7))) D 3320
      IF (XLALFA(71).LT.-78.) GO TO 300                                 D 3330
      ALFA(71)=10.**XLALFA(71)                                          D 3340
  300 CONTINUE                                                          D 3350
C                                                                       D 3360
C                                                                       D 3370
C     LITHIUM, STRONTIUM, BARIUM SPECIES                                D 3380
      C1=KT(126)*ALFA(27)/GAMMA(82)                                     D 3390
      C2=KT(127)*ALFA(6)/GAMMA(83)                                      D 3400
      MI(81)=LITOT/(1.0+GAMMA(81)*(C1+C2))                              D 3410
      ALFA(81)=MI(81)*GAMMA(81)                                         D 3420
      MI(82)=C1*ALFA(81)                                                D 3430
      MI(83)=C2*ALFA(81)                                                D 3440
      C1=KT(130)*ALFA(27)/GAMMA(89)                                     D 3450
      MI(88)=SRTOT/(1.0+GAMMA(88)*C1)                                   D 3460
      MI(89)=GAMMA(88)*MI(88)*C1                                        D 3470
      C1=KT(131)*ALFA(27)/GAMMA(91)                                     D 3480
      MI(90)=BATOT/(1.0+GAMMA(90)*C1)                                   D 3490
      MI(91)=GAMMA(90)*MI(90)*C1                                        D 3500
      DO 310 I=1,6                                                      D 3510
      ALFA(LIST3(I))=MI(LIST3(I))*GAMMA(LIST3(I))                       D 3520
  310 CONTINUE                                                          D 3530
      S1=0.0                                                            D 3540
      S2=0.0                                                            D 3550
      S3=0.0                                                            D 3560
      S4=0.0                                                            D 3570
      S5=0.0                                                            D 3580
      ANALCO=CO2TIT                                                     D 3590
C     MASS BALANCE ON CARBON                                            D 3600
      IF (CO2TIT.LE.0.0) GO TO 370                                      D 3610
      ACT=KT(69)*ALFA(64)                                               D 3620
      SUM=0.0                                                           D 3630
      SUM1=0.0                                                          D 3640
      N=NPAIR(1)                                                        D 3650
      DO 320 I=1,N                                                      D 3660
      MI(L1M(I))=KT(L1K(I))*ALFA(L1C(I))/GAMMA(L1M(I))                  D 3670
      IF (L1A(I).EQ.7) MI(L1M(I))=MI(L1M(I))*ACT                        D 3680
      SUM=SUM+MI(L1M(I))                                                D 3690
      SUM1=SUM1+L1ALK(I)*MI(L1M(I))                                     D 3700
  320 CONTINUE                                                          D 3710
      IF (CORALK.NE.2) GO TO 340                                        D 3720
      MI(18)=ANALCO/(1.0+GAMMA(18)*SUM)                                 D 3730
      ALFA(18)=MI(18)*GAMMA(18)                                         D 3740
      DO 330 I=1,N                                                      D 3750
      MI(L1M(I))=MI(L1M(I))*ALFA(18)                                    D 3760
      ALFA(L1M(I))=MI(L1M(I))*GAMMA(L1M(I))                             D 3770
      S1=S1+MI(L1M(I))                                                  D 3780
  330 CONTINUE                                                          D 3790
      S1=S1+MI(18)                                                      D 3800
      GO TO 370                                                         D 3810
  340 CONTINUE                                                          D 3820
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      IF (CORALK.EQ.1) GO TO 350                                        D 3830
      ANALCO=CO2TIT-MI(25)-2.0*MI(26)-MI(27)-MI(37)-2.0*MI(45)-MI(47)-MI D 3840
     1(54)-MI(67)-2.0*MI(68)-MI(82)                                     D 3850
  350 CONTINUE                                                          D 3860
      MI(18)=ANALCO/(2.0+GAMMA(18)*SUM1)                                D 3870
      ALFA(18)=MI(18)*GAMMA(18)                                         D 3880
      DO 360 I=1,N                                                      D 3890
      MI(L1M(I))=MI(L1M(I))*ALFA(18)                                    D 3900
      ALFA(L1M(I))=MI(L1M(I))*GAMMA(L1M(I))                             D 3910
      S1=S1+L1ALK(I)*MI(L1M(I))                                         D 3920
  360 CONTINUE                                                          D 3930
      S1=S1+2.0*MI(18)                                                  D 3940
  370 CONTINUE                                                          D 3950
C     MASS BALANCE ON SULFATE                                           D 3960
      IF (SO4TOT.LE.0.0) GO TO 410                                      D 3970
      N=NPAIR(2)                                                        D 3980
      DO 380 I=1,N                                                      D 3990
      MI(L2M(I))=KT(L2K(I))*ALFA(L2C(I))/GAMMA(L2M(I))                  D 4000
  380 CONTINUE                                                          D 4010
      MI(15)=MI(15)/TEMPE                                               D 4020
      MI(60)=MI(60)*ALFA(6)                                             D 4030
      MI(96)=MI(96)*ALFA(64)                                            D 4040
      SUM=MI(60)                                                        D 4050
      DO 390 I=1,N                                                      D 4060
      SUM=SUM+MI(L2M(I))                                                D 4070
  390 CONTINUE                                                          D 4080
      MI(6)=SO4TOT/(1.0+GAMMA(6)*SUM)                                   D 4090
      ALFA(6)=MI(6)*GAMMA(6)                                            D 4100
      DO 400 I=1,N                                                      D 4110
      MI(L2M(I))=MI(L2M(I))*ALFA(6)                                     D 4120
      ALFA(L2M(I))=MI(L2M(I))*GAMMA(L2M(I))                             D 4130
      S2=S2+MI(L2M(I))                                                  D 4140
  400 CONTINUE                                                          D 4150
      S2=S2+MI(6)+MI(60)                                                D 4160
  410 CONTINUE                                                          D 4170
C     MASS BALANCE ON FLUORIDE                                          D 4180
