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MIX2: A COMPUTER PROGRAM FOR MODELING CHEMICAL REACTIONS IN NATURAL WATERS

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ABSTRACT

MIX2 is a FORTRAN IV computer program that utilizes an aqueous model and the constraints of mass balance and electrical balance to compute the pH and equilibrium distribution of inorganic species as a result of net reaction progress in the closed system: CaO-MgO-Na_2O-K_2O-CO_2-H_2SO_4-HCl-H_2O. The program considers three general classes of problems involving net reaction progress: 1) mixing of two solutions in fixed volume, 2) titration of one solution into another (variable volume), and 3) the addition or subtraction of a net stoichiometric reaction to or from an aqueous solution. In addition, MIX2 will follow one phase boundary through any of the above classes of problems.

This report presents the theory and method of calculation used by MIX2, describes the input to the program, presents results of two test cases, and provides a program listing.

INTRODUCTION

MIX2 is a FORTRAN IV computer program that utilizes an aqueous model and the constraints of mass balance and electrical balance to compute the pH and equilibrium distribution of inorganic species as a result of net reaction progress in the closed system: CaO-MgO-Na_2O-K_2O-CO_2-H_2SO_4-HCl-H_2O. The program considers three general classes of problems involving net reaction progress: 1) mixing of two solutions in fixed volume, 2) titration of one solution into another (variable volume), and 3) the addition or subtraction of a net stoichiometric reaction to or from an aqueous solution. In addition, MIX2 will follow one phase boundary through any of the above classes of probelms.

There are a number of problems in natural water systems, and in the laboratory, that can be modeled by MIX2. For example, MIX2 can model chemical reactions in problems such as sea water encroachment of a fresh water aquifer, Plummer (1975), the testing of proposed inorganic reaction paths in heterogeneous evolving systems, predicting the amount of accompanying mineralogic transfer in reacting heterogeneous systems, predicting the solubility of minerals in aqueous solutions, and testing proposed aqueous models by simulating laboratory experiments.

The purpose of this report is to briefly present the theory and method of calculation used by MIX2, describe the input to the program, present test cases suitable for comparison (Table 3), and make available a listing of MIX2 (Table 4).

METHODS

Aqueous Model

The aqueous model of MIX2 is similar to that of WATEQ (Truesdell and Jones, 1974), except that fewer species are used. The species considered and thermochemical data (which are valid from 0 to 50°C (Celsius) at one atmosphere total pressure) are shown in Table 1. Individual ion activity coefficients of changed species are computed from extended Debye-Hückel theory (Robinson and Stokes, 1955)

$$\log \gamma = \frac{-A z^2 \sqrt{I}}{1 + B a \sqrt{I}} + b I \qquad (1)$$

where z is the ion charge and I is ionic strength. In equation (1), the parameters a and b have been estimated for the major ions by Truesdell and Jones (1974) and are given in Table 2. The constants A and B of equation (1) are calculated from the density and dielectric constant of water as a function of temperature (Hamer, 1968; see also Truesdell and Jones, 1974). As shown by Truesdell and Jones (1974, p. 242), the computed activity coefficients for the major ions (Table 2) are near the mean salt values to ionic strengths of 4.0.

Activity coefficients of neutral species are estimated from the relation

$$\log \gamma^{o} = 0.1I, \qquad (2)$$

except for $\gamma_{H_2CO_3}$ which has been computed from the Henry's Law constants of Harned and Davis (1943) (for the solubility of CO_2 in NaCl solutions) by Wigley and Plummer (1975). The analytical expression for $\gamma_{H_2CO_3}$ is given as a footnote to Table 1.

The mass action and mass balance equations in the aqueous model of MIX2 are programmed in a manner similar to WATEQ (Truesdell and Jones, 1974). An advantage of this programming method (see Truesdell and Jones, 1974) is that important changes in the model can be accomplished quite simply. The only significant programming difference between the aqueous models of MIX2 and WATEQ is the method of convergence on mass balance for the anions used by MIX2 which is as much as 10 times faster than that of WATEQ. MIX2 solves both cation and anion mass balance in the manner described for cation mass balance by Truesdell and Jones (1974); a method similar to that of Wigley (1971).

Numerical Convergence

MIX2 performs three functions that require an iterative procedure:

1) Solving mass action and mass balance equations in the aqueous model given pH and total composition of the solution.

2) Finding the pH of a solution necessary for both mass and charge balance.

3) Finding the number of moles of a specified mineral to be dissolved or precipitated in order to bring the solution to equilibrium with the mineral and accompanying mass and charge balance.

Because of the number of iterative calculations made by MIX2, it is essential that the speed of these calculations be optimized.

Probably little can be done to speed convergence on mass action and mass balance in the aqueous model. For example, MIX2 solves the aqueous model for a simple carbonate solution to better than 1.0×10^{-15} moles per 1000g H_2O (molality difference between computed mass of carbon and actual carbon) in six iterations, and seawater is solved to the same precision in 14 iterations (see Table 3). These required iterations on the aqueous model compound rapidly, however, in solving for solution pH following chemical reaction (case 2) and particularly in finding phase boundaries (case 3).