      IF (FTOT.LE.0.0) GO TO 450                                        D 4190
      N=NPAIR(3)                                                        D 4200
      DO 420 I=1,N                                                      D 4210
      MI(L3M(I))=KT(L3K(I))*ALFA(L3C(I))/GAMMA(L3M(I))                  D 4220
  420 CONTINUE                                                          D 4230
      MI(56)=MI(56)*ALFA(62)                                            D 4240
      MI(57)=MI(57)*ALFA(62)*ALFA(62)                                   D 4250
      MI(58)=MI(58)*ALFA(62)*ALFA(62)*ALFA(62)                          D 4260
      SUM=MI(56)+2.0*MI(57)+3.0*MI(58)                                  D 4270
      DO 430 I=1,N                                                      D 4280
      SUM=SUM+MI(L3M(I))                                                D 4290
  430 CONTINUE                                                          D 4300
      MI(62)=FTOT/(1.0+GAMMA(62)*SUM)                                   D 4310
      ALFA(62)=MI(62)*GAMMA(62)                                         D 4320
      DO 440 I=1,N                                                      D 4330
      MI(L3M(I))=MI(L3M(I))*ALFA(62)                                    D 4340
      ALFA(L3M(I))=MI(L3M(I))*GAMMA(L3M(I))                             D 4350
      S3=S3+MI(L3M(I))                                                  D 4360
  440 CONTINUE                                                          D 4370
      S3=S3+MI(62)+MI(56)+2.0*MI(57)+3.0*MI(58)                         D 4380
  450 CONTINUE                                                          D 4390
C     MASS BALANCE ON PHOSPHATE                                         D 4400
      IF (PTOT.LE.0.0) GO TO 490                                        D 4410
      N=NPAIR(4)                                                        D 4420
      C1=KT(16)*ALFA(64)                                                D 4430
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      C2=KT(17)*ALFA(64)*ALFA(64)                                        D 4440
      DO 460 I=1,N                                                       D 4450
      MI(L4M(I))=KT(L4K(I))*ALFA(L4C(I))/GAMMA(L4M(I))                   D 4460
      IF (L4A(I).EQ.47) MI(L4M(I))=MI(L4M(I))*C1                         D 4470
      IF (L4A(I).EQ.48) MI(L4M(I))=MI(L4M(I))*C2                         D 4480
  460 CONTINUE                                                           D 4490
      MI(13)=MI(13)/TENMPE                                               D 4500
      MI(48)=MI(48)*ALFA(64)                                             D 4510
      MI(99)=MI(99)/TENMPE                                               D 4520
      SUM=0.0                                                            D 4530
      DO 470 I=1,N                                                       D 4540
      SUM=SUM+MI(L4M(I))                                                 D 4550
  470 CONTINUE                                                           D 4560
      MI(45)=PTOT/(1.0+GAMMA(45)*SUM)                                    D 4570
      ALFA(45)=MI(45)*GAMMA(45)                                          D 4580
      DO 480 I=1,N                                                       D 4590
      MI(L4M(I))=MI(L4M(I))*ALFA(45)                                     D 4600
      ALFA(L4M(I))=MI(L4M(I))*GAMMA(L4M(I))                              D 4610
      S4=S4+MI(L4M(I))                                                   D 4620
  480 CONTINUE                                                           D 4630
      S4=S4+MI(45)                                                       D 4640
  490 CONTINUE                                                           D 4650
C     MASS BALANCE ON CHLORIDE                                           D 4660
      IF (CLTOT.LE.0.0) GO TO 530                                        D 4670
      N=NPAIR(5)                                                         D 4680
      DO 500 I=1,N                                                       D 4690
      MI(L5M(I))=KT(L5K(I))*ALFA(L5C(I))/GAMMA(L5M(I))                   D 4700
  500 CONTINUE                                                           D 4710
      MI(16)=MI(16)/TENMPE                                               D 4720
      MI(28)=MI(28)*ALFA(5)/TENMPE                                       D 4730
      MI(33)=MI(33)*ALFA(5)*ALFA(5)/TENMPE                               D 4740
      MI(104)=MI(104)*ALFA(5)                                            D 4750
      MI(105)=MI(105)*ALFA(5)*ALFA(5)                                    D 4760
      SUM=MI(28)+2.0*MI(33)+MI(104)+2.0*MI(105)                          D 4770
      DO 510 I=1,N                                                       D 4780
      SUM=SUM+MI(L5M(I))                                                 D 4790
  510 CONTINUE                                                           D 4800
      MI(5)=CLTOT/(1.0+GAMMA(5)*SUM)                                     D 4810
      ALFA(5)=MI(5)*GAMMA(5)                                             D 4820
      DO 520 I=1,N                                                       D 4830
      MI(L5M(I))=MI(L5M(I))*ALFA(5)                                      D 4840
      ALFA(L5M(I))=MI(L5M(I))*GAMMA(L5M(I))                              D 4850
      S5=S5+MI(L5M(I))                                                   D 4860
  520 CONTINUE                                                           D 4870
      S5=S5+MI(5)+MI(28)+2.0*MI(33)+MI(104)+2.0*MI(105)                  D 4880
  530 CONTINUE                                                           D 4890
      ALFA(85)=MI(85)*GAMMA(85)                                          D 4900
      ALFA(98)=MI(98)*GAMMA(98)                                          D 4910
      ALFA(27)=AH2O*KW*TENPH                                             D 4920
      MI(27)=ALFA(27)/GAMMA(27)                                          D 4930
      MI(64)=1E0/(TENPH*GAMMA(64))                                       D 4940
      TEST1=S1-ANALCO                                                    D 4950
      TEST2=S2-SO4TOT                                                    D 4960
      TEST3=S3-FTOT                                                      D 4970
      TEST4=S4-PTOT                                                      D 4980
      TEST5=S5-CLTOT                                                     D 4990
      RBIT=0                                                             D 5000
      IF (S1.EQ.0.0.OR.ANALCO.LE.0.0) GO TO 540                          D 5010
      IF (ABS(TEST1).GT.EROR1*ANALCO) RBIT=1                             D 5020
      GO TO 550                                                          D 5030
  540 ANALCO=0.0                                                         D 5040
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  550 CONTINUE                                                          D 5050
      IF (S2.EQ.0.0) GO TO 560                                          D 5060
      IF (ABS(TEST2).GT.EROR2*SO4TOT) RBIT=1                            D 5070
  560 CONTINUE                                                          D 5080
      IF (S3.EQ.0.0) GO TO 570                                          D 5090
      IF (ABS(TEST3).GT.EROR3*FTOT) RBIT=1                              D 5100
  570 CONTINUE                                                          D 5110
      IF (S4.EQ.0.0) GO TO 580                                          D 5120
      IF (ABS(TEST4).GT.EROR4*PTOT) RBIT=1                              D 5130
  580 CONTINUE                                                          D 5140
      IF (S5.EQ.0.0) GO TO 590                                          D 5150
      IF (ABS(TEST5).GT.EROR5*CLTOT) RBIT=1                             D 5160
  590 CONTINUE                                                          D 5170
      IF (PRT(2).NE.0) GO TO 600                                        D 5180
      PRINT 610, ITER,TEST1,TEST2,TEST3,TEST4,TEST5                     D 5190
  600 CONTINUE                                                          D 5200
      RETURN                                                            D 5210
C                                                                       D 5220
  610 FORMAT (1H ,19X,I3,5X,5(1PE13.6,3X))                              D 5230
      END                                                               D 5240-
      SUBROUTINE PRINT                                                  E   10
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST4(104),LIST5(8),PRT(4)      E   20
      INTEGER PECALC,PECK                                               F   30
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT E   40
     1OT,MGTOT,LITOT,NH4TOT,KW,RATIO1(10),RATIO2(10),RATIO3(8),XLGAM(120 F   50
     2)                                                                 E   60
      REAL *8NSPEC(120),NREACT(200)                                     E   70
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P E   80
     1ESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA E   90
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120), E  100
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI( E  110
     4120),ITER,RBIT,CISAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT E  120
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT E  130
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC, E  140
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                         E  150
      DATA LIST4/1,2,3,4,64,5,6,7,18,86,27,62,98,19,23,22,21,20,29,32,30 F  160
     1,31,49,44,43,42,94,46,95,63,96,93,24,25,26,14,67,68,8,9,10,11,12,7 E  170
     27,78,79,80,13,100,65,99,15,16,28,33,34,101,102,106,107,111,109,110 F  180
     3,103,104,105,108,112,113,115,51,52,53,54,55,56,57,58,59,60,45,47,4 E  190
     4R,40,73,41,75,74,76,61,50,36,37,85,38,39,92,81,82,83,88,89,90,91/ F  200
      DATA LIST5/1,2,3,4,51,8,6,7/                                      E  210
      CEPMAN=0.0                                                        E  220
      CEPMCT=0.0                                                        E  230
      DO 20 I=1,D                                                       E  240
      IF (Z(I).GT.0) GO TO 10                                           E  250
      CEPMAN=CEPMAN-Z(I)*MI(I)                                          E  260
      GO TO 20                                                          E  270
   10 CEPMCT=CEPMCT+Z(I)*MI(I)                                          E  280
   20 CONTINUE                                                          E  290
      CEPMAN=CEPMAN*1000.                                               E  300
      CEPMCT=CEPMCT*1000.                                               E  310
      S1=MI(7)+MI(18)+MI(21)+MI(22)+MI(30)+MI(31)+MI(42)+MI(49)+MI(86)+M E  320
     1I(111)+MI(43)                                                     E  330
      PCO2=0.0                                                          E  340
      IF (ALFA(86).GT.0.0) GO TO 30                                     E  350
      GO TO 40                                                          E  360
   30 PCO2=10.**(ALOG10(ALFA(86))-2385.73/T-1.5264E-2*T+14.0184)        E  370
      XLPCO2=ALOG10(PCO2)                                               E  380
   40 CONTINUE                                                          E  390
      EHPE=PE*C*R*T/F                                                   E  400
      PRINT 110                                                         E  410
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      PRINT 110                                                          F  420
      PRINT 120, AH2O,EPMCAT,CEPMCT,PH,PCO2,EPMAN,CEPMAN,XLPCO2,ALFA(70) E  430
     1,EHP,PE,TEMP,ALFA(71),PES,S1,PEDO,DENS,PESATO,MU,TDS               E  440
      PRINT 130, PE,EHPE                                                 E  450
      PRINT 140                                                          E  460
      DUM=10.**(-70)                                                     F  470
      DO 50 I=1,D                                                        E  480
      CUNITS(I)=0.0                                                      E  490
      IF (MI(I).LT.DUM) GO TO 50                                         E  500
      CUNITS(I)=MI(I)*1000.*GFW(I)*(1.0-1.0E-06*CISAVE)                  E  510
      XLMI(I)=ALOG10(MI(I))                                              E  520
      XLALFA(I)=ALOG10(ALFA(I))                                          E  530
      XLGAM(I)=ALOG10(GAMMA(I))                                          E  540
   50 CONTINUE                                                           E  550
      DO 80 I=1,104                                                      E  560
      IF (MI(LIST4(I)).LT.DUM) GO TO 80                                  E  570
      IF (ISPEC.EQ.0) GO TO 70                                           E  580
      DO 60 J=1,ISPEC                                                    E  590
      IF (LIST4(I).EQ.KSPEC(J)) GO TO 70                                 F  600
   60 CONTINUE                                                           F  610
      GO TO 80                                                           E  620
   70 CONTINUE                                                           E  630
      PRINT 150, LIST4(I),NSPEC(LIST4(I)),Z(LIST4(I)),CUNITS(LIST4(I)),M E  640