In solving cases (2) and (3) above, MIX2 uses an optimized numerical convergence scheme of scanning functional relationships until roots are crossed, followed by linear and second order approximation. As shown in Table 3, this method of convergence is quite rapid, requiring roughly 4 to 7 iterations each for cases (2) and (3). The number of iterations on the aqueous model compound rapidly, however, when phase boundaries are solved, because each iteration on the phase boundary necessitates iteration on pH - charge balance which in turn requires iteration on mass action - mass balance in the aqueous model. Thus, for example, in finding the number of moles of a specified mineral to be dissolved or precipitated (to 3 significant figures) and defining the pH of that solution (to 3 decimal places) can require as many as 686 iterations (7x7x14) of the aqueous model for solutions similar to seawater (when convergence to better than 10^{-15} on mass balance is required). The test cases of Table 3 show that this estimate of number of iterations is an extreme value. Many cases can be solved to high precision in several hundred iterations of the aqueous model, and this estimate of required iterations can be reduced further when less accuracy of computed results is warranted. We discuss in more detail below the numerical convergence procedure in solving cases (2) and (3).

Case 2. There is one unique value of pH of a solution that, through convergence on mass balance in the aqueous model, will result in perfect charge balance. Perfect charge balance is defined by the equation

$$\Sigma\, m_i z_i = 0 \qquad (3)$$

where m_i is the molality of the ith ion and z_i is it's charge. Numerical convergence on charge balance is, of course, limited by the precision of the computer, and thus, only approaches zero. pH values less than the unique value causing perfect charge balance yield a positive charge imbalance and pH values greater than that unique value result in negative charge imbalance.

MIX2 uses the following procedure to find the value of pH resulting in perfect charge balance, within the prescribed limits of the calculation:

1) Scan pH as a function of charge balance (an approximately parabolic function for most natural waters) until the root is crossed, as indicated by a change in sign of electrical balance and converging on mass balance in the aqueous model with each new estimate of pH.

2) Obtain a first order estimate of the unique value of pH from a linear relation between the point (point (X,Y) = point (pH, electrical balance)) above the root and the point below the root, and return to the aqueous model for convergence on mass balance to find the new corresponding value of charge balance.

3) Obtain a second order estimate of the unique value of pH using a parabolic solution to the three values from step 2 (above), and return to the aqueous model for convergence on mass balance to find the corresponding charge balance. At this point, MIX2 has knowledge of four points on the pH - electrical balance curve. Because of the nature of the pH - electrical balance curve, the 4th point, obtained by the second order approximation, is closer to the root than any of the other 3 points, and is therefore retained. Two of the remaining 3 points lie on the same side of the root. The absolute values of the electrical balance of these two points are compared and the point farthest from the root is discarded.

4) Repeat step 3 (above) until the required precision is obtained.

Once the root is crossed, this procedure usually finds pH to 3 decimal places in 2-3 steps, which compares with 20 or more steps by interval halving techniques. It is important that the root be crossed in as few steps as possible; MIX2 scans initially at 0.2pH (in the direction of the root based on the sign of electrical balance), and if not crossed on the first step, the scanning increment is increased to 1.0pH unit.

Case 3.

Case 3, that of locating a phase boundary, is essentially identical (mathematically) to that of finding the unique value of pH (case 2), where pH is replaced by the term "XMOL", the number of moles of the appropriate mineral to be added to or removed from the solution to bring the solution to equilibrium with the mineral, and electrical balance is replaced by the corresponding saturation index

(SI) of the mineral. Saturation index is defined by

$$SI = \log \frac{IAP}{K} \qquad (4)$$

where IAP is the ion activity product of the mineral in solution and K is the thermodynamic equilibrium constant. Negative values of SI correspond to undersaturation and positive values indicate supersaturation. In finding a phase boundary, each new estimate of XMOL revises the total masses of appropriate species in solution which requires iteration on mass and charge balance (case 2) to define the new pH, distribution of species and resultant mineral saturation index corresponding to the estimate of XMOL.

General Calculation Procedure

Having described some of the details of the aqueous model and numerical convergence procedure of MIX2, we can discuss the overall calculation scheme of the program. All calculations of MIX2 are performed in double precision, necessary for the required convergence on an IBM 370/155. The initial data to MIX2 define the various options and required parameters for the job to follow. The total mass composition, pH, temperature and density of initial solution is read and the units of concentration are converted to molality, if not entered as molality. All equilibrium constants and other temperature dependent data are computed at the temperature of the input solution.

Because the constraint of charge balance will be utilized later in the program to determine solution pH, it is essential that the initial solution be balanced in charge through the aqueous model in accordance with the initial pH. Charge balance in the initial solution is accomplished by adding chloride or potassium (as determined by the initial charge imbalance) using the same numerical procedure described above for finding the pH of solutions.

So that any possible errors in later solutions, owing to differences in extent of convergence, will be negligible, the initial solutions are converged on mass balance and charge balance to $\leq \pm 10^{-15}$. Also with the choice of the appropriate input option (described in a later section of this report), the pH of an initial solution can be adjusted rather than total chloride or potassium content in determining initial charge balance.