     1I(LIST4(I)),XLMI(LIST4(I)),ALFA(LIST4(I)),XLALFA(LIST4(I)),GAMMA(L E  650
     2IST4(I)),XLGAM(LIST4(I))                                           E  660
   80 CONTINUE                                                           E  670
      IF (PRT(3).NE.0) GO TO 100                                         E  680
C                                                                        E  690
C                                                                        E  700
C     CALCULATION OF MOLAR RATIOS AND LOG ACTIVITY RATIOS.               E  710
      DO 90 I=1,8                                                        E  720
      IF (ANALMI(LIST5(I)).LT.1E-30) ANALMI(LIST5(I))=1E-30              F  730
      IF (MI(LIST5(I)).LT.1E-30) MI(LIST5(I))=1E-30                      E  740
      IF (MI(LIST5(I)).LT.1E-30) XLALFA(LIST5(I))=-30.                   E  750
      RATIO1(I)=ANALMI(5)/ANALMI(LIST5(I))                               E  760
      RATIO2(I)=MI(5)/MI(LIST5(I))                                       E  770
   90 CONTINUE                                                           E  780
      RATIO1(9)=ANALMI(1)/ANALMI(2)                                      F  790
      RATIO1(10)=ANALMI(3)/ANALMI(4)                                     F  800
      RATIO2(9)=MI(1)/MI(2)                                              E  810
      RATIO2(10)=MI(3)/MI(4)                                             F  820
      RATIO3(1)=XLALFA(1)+PH*2.                                          E  830
      RATIO3(2)=XLALFA(2)+PH*2.                                          F  840
      RATIO3(3)=XLALFA(3)+PH                                             E  850
      RATIO3(4)=XLALFA(4)+PH                                             E  860
      RATIO3(5)=XLALFA(51)+PH*3.                                         E  870
      RATIO3(6)=XLALFA(8)+PH*2.                                          E  880
      RATIO3(7)=XLALFA(1)-XLALFA(2)                                      E  890
      RATIO3(8)=XLALFA(3)-XLALFA(4)                                      F  900
      PRINT 110                                                          F  910
      PRINT 160, (RATIO1(I),RATIO2(I),RATIO3(I),I=1,8),(RATIO1(I),RATIO2 E  920
     1(I),I=9,10)                                                        E  930
  100 CONTINUE                                                           E  940
      RETURN                                                             E  950
C                                                                        E  960
C                                                                        E  970
  110 FORMAT (//)                                                        E  980
  120 FORMAT (//,46X,'****DESCRIPTION OF SOLUTION ****',//,27X,'ANALYTIC E  990
     1AL  COMPUTED',13X,'PH',16X,'ACTIVITY H2O = ',F7.4,/,20X,'EPMCAT ', F 1000
     2F9.3,3X,F9.3,10X,F6.3,14X,'PCO2 = ',1PE13.6,/,20X,'EPMAN  ',0PF9.3 E 1010
     3.3X,F9.3,30X,'LOG PCO2 = ',F8.4,/,56X,'TEMPERATURE',11X,'PO2 = ',1 E 1020
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     4PE13.6,/,20X,'EH = ',0PF6.4,2X,'PE = ',F7.3,11X,F6.2,' DEG C',10X, E 1030
     5'FCH4 = ',1PE13.6,/,20X,'PE CALC S = ',E13.6,33X,'CO2 TOT = ',E13. E 1040
     66,/,20X,'PE CALC DOX=',E13.6,10X,'IONIC STRENGTH',9X,'DENSITY = ', E 1050
     70PF8.4,/,20X,'PE SATO DOX=',1PE13.6,10X,E13.6,10X,'TDS = '0PF9.1,' E 1060
     8MG/L',/)                                                          E 1070
  130 FORMAT (11X,'IN COMPUTING THE DISTRIBUTION OF SPECIES, PE = ',F7.3 E 1080
     1,5X,'EQUIVALENT EH =',F7.3,'VOLTS',//)                            E 1090
  140 FORMAT (///,52X,'----------------------',/,52X,'DISTRIBUTION OF S F 1100
     1PECIES',/,52X,'----------------------',//,7X,'I',2X,'SPECIES',10X F 1110
     2,'PPM',11X,'MOLALITY',8X,'LOG MOL',6X,'ACTIVITY',8X,'LOG ACT',5X,' E 1120
     3ACT. COEFF.',5X,'LOG A COF',/)                                    E 1130
  150 FORMAT (1H ,5X,I3,1X,A8,I3,2X,1PE12.5,4X,E12.5,4X,0PF9.4,4X,1PE12. E 1140
     15,4X,0PF9.4,4X,1PE12.5,4X,0PF9.4)                                 E 1150
  160 FORMAT (//,18X,'MOLE RATIOS FROM ANALYTICAL MOLALITY   MOLE RATIOS F 1160
     1 FROM COMPUTED MOLALITY   LOG ACTIVITY RATIOS',/,18X,'------------ F 1170
     2----------------------   ------------------------------   -- E 1180
     3----------------',/,25X,'CL/CA    = ',1PE11.4,17X,'CL/CA    = ',E11 E 1190
     4.4,9X,'LOG CA/H2 = ',0PF9.4,/,25X,'CL/MG    = ',1PE11.4,17X,'CL/MG  E 1200
     5   = ',E11.4,9X,'LOG MG/H2 = ',0PF9.4,/,25X,'CL/NA    = ',1PE11.4,17 F 1210
     6X,'CL/NA    = ',E11.4,9X,'LOG NA/H1 = ',0PF9.4,/,25X,'CL/K     = ',1 F 1220
     7PE11.4,17X,'CL/K     = ',E11.4,9X,'LOG K/H1  = ',0PF9.4,/,25X,'CL/A F 1230
     8L    = ',1PE11.4,17X,'CL/AL    = ',E11.4,9X,'LOG AL/H3 = ',0PF9.4,/, E 1240
     925X,'CL/FE    = ',1PE11.4,17X,'CL/FE    = ',E11.4,9X,'LOG FE/H2 = ', E 1250
     $0PF9.4,/,25X,'CL/SO4   = ',1PE11.4,17X,'CL/SO4   = ',E11.4,9X,'LOG C F 1260
     $A/MG = ',0PF9.4,/,25X,'CL/HCO3 = ',1PE11.4,17X,'CL/HCO3 = ',E11.4, E 1270
     $9X,'LOG NA/K  = ',0PF9.4,/,25X,'CA/MG    = ',1PE11.4,17X,'CA/MG    = E 1280
     $ ',E11.4,/,25X,'NA/K     = ',E11.4,17X,'NA/K     = ',E11.4)       E 1290
      END                                                               E 1300-
      SUBROUTINE SAT                                                    F   10
      INTEGER D,E,DD,RBIT,CORALK,Z(120),LIST6(24),PRT(4)                F   20
      INTEGER PECALC,PECK                                               F   30
      DIMENSION LIST7(101), LIST8(15)                                   F   40
      REAL MI(120),KT(200),LOGKT(200),LOGKTO(200),MNTOT,LH2O,MU,NATOT,KT F   50
     1OT,MGTOT,LITOT,NH4TOT,KW                                          F   60
      REAL *8NSPEC(120),NREACT(200)                                     F   70
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,PE,PES,PEDC,P F   80
     1ESATO,PECK,PECALC,PH,TEMPE,TENPH,ALFA(120),GAMMA(120),AP(200),XLA F   90
     2LFA(120),Z,CUNITS(120),ANALMI(120),NSPEC,NREACT,GFW(120),DHA(120), F  100
     3DH(200),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XLMI( F  110
     4120),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(200),CO2TIT,ANALCO,SITOT,CAT F  120
     5OT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4TOT F  130
     6,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(20),EPMCAT,EPMAN,NEQU,ISPEC, F  140
     7KSPEC(120),IMIN,KMIN(200),TDS,IDAVES,IPRT                         F  150
      DATA LIST6/1,2,3,4,5,6,7,8,9,11,18,24,27,40,45,47,51,54,62,67,88,9 F  160
     10,101,102/                                                        F  170
      DATA LIST7/40,41,141,51,43,18,114,42,22,151,145,49,53,20,13,144,98 F  180
     1,50,21,30,57,100,29,12,56,113,120,97,63,28,52,111,112,119,19,65,48 F  190
     2,109,118,39,96,46,47,44,129,148,68,99,110,11,108,64,116,117,58,67, F  200
     359,61,150,55,45,142,115,54,102,37,10,101,147,143,38,66,62,32,60,10 F  210
     47,146,154,155,156,172,173,174,175,176,177,178,179,180,181,183,184, F  220
     5185,186,187,188,189,190,191,192,193/                              F  230
      DATA LIST8/107,108,109,110,111,112,113,114,115,119,120,173,174,175 F  240
     1,177/                                                             F  250
C                                                                       F  260
C                                                                       F  270
C     CALCULATION OF ION ACTIVITY PRODUCTS                              F  280
      DO 20 I=1,24                                                      F  290
      IF (ALFA(LIST6(I)).LT.1.E-40) GO TO 10                            F  300
      ALFA(LIST6(I))=ALOG10(ALFA(LIST6(I)))                             F  310
      GO TO 20                                                          F  320
   10 ALFA(LIST6(I))=-2E4                                               F  330
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20 CONTINUE                                                              F  340
   AP(10)=ALFA(8)+ALFA(18)                                               F  350
   AP(11)=ALFA(2)+ALFA(18)                                               F  360
   AP(12)=ALFA(1)+AP(11)+ALFA(18)                                        F  370
   AP(13)=ALFA(1)+ALFA(18)                                               F  380
   AP(18)=ALFA(1)+ALFA(6)                                                F  390
   AP(19)=AP(18)+2E0*LH20                                                F  400
   AP(20)=ALFA(2)+2E0*ALFA(27)                                           F  410
   AP(21)=3E0*ALFA(2)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH20                 F  420
   AP(22)=AP(13)                                                         F  430
   AP(28)=2E0*ALFA(2)+ALFA(24)+4E0*(ALFA(27)-LH20)                       F  440
   AP(29)=ALFA(1)+ALFA(2)+2E0*ALFA(24)+4E0*ALFA(27)-6E0*LH20             F  450
   AP(30)=ALFA(2)+ALFA(24)+2E0*ALFA(27)-3E0*LH20                         F  460
   AP(32)=2E0*ALFA(1)+5E0*ALFA(2)+8E0*ALFA(24)+14E0*ALFA(27)-22E0*LH2    F  470
  10                                                                     F  480
   AP(37)=2E0*ALFA(2)+3E0*ALFA(24)+4E0*ALFA(27)-4.5E0*LH20               F  490
   AP(38)=3E0*ALFA(2)+4E0*ALFA(24)+6E0*ALFA(27)-1E1*LH20                 F  500
   AP(39)=4E0*ALFA(2)+3E0*ALFA(18)+2E0*ALFA(27)+3E0*LH20                 F  510
   AP(40)=ALFA(4)+ALFA(54)+3E0*ALFA(24)-8E0*LH20                         F  520
   AP(41)=AP(40)-ALFA(4)+ALFA(3)                                         F  530
   AP(42)=ALFA(1)+2E0*(ALFA(54)+ALFA(24))-8E0*LH20                       F  540
   AP(43)=ALFA(3)+ALFA(54)+2E0*ALFA(24)-5E0*LH20                         F  550
   AP(44)=ALFA(4)+3E0*(ALFA(54)+ALFA(24))-2E0*PH-12E0*LH20               F  560
   AP(45)=ALFA(4)+ALFA(54)+3E0*(ALFA(2)+ALFA(24))+6E0*ALFA(27)-1E1*LH    F  570
  12C                                                                    F  580
   AP(46)=.6E0*ALFA(4)+.25E0*ALFA(2)+2.3E0*ALFA(54)+3.5E0*ALFA(24)-1.    F  590
  12E0*PH-11.2E0*LH2C                                                    F  600
   AP(47)=2E0*(ALFA(54)+ALFA(24)-PH)-7E0*LH2C                            F  610
   AP(48)=AP(47)                                                         F  620
   C1=(SQRT(MI(1)*GAMMA(1)+MI(2)*GAMMA(2)+MI(3)*GAMMA(3)))               F  630
   IF (C1.GT.0.0) C1=ALOG10(C1)                                          F  640
   IF (C1.LE.0.0) C1=-2E4                                                F  650
   AP(49)=.33E0*C1+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0*LH2C      F  660
   AP(50)=5E0*ALFA(2)+2E0*ALFA(54)+3E0*ALFA(24)+8E0*ALFA(27)-1E1*LH20    F  670
   AP(51)=ALFA(4)+3E0*ALFA(51)+6E0*ALFA(27)+2E0*ALFA(6)                  F  680
   AP(52)=ALFA(51)+3E0*ALFA(27)                                          F  690
   AP(53)=AP(52)-LH2C                                                    F  700
   AP(54)=2E0*ALFA(54)+4E0*ALFA(24)-2E0*PH-12.0*LH20                     F  710
   AP(55)=.5E0*(ALFA(3)+ALFA(4))+ALFA(54)+3E0*ALFA(24)-7E0*LH20          F  720
   AP(56)=ALFA(3)+ALFA(54)+3.5E0*ALFA(24)-6E0*LH20                       F  730
   C2=(MI(3)*GAMMA(3)+MI(4)*GAMMA(4))                                    F  740
   IF (C2.GT.0.0) C2=ALOG10(C2)                                          F  750
   IF (C2.LE.0.0) C1=-2E4                                                F  760
   AP(57)=.5E0*C2+ALFA(54)+5E0*ALFA(24)-8.5E0*LH20                       F  770
   AP(58)=.5E0*C2+ALFA(54)+4.5E0*ALFA(24)-8E0*LH20                       F  780
   AP(59)=ALFA(3)+ALFA(7)                                                F  790
   AP(60)=3E0*ALFA(3)+ALFA(7)+ALFA(18)+2E0*LH20                          F  800
   AP(62)=2E0*ALFA(3)+ALFA(18)+LH20                                      F  810
   AP(61)=AP(62)+9E0*LH20                                                F  820
   AP(63)=ALFA(1)+2E0*ALFA(62)                                           F  830
   AP(64)=.167E0*ALFA(1)+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0*    F  840
  1LH20                                                                  F  850
   AP(65)=ALFA(3)+ALFA(5)                                                F  860
   AP(66)=2E0*ALFA(3)+ALFA(6)                                            F  870
   AP(67)=AP(66)+1E1*LH20                                                F  880
   AP(68)=ALFA(8)+ALFA(67)+PH                                            F  890
   AP(96)=5E0*ALFA(1)+3E0*(ALFA(47)-LH20)+4E0*ALFA(27)                   F  900
   AP(97)=5E0*ALFA(1)+3E0*(ALFA(47)-LH20)+3E0*ALFA(27)+ALFA(62)          F  910
   AP(98)=ALFA(24)-2E0*LH2C                                              F  920
   AP(99)=ALFA(4)+7E0*ALFA(24)+PH-9E0*LH20                               F  930
   AP(100)=AP(98)                                                        F  940
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      AP(101)=AP(98)                                                    F  950
      AP(102)=AP(98)                                                    F  960
      IF (ABS(PE).LT.20.0) GO TO 30                                     F  970
      GO TO 40                                                          F  980
   30 CONTINUE                                                          F  990
      AP(107)=3E0*ALFA(8)+2E0*ALFA(45)+8E0*LH2O                         F 1000
      AP(108)=3E0*ALFA(9)-2E0*PE+4E0*LH2O+8E0*PH                        F 1010
      AP(109)=2E0*ALFA(9)+3E0*LH2O+6E0*PH                               F 1020
      AP(110)=AP(109)                                                   F 1030
      AP(111)=ALFA(9)+3E0*ALFA(27)-LH2O                                 F 1040
      AP(112)=3E0*ALFA(8)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH2O            F 1050
      AP(113)=ALFA(9)+3E0*(LH2O+PH)                                     F 1060
      AP(114)=AP(45)+3E0*(ALFA(8)-ALFA(2))                              F 1070
      AP(115)=ALFA(8)+2E0*(ALFA(67)+PE+PH)                              F 1080
      AP(119)=3E0*ALFA(8)+4E0*ALFA(67)+2E0*PE+4E0*PH                    F 1090
      AP(120)=AP(68)                                                    F 1100
      AP(173)=ALFA(102)+2*LH2O+4*PH+PE                                  F 1110
      AP(174)=AP(173)                                                   F 1120
      AP(175)=AP(173)                                                   F 1130
      AP(177)=3*ALFA(101)+4*LH2O+8*PH+2*PE                              F 1140
      GO TO 60                                                          F 1150
   40 CONTINUE                                                          F 1160
      DO 50 I=1,15                                                      F 1170
      JK=LIST8(I)                                                       F 1180
      AP(JK)=-6000.                                                     F 1190
   50 CONTINUE                                                          F 1200
      PECK=1                                                            F 1210
   60 CONTINUE                                                          F 1220
      AP(116)=.29*ALFA(2)+.23*ALFA(9)+1.58*ALFA(54)+3.93*ALFA(24)-10.*LH F 1230
     12O                                                                F 1240
      AP(117)=.45*ALFA(2)+.34*ALFA(9)+1.47*ALFA(54)+3.82*ALFA(24)-9.2*LH F 1250
     12O+.76*PH                                                         F 1260
      AP(118)=3E0*ALFA(2)+ALFA(1)+4E0*ALFA(18)                          F 1270
      AP(129)=ALFA(1)+2E0*ALFA(54)+4E0*ALFA(24)-8E0*LH2O                F 1280
      AP(141)=AP(52)                                                    F 1290
      AP(142)=2E0*(ALFA(1)+ALFA(54)+PH)+3E0*ALFA(24)-8E0*LH2O           F 1300
      AP(143)=ALFA(88)+ALFA(18)                                         F 1310
      AP(144)=ALFA(88)+ALFA(6)                                          F 1320
      AP(145)=ALFA(90)+ALFA(6)                                          F 1330
      AP(146)=ALFA(90)+ALFA(18)                                         F 1340
      AP(147)=ALFA(9)+ALFA(45)+2E0*LH2O                                 F 1350
      AP(148)=2E0*ALFA(1)+4E0*ALFA(54)+8E0*ALFA(24)-17E0*LH2O           F 1360
      AP(150)=ALFA(2)+ALFA(18)+3E0*LH2O                                 F 1370
      AP(151)=2E0*ALFA(1)+ALFA(18)+2E0*ALFA(27)+3E0*LH2O                F 1380
      AP(172)=ALFA(101)+LH2O+2*PH                                       F 1390
      AP(176)=2*ALFA(102)+3*LH2O+6*PH                                   F 1400
      AP(178)=ALFA(101)+2*ALFA(27)                                      F 1410
      AP(179)=ALFA(102)+3*ALFA(27)                                      F 1420
      AP(180)=ALFA(102)+2*LH2O+3*PH                                     F 1430
      AP(181)=ALFA(101)+ALFA(18)                                        F 1440
      AP(183)=ALFA(101)+2*ALFA(5)                                       F 1450
      AP(184)=AP(183)+LH2O                                              F 1460
      AP(185)=AP(183)+2*LH2O                                            F 1470
      AP(186)=AP(183)+4*LH2O                                            F 1480
      AP(187)=2*ALFA(101)+ALFA(24)+4*PH                                 F 1490
      AP(188)=2*ALFA(101)+ALFA(24)+2*PH-LH2O                            F 1500
      AP(189)=ALFA(101)+ALFA(67)+PH                                     F 1510
      AP(190)=ALFA(101)+ALFA(6)                                         F 1520
      AP(191)=2*ALFA(102)+3*ALFA(6)                                     F 1530
      AP(192)=3*ALFA(101)+2*ALFA(45)                                    F 1540
      AP(193)=ALFA(101)+ALFA(47)                                        F 1550
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      AP(154)=AP(37)                                                    F 1560
      AP(155)=AP(52)-LH2O                                               F 1570
      AP(156)=AP(129)-2*LH2O                                            F 1580
      PRINT 140                                                         F 1590
      PRINT 150                                                         F 1600
      DO 100 I=1,102                                                    F 1610
      IF (IMIN.EQ.0) GO TO 80                                           F 1620
      K=0                                                               F 1630
      DO 70 J=1,IMIN                                                    F 1640
      IF (LIST7(I).EQ.KMIN(J)) K=1                                      F 1650
   70 CONTINUE                                                          F 1660
      IF (K.EQ.1) GO TO 80                                              F 1670
      GO TO 100                                                         F 1680
   80 CONTINUE                                                          F 1690
      IF (AP(LIST7(I)).LT.-77.0.OR.AP(LIST7(I)).GT.75.0) GO TO 90       F 1700
      IF (LCHEK(LIST7(I)).EQ.1) GO TO 90                                F 1710
      DUM=AP(LIST7(I))-ALOG10(KT(LIST7(I)))                             F 1720
      IF (DUM.GT.75.) GO TO 90                                          F 1730
      XIAP=10.**AP(LIST7(I))                                            F 1740
      RAT=XIAP/KT(LIST7(I))                                             F 1750
      XLRAT=ALOG10(RAT)                                                 F 1760
      DELGR=C*R*T*XLRAT                                                 F 1770
      PRINT 160, LIST7(I),NREACT(LIST7(I)),XIAP,KT(LIST7(I)),AP(LIST7(I) F 1780
     1),LOGKT(LIST7(I)),RAT,XLRAT,DELGR                                 F 1790
      GO TO 100                                                         F 1800
   90 IF (AP(LIST7(I)).LT.-5000.0.OR.AP(LIST7(I)).GT.5000.0) GO TO 100  F 1810
      XLRAT=AP(LIST7(I))-LOGKT(LIST7(I))                                F 1820
      DELGR=C*R*T*XLRAT                                                 F 1830
      PRINT 170, LIST7(I),NREACT(LIST7(I)),AP(LIST7(I)),LOGKT(LIST7(I)), F 1840
     1XLRAT,DELGR                                                       F 1850
  100 CONTINUE                                                          F 1860
      IF (PECK.EQ.1.AND.PECALC.NE.0) GO TO 110                          F 1870
      GO TO 130                                                         F 1880
  110 PRINT 180                                                         F 1890
      DO 120 I=1,15                                                     F 1900
      PRINT 190, NREACT(LIST8(I))                                       F 1910
  120 CONTINUE                                                          F 1920
  130 CONTINUE                                                          F 1930
      RETURN                                                            F 1940
C                                                                       F 1950
  140 FORMAT (//)                                                       F 1960
  150 FORMAT (//,22X,'PHASE',9X,'IAP',10X,'KT',8X,'LOG IAP',4X,'LOG KT', F 1970
     16X,'IAP/KT',6X,'LOG IAP/KT',5X,'DELGR',/)                         F 1980
  160 FORMAT (1H ,17X,I3,1X,A8,2(2X,1PE11.4),2(2X,0PF9.4),2X,1PE11.4,2(2 F 1990
     1X,0PF10.5))                                                       F 2000
  170 FORMAT (1H ,17X,I3,1X,A8,28X,2(F9.4,2X),11X,2(2X,F10.5))          F 2010
  180 FORMAT (///,20X,'PE IS GREATER THAN 20 OR LESS THAN -20',/,20X,'AN F 2020
     1D THE FOLLOWING MINERAL REACTIONS HAVE BEEN DISREGARDED',/)       F 2030
  190 FORMAT (1H ,20X,A8)                                               F 2040
      END                                                               F 2050-
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NUMBER	MINERAL NAMES	MINERAL OR SPECIES ABR.	REACTION
1	-----	KFE +3	$Fe^{+2} = Fe^{+3} + e^{-}$
2	-----	KFEH+2	$Fe^{+2} + H_2O = FeOH^{+2} + e^{-} + H^{+}$
3	-----	KFEOH+	$Fe^{+2} + H_2O = FeOH^{+} + H^{+}$
4	-----	KFEOOH	$Fe^{+2} + 2H_2O = FeOOH^{-} + 3H^{+}$
5	-----	KFESO4	$Fe^{+2} + SO_4^{-2} = FeSO_4^{+} + e^{-}$
6	-----	KFECL	$Fe^{+2} + Cl^{-} = FeCl^{+2} + e^{-}$
7	-----	KFECL2	$Fe^{+2} + 2Cl^{-} = FeCl_2^{+} + e^{-}$
8	-----	KFECL3	$Fe^{+2} + 3Cl^{-} = FeCl_3^{\circ} + e^{-}$
9	-----	KFESO	$Fe^{+2} + SO_4^{-2} = FeSO_4^{\circ}$
10	siderite	SIDERITE	$FeCO_3 = Fe^{+2} + CO_3^{-2}$
11	magnesite	MAGNESIT	$MgCO_3 = Mg^{+2} + CO_3^{-2}$
12	dolomite	DOLOMITE	$CaMg(CO_3)_2 = Ca^{+2} + Mg^{+2} + 2CO_3^{-2}$
13	calcite	CALCITE	$CaCO_3 = Ca^{+2} + CO_3^{-2}$
14	-----	KH3SIO	$H_4SiO_4 = H_3SiO_4^{-} + H^{+}$
15	-----	KH2SIO	$H_4SiO_4 = H_2SiO_4^{-2} + 2H^{+}$
16	-----	KHPO4	$H^{+} + PO_4^{-3} = HPO_4^{-2}$
17	-----	KH2PO4	$2H^{+} + PO_4^{-3} = H_2PO_4^{-}$
18	anhydrite	ANHYDRIT	$CaSO_4 = Ca^{+2} + SO_4^{-2}$

19	gypsum	GYPSUM	$CaSO_4 \cdot 2H_2O = Ca^{+2} + SO_4^{-2} + 2H_2O$
20	brucite	BRUCITE	$Mg(OH)_2 = Mg^{+2} + 2OH^-$
21	chrysotile	CHRYSOTL	$Mg_3Si_2O_5(OH)_4 + 5H_2O = 3Mg^{+2} + 2H_4SiO_4 + 6OH^-$
22	aragonite	ARAGONIT	$CaCO_3 = Ca^{+2} + CO_3^{-2}$
23	-----	KMGF	$Mg^{+2} + F^- = MgF^+$
24	-----	KCASO4	$Ca^{+2} + SO_4^{-2} = CaSO_4^\circ$
25	-----	KMGOH	$Mg^{+2} + OH^- = MgOH^+$
26	-----	KH3BO3	$H_3BO_3 = H^+ + H_2BO_3^-$
27	-----	KNH3	$NH_4^+ = NH_3 + H^+$
28	forsterite	FORSTRIT	$Mg_2SiO_4 + 4H_2O = 2Mg^{+2} + 2H_4SiO_4 + 4OH^-$
29	diopside	DIOPSIDE	$CaMgSi_2O_6 + 6H_2O = Ca^{+2} + Mg^{+2} + 2H_4SiO_4 + 4OH^-$
30	clinoenstatite	CLENSTIT	$MgSiO_3 + 3H_2O = Mg^{2+} + H_4SiO_4 + 2OH^-$
31	-----	KNAHPO	$Na^+ + HPO_4^{-2} = NaHPO_4^-$
32	tremolite	TREMOLIT	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 22H_2O = 2Ca^{+2} + 5Mg^{+2} + 8H_4SiO_4 + 14OH^-$
33	-----	KKHPO	$K^+ + HPO_4^{-2} = KHPO_4^-$
34	-----	KMGHPO	$Mg^{+2} + HPO_4^{-2} = MgHPO_4^\circ$
35	-----	KCAHPO	$Ca^{+2} + HPO_4^{-2} = CaHPO_4^\circ$
36	-----	KH2CO3	$HCO_3^- + H^+ = H_2CO_3^*$
37	sepiolite	SEPIALIT	$Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O + 4.5H_2O = 2Mg^{+2} + 3H_4SiO_4 + 4(OH)^-$

38	talc	TALC	$Mg_3Si_4O_{10}(OH)_2 + 10H_2O = 3Mg^{+2} + 4H_4SiO_4 + 6OH^-$
39	hydromagnesite	HYDMAG	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O = 5Mg^{+2} + 4CO_3^{-2} + 2OH^- + 4H_2O$
40	adularia	ADULAR	$KAlSi_3O_8 + 8H_2O = K^+ + Al(OH)_4^- + 3H_4SiO_4$
41	albite	ALBITE	$NaAlSi_3O_8 + 8H_2O = Na^+ + Al(OH)_4^- + 3H_4SiO_4$
42	anorthite	ANORTH	$CaAl_2Si_2O_8 + 8H_2O = Ca^{+2} + 2Al(OH)_4^- + 2H_4SiO_4$
43	analcime	ANALCM	$NaAlSi_2O_6 \cdot H_2O + 5H_2O = Na^+ + Al(OH)_4^- + 2H_4SiO_4$
44	muscovite	KMICA	$KAl_3Si_3O_{10}(OH)_2 + 12H_2O = K^+ + 3Al(OH)_4^- + 3H_4SiO_4 + 2H^+$
45	phlogopite	PHLOG	$KMg_3AlSi_3O_{10}(OH)_2 + 10H_2O = K^+ + 3Mg^{+2} + Al(OH)_4^- + 3H_4SiO_4 + 6OH^-$
46	illite	ILLITE	$K_{.6}Mg_{.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 11.2H_2O = .6K^+ + .25Mg^{+2} + 2.3Al(OH)_4^- + 3.5H_4SiO_4 + 1.2H^+$
47	kaolinite	KAOLIN	$Al_2Si_2O_5(OH)_4 + 7H_2O = 2Al(OH)_4^- + 2H_4SiO_4 + 2H^+$
48	halloysite	HALLOY	$Al_2Si_2O_5(OH)_4 + 7H_2O = 2Al(OH)_4^- + 2H_4SiO_4 + 2H^+$
49	beidellite	BEIDEL	$(Na,K,\frac{1}{2}Mg)_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O = .33(Na,K,\frac{1}{2}Mg)^+ + 2.33Al(OH)_4^- + 3.67H_4SiO_4 + 2H^+$
50	chlorite	CHLOR	$Mg_5Al_2Si_3O_{10}(OH)_8 + 10H_2O = 5Mg^{+2} + 2Al(OH)_4^- + 3H_4SiO_4 + 8OH^-$
51	alunite	ALUNIT	$KAl_3(SO_4)_2(OH)_6 = K^+ + 3Al^{+3} + 2SO_4^{-2} + 6OH^-$
52	gibbsite	GIBCRS	$Al(OH)_3 = Al^{+3} + 3OH^-$
53	boehmite	BOEHM	$AlO(OH) + H_2O = Al^{+3} + 3OH^-$
54	pyrophyllite	PYROPH	$Al_2Si_4O_{10}(OH)_2 + 12H_2O = 2Al(OH)_4^- + 4H_4SiO_4 + 2H^+$
55	phillipsite	PHILIP	$Na_{.5}K_{.5}AlSi_3O_8 \cdot H_2O + 7H_2O = 0.5Na^+ + 0.5K^+ + Al(OH)_4^- + 3H_4SiO_4$
56	erionite	ERION	$NaAlSi_{3.5}O_9 \cdot 3H_2O + 6H_2O = Na^+ + Al(OH)_4^- + 3.5H_4SiO_4$

57	clinoptilolite	CLINOP	$(K,Na)AlSi_5O_{12}\cdot 3.5H_2O + 8.5H_2O = (K,Na)^+ + Al(OH)_4^- + 5H_4SiO_4$
58	mordenite	MORDEN	$(Na,K)AlSi_{4.5}O_{11}\cdot 3H_2O + 8H_2O = (Na,K)^+ + Al(OH)_4^- + 4.5H_4SiO_4$
59	nahcolite	NAHCOL	$NaHCO_3 = Na^+ + HCO_3^-$
60	trona	TRONA	$NaHCO_3\cdot Na_2CO_3\cdot 2H_2O = 3Na^+ + HCO_3^- + CO_3^{-2} + 2H_2O$
61	natron	NATRON	$Na_2CO_3\cdot 10H_2O = 2Na^+ + CO_3^{-2} + 10H_2O$
62	thermonatrite	THRNAT	$Na_2CO_3\cdot H_2O = 2Na^+ + CO_3^{-2} + H_2O$
63	fluorite	FLUOR	$CaF_2 = Ca^{+2} + 2F^-$
64	Ca-montmorillonite	MONTCA	$Ca_{.17}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O = .17Ca^{+2} + 2.33Al(OH)_4^- + 3.67H_4SiO_4 + 2H^+$
65	halite	HALITE	$NaCl = Na^+ + Cl^-$
66	thenardite	THENAR	$Na_2SO_4 = 2Na^+ + SO_4^{-2}$
67	mirabilite	MIRABI	$Na_2SO_4\cdot 10H_2O = 2Na^+ + SO_4^{-2} + 10H_2O$
68	mackinawite	MACKIT	$FeS + H^+ = Fe^{+2} + HS^-$
69	-----	KHCO3	$CO_3^{-2} + H^+ \rightleftharpoons HCO_3^-$
70	-----	KNACO3	$Na^+ + CO_3^{-2} = NaCO_3^-$
71	-----	KNAHCO3	$Na^+ + HCO_3^- = NaHCO_3^\circ$
72	-----	KNASO4	$Na^+ + SO_4^{-2} = NaSO_4^-$
73	-----	KKSO4	$K^+ + SO_4^{-2} = KSO_4^-$
74	-----	KMGCO3	$Mg^{+2} + CO_3^{-2} = MgCO_3^\circ$
75	-----	KMGHCO3	$Mg^{+2} + HCO_3^- = MgHCO_3^+$

76	-----	KMGSO4	$Mg^{+2} + SO_4^{-2} = MgSO_4^{\circ}$
77	-----	KCAOH	$Ca^{+2} + OH^{-} = CaOH^{+}$
78	-----	KCAHCO3	$Ca^{+2} + HCO_3^{-} = CaHCO_3^{+}$
79	-----	KCACO3	$Ca^{+2} + CO_3^{-2} = CaCO_3^{\circ}$
80	-----	KCAF+	$Ca^{+2} + F^{-} = CaF^{+}$
81	-----	KALOH	$Al^{+3} + OH^{-} = AlOH^{+2}$
82	-----	KALOH2	$Al^{+3} + 2OH^{-} = Al(OH)_2^{+}$
83	-----	KALOH4	$Al^{+3} + 4OH^{-} = Al(OH)_4^{-}$
84	-----	KALF	$Al^{+3} + F^{-} = AlF^{+2}$
85	-----	KALF2	$Al^{+3} + 2F^{-} = AlF_2^{+}$
86	-----	KALF3	$Al^{+3} + 3F^{-} = AlF_3^{\circ}$
87	-----	KALF4	$Al^{+3} + 4F^{-} = AlF_4^{-}$
88	-----	KALSO4	$Al^{+3} + SO_4^{-2} = AlSO_4^{+}$
89	-----	KASO42	$Al^{+3} + 2SO_4^{-2} = Al(SO_4)_2^{-}$
90	-----	KHSO4	$H^{+} + SO_4^{-2} = HSO_4^{-}$
91	-----	KH2SC	$SO_4^{-2} + 10H^{+} + 8e^{-} = H_2S + 4H_2O$
92	-----	KH2S	$H_2S = H^{+} + HS^{-}$
93	-----	KHS	$HS^{-} \rightleftharpoons H^{+} + S^{-2}$
94	-----	KOXY	$.5H_2O = .25O_2 + H^{+} + e^{-}$

95	-----	KCH4	$HCO_3^- + 8e^- + 9H^+ = CH_4 + 3H_2O$
96	hydroxyapatite	HYXAPT	$Ca_5(PO_4)_3(OH) + 3H_2O = 5Ca^{+2} + 3HPO_4^{-2} + 4OH^-$
97	fluorapatite	FLUAPT	$Ca_5(PO_4)_3F + 3H_2O = 5Ca^{+2} + 3HPO_4^{-2} + 3OH^- + F^-$
98	chalcedony	CHALC	$SiO_2 + 2H_2O = H_4SiO_4$
99	magadiite	MAGADI	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O = Na^+ + 7H_4SiO_4$
100	cristobalite	CRISTO	$SiO_2 + 2H_2O = H_4SiO_4$
101	silica gel	SILGEL	$SiO_2 + 2H_2O = H_4SiO_4$
102	quartz	QUARTZ	$SiO_2 + 2H_2O = H_4SiO_4$
103	-----	KFEOH2	$Fe^{+2} + 2H_2O = Fe(OH)_2^+ + 2H^+ + e^-$
104	-----	KFEOH3	$Fe^{+2} + 3H_2O = Fe(OH)_3^o + 3H^+ + e^-$
105	-----	KFEOH4	$Fe^{+2} + 4H_2O = Fe(OH)_4^- + 4H^+ + e^-$
106	-----	KFEOH2	$Fe^{+2} + 2H_2O = Fe(OH)_2^o + 2H^+$
107	vivianite	VIVIAN	$Fe_3(PO_4)_2 \cdot 8H_2O = 3Fe^{+2} + 2PO_4^{-3} + 8H_2O$
108	magnetite	MAGNET	$Fe_3O_4 + 8H^+ = 3Fe^{+3} + 4H_2O + e^-$
109	hematite	HEMATI	$Fe_2O_3 + 6H^+ = 2Fe^{+3} + 3H_2O$
110	maghemite	MAGHEM	$Fe_2O_3 + 6H^+ = 2Fe^{+3} + 3H_2O$
111	goethite	GOETH	$FeO(OH) + H_2O = Fe^{+3} + 3OH^-$
112	greenalite	GREENA	$Fe_3Si_2O_5(OH)_4 + 5H_2O = 3Fe^{+2} + 2H_2SiO_4 + 6OH^-$
113	amorphous $Fe(OH)_3$	FEOH3A	$Fe(OH)_3 + 3H^+ = Fe^{+3} + 3H_2O$

114	annite	ANNITE	$KFE_3AlSi_3O_{10}(OH)_2 + 10H_2O = K^+ + 3Fe^{+2} + Al(OH)_4^- + 3H_4SiO_4 + 6OH^-$
115	pyrite	PYRITE	$FeS_2 + 2H^+ + 2e^- = Fe^{+2} + 2HS^-$
116	montmorillonite	MONTBF	$(H,Na,K)_{0.28}Mg_{0.29}Fe^{3+}_{0.23}Al_{1.58}Si_{3.93}O_{10}(OH)_2 + 10.04H_2O =$ $0.28(H,Na,K)^+ + 0.29Mg^{+2} + 0.23Fe^{+3} + 1.58\ Al(OH)_4^-$ $+3.93\ H_4SiO_4$
117	montmorillonite	MONTAB	$(H,Na,K)_{0.42}Mg_{0.45}Fe^{+3}_{0.34}Al_{1.47}Si_{3.82}O_{10}(OH)_2 + 9.16H_2O + 0.84H^+$ $=0.42(H,Na,K)^+ + 0.45Mg^{+2} + 0.34Fe^{+3} + 1.47Al(OH)_4^- + 3.82\ H_4SiO_4$
118	huntite	HUNTITE	$CaMg_3(CO_3)_4 = 3Mg^{+2} + Ca^{+2} + 4CO_3^{-2}$
119	greigite	GREGITE	$Fe_3S_4 + 4H^+ + 2e^- = 3Fe^{+2} + 4HS^-$
120	amorphous FeS	FESPPT	$FeS + H^+ = Fe^{+2} + HS^-$
121	--------	KFEH2P	$Fe^{+2} + H_2PO_4^- = FeH_2PO_4^+$
122	--------	KCAPO4	$Ca^{+2} + PO_4^{-3} = CaPO_4^-$
123	--------	KCAH2P	$Ca^{+2} + H_2PO_4^- = CaH_2PO_4^+$
124	--------	KMGPO4	$Mg^{+2} + PO_4^{-3} = MgPO_4^-$
125	---------	KMGH2P	$Mg^{+2} + H_2PO_4^- = MgH_2PO_4^+$
126	---------	KLIOH	$Li^+ + OH^- = LiOH^o$
127	---------	KLISO4	$Li^+ + SO_4^{-2} = LiSO_4^-$
128	---------	KNH4R	$NO_3^- + 10H^+ + 8e^- = NH_4^+ + 3H_2O$
129	Laumontite	LAUMON	$CaAl_2Si_4O_{12}\cdot 4H_2O + 8H_2O = Ca^{+2} + 2Al(OH)_4^- + 4H_4SiO_4$
130	---------	KSROH	$Sr^{+2} + OH^- = SrOH^+$
131	---------	KBAOH	$Ba^{+2} + OH^- = BaOH^+$
132	---------	KNH4SO	$NH_4^+ + SO_4^{-2} = NH_4SO_4^-$

133	-----	KHCL	$H^+ + Cl^- = HCl^\circ$
134	-----	KNACL	$Na^+ + Cl^- = NaCl^\circ$
135	-----	KKCL	$K^+ + Cl^- = KCl^\circ$
136	-----	KH2SO4	$2H^+ + SO_4^{-2} = H_2SO_4^o$
137	-----	KO2SATO	$0.5H_2O = 0.25O_{2(aq)} + H^+ + e^-$
138	-----	KCO2	$CO_{2(g)} + H_2O = H_2CO_3^*$
139	-----	KFEHPO	$Fe^{+2} + HPO_4^{-2} = FeHPO_4^o$
140	-----	KFEHP+	$Fe^{+2} + HPO_4^{-2} = FeHPO_4^+ + e^-$
141	amorphous $Al(OH)_3$	ALOH3A	$Al(OH)_3 = Al^{+3} + 3OH^-$
142	prehnite	PREHNT	$Ca_2Al_2Si_3O_{10}(OH)_2 + 8H_2O + 2H^+ = 2Ca^{+2} + 2Al(OH)_4^- + 3H_4SiO_4$
143	strontianite	STRONT	$SrCO_3 = Sr^{+2} + CO_3^{-2}$
144	celestite	CELEST	$SrSO_4 = Sr^{+2} + SO_4^{-2}$
145	barite	BARITE	$BaSO_4 = Ba^{+2} + SO_4^{-2}$
146	witherite	WITHERIT	$BaCO_3 = Ba^{+2} + CO_3^{-2}$
147	strengite	STRENGIT	$FePO_4 \cdot 2H_2O = Fe^{+3} + PO_4^{-3} + 2H_2O$
148	leonhardite	LEON	$Ca_2Al_4Si_8O_{24} \cdot 7H_2O + 17H_2O = 2Ca^{+2} + 4Al(OH)_4^- + 8H_4SiO_4$
149	-----	BLANK	
150	nesquehonite	NESQUE	$MgCO_3 \cdot 3H_2O = Mg^{+2} + CO_3^{-2} + 3H_2O$
151	artinite	ARTIN	$Mg_2(OH)_2CO_3 \cdot 3H_2O = 2Mg^{+2} + CO_3^{-2} + 2OH^- + 3H_2O$

152	-----	KO2AQ	$0.5H_2O = 0.25O_2(aq) + H^+ + e^-$
153	-----	KW	$H_2O = H^+ + OH^-$
154	sepiolite	SEP PT	$Mg_2Si_3O_{7.5}(OH).3H_2O + 4.5H_2O = 2Mg^{+2} + 3H_4SiO_4 + 4OH^-$
155	diaspore	DIASP	$AlOOH + H_2O = Al^{+3} + 3OH^-$
156	wairakite	WAIRKT	$CaAl_2Si_4O_{12}.2H_2O + 10H_2O = Ca^{+2} + 2Al(OH)_4^- + 4H_4SiO_4$
157	-----	KFEHP2	$Fe^{+2} + H_2PO_4^- = FeH_2PO_4^{+2} + e^-$
158	-----	KMN3+	$Mn^{+2} = Mn^{+3} + e^-$
159	-----	KMNCL+	$Mn^{+2} + Cl^- = MnCl^+$
160	-----	KMNCL2	$Mn^{+2} + 2Cl^- = MnCl_2^o$
161	-----	KMNCL3-	$Mn^{+2} + 3Cl^- = MnCl_3^-$
162	-----	KMNOH+	$Mn^{+2} + OH^- = MnOH^+$
163	-----	KMN(OH)3	$Mn^{+2} + 3OH^- = Mn(OH)_3^-$
164	-----	KMNF+	$Mn^{+2} + F^- + MnF^+$
165	-----	KMNSO4	$Mn^{+2} + SO_4^= = MnSO_4^o$
166	-----	KMNNO3,2	$Mn^{+2} + 2NO_3^- = Mn(NO_3)_2^o$
167	-----	KMNHCO3+	$Mn^{+2} + HCO_3^- = MnHCO_3^+$

168	-----	KMNO4-	$Mn^{+2} + 4H_2O = MnO_4^- + 8H^+ + 5e^-$
169	-----	KMNO4--	$Mn^{+2} + 4H_2O = MnO_4^{--} + 8H^+ + 4e^-$
170	-----	BLANK	
171	-----	KHMNO2--	$Mn^{+2} + 2H_2O = HMnO_2^- + 3H^+$
172	manganosite	MANGANO	$MnO + 2H^+ = Mn^{+2} + H_2O$
173	pyrolusite	PYROLUST	$MnO_2 + 4H^+ + e^- = Mn^{+3} + 2H_2O$
174	δ, birnessite	BIRNSITE	$MnO_2 + 4H^+ + e^- = Mn^{+3} + 2H_2O$
175	nsutite	NUSTITE	$MnO_2 + 4H^+ + e^- = Mn^{+3} = 2H_2O$
176	bixbyite	BIXBYITE	$Mn_2O_3 + 6H^+ = 2Mn^{+3} + 3H_2O$
177	hausmanite	HAUSMITE	$Mn_3O_4 + 8H^+ + 2e^- = 3Mn^{+2} + 4H_2O$
178	pyrochrosite	MNOH2	$Mn(OH)_2 = Mn^{+2} + 2OH^-$
179	$Mn(OH)_3$	MNOH3	$Mn(OH)_3 = Mn^{+3} + 3OH^-$
180	manganite	MANGANIT	$MnOOH + 3H^+ = Mn^{+3} = 2H_2O$
181	rhodochrosite	RHODOCHR	$MnCO_3 = Mn^{+2} + CO_3^=$
182	--------	BLANK	

183	$MnCl_2$	MNCL2	$MnCl_2 = Mn^{+2} + 2Cl^-$
184	$MnCl_2.H_2O$	MNCL2,1W	$MnCl_2.H_2O = Mn^{+2} + 2Cl^- + H_2O$
185	$MnCl_2.2H_2O$	MNCL2,2W	$MnCl_2.2H_2O = Mn^{+2} + 2Cl^- + 2H_2O$
186	$MnCl_2.4H_2O$	MNCL2,4W	$MnCl_2 \cdot 4H_2O = Mn^{+2} + 2Cl^- + 4H_2O$
187	tephroite	TEPHRITE	$Mn_2SiO_4 + 4H^+ = 2Mn^{+2} + H_4SiO_4$
188	rhodonite	RHODONIT	$MnSiO_3 + 2H^+ + H_2O = Mn^{+2} + H_4SiO_4$
189	MnS(green)	MNS GRN	$MnS + H^+ = Mn^{+2} + HS^-$
190	$MnSO_4$	$MNSO_4$	$MnSO_4 = Mn^{+2} + SO_4^{-2}$
191	$Mn_2(SO_4)3$	MN2S04,3	$Mn_2(SO_4)_3 = 2Mn^{+3} + 3SO_4^{-2}$
192	$Mn_3(PO_4)_2$	MN3P04,2	$Mn_3(PO_4)_2 = 3Mn^{+2} + 2PO_4^{-3}$
193	$MnHPO_4$	MNHP04	$MnHPO_4 = Mn^{+2} + HPO_4^{-2}$

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