If two solutions are to be mixed, or a solution is to be titrated into the initial solution, the second solution is entered and convergence on charge and mass balance, at the temperature of the second solution, is followed in an identical manner as with solution 1. If the temperatures of the two solutions differ, the temperature of of mixtures is estimated linearly from the end-member temperatures and all calculations are performed at the new temperature. Possible

temperature effects resulting from heats of reaction are not considered.

If a net reaction is to be added to the initial solution, the stoichiometric coefficients of each component in the net reaction, $\overline{X}$, are entered along with values of total moles of that net reaction to be added to the solution. The net stoichiometric reaction must be perfectly charge balanced, that is,

$$2\ (\overline{X}_{Ca^{++}} + \overline{X}_{Mg^{++}}) + \overline{X}_{Na^{+}} + \overline{X}_{K^{+}} = \overline{X}_{Cl^{-}} + 2\ (\overline{X}_{SO_4^{--}} + \overline{X}_{CO_3^{--}}) \qquad (8)$$

except for the cases of adding acids or bases to solution, such as in the oxidation of organic matter where $\overline{X}_{CO_3^{--}}$ is taken as $\overline{X}_{CO_2}$.

For example, suppose that along a presumed flow path in an aquifer, analytical data suggest that the net reaction is, relatively, 2.7 moles of calcite + 0.5 moles of dolomite + 0.1 moles of CH_2O (organic matter) per mole of gypsum. The stoichiometric coefficients for the net reaction could be written $\overline{X}_{Ca^{++}} = 4.2$, $\overline{X}_{Mg^{++}} = 0.5$, $\overline{X}_{CO_3^{--}}$ 3.8, and $\overline{X}_{SO_4^{--}} = 1.0$, with the remaining $\overline{X}$ values equal to zero. The total mass composition of the solution is computed at any point in reaction progress from the total concentrations in the initial solution, the stoichiometric coefficients of the net reaction, and the number of moles of the net reaction to be added to the solution, XMIX; i.e.,

$$C_{TOT}(\alpha) = C_{TOT}\ (\text{initial}) + \text{XMIX} \cdot \overline{X} \qquad (9)$$

where C_{TOT} is the total molality of the species in solution and α indicates the desired amount of reaction progress. If, based on the net stoichiometric reaction, the total molality of sulfate added to the initial solution at α is to be 3.0 mmoles, XMIX (equation 9) becomes 0.003. After the step in reaction progress is taken, MIX2 returns to the iterative convergence procedure of finding pH resulting in both charge and mass balance.

If the appropriate options are specified in the input data, MIX2 will follow any mineral phase boundary that can be defined in the chemical system of the aqueous model. The phase boundary is defined by entering the number of moles of each component in one mole of the mineral, PHAS (I), and the desired value of the equilibrium constant to be followed. For example, if it is desired to maintain the ion activity product of dolomite at $10^{-16.85}$, one would enter PHAS (Ca^{++}) = 1.0, PHAS (Mg^{++}) = 1.0, PHAS (CO_3^{--}) = 2.0 and a log value of the "equilibrium" constant, KPHAS, of -16.85. All other

values of PHAS(I) would be zero. MIX2 is capable of following one phase boundary during, mixing, titrating, or dissolution - precipitation reaction steps.

INPUT

The number of data cards required by MIX2 is variable and depends on the nature of the problem being solved. We have listed below the data requirements for all possible situations considered by MIX2 in the sequence in which the cards would be input. The actual input cards required for a particular problem should be evident from the description of the input variables.

Card	Variables	Format
1	IOPT1, IOPT2, IOPT3, IOPT4, IOPT5, IOPT6, IOPT8, IOPT9, IOPT10, NMIX, VO, CLOSE, HCLOSE, STPSIZ	(9I1, I5 4D10.3)
2	COEF(I), (I = 1,7)	(7D10.3)
3	PHAS (I), (I = 1,7), KPHAS	(8D10.3)
4	XMIX (I), (I = 1, NMIX)	(8D10.3)
5	TITLE	(20A4)
6	TEMP, PH, DENS, FLAG, IHOLD, IOPT7, CUNITS(7)	(3D10.3, 1X, 3I1, 1X, D12.5)
7	CUNITS (I), (I = 1,6)	(6D12.5)
7 + n	n cards containing optional input pertaining to Solution 1 are read here	(A4, 1X, 5 (I3, D12.5))
8 + n	Blank card required to denote end of data input for Solution 1	
9 + n -- 12 + n + m	Repeat cards 5 through 8 + n for solution 2, if IOPT4 equals 0 or 1, where solution 2 contains m optional input cards. If IOPT4 = 2, omit cards 9 + n --12 + n + m	

Description of Input Variables

IOPT1 Equals 0 prints thermochemical data, equals 1 omits print of thermochemical data.

IOPT2 Equals 0 prints convergence iterations on electrical balance for initial solutions, equals 1 to omit print.

IOPT3 Equals 0 prints convergence iterations on pH, equals 1 to omit print.

IOPT4 Equals 0 if solution 1 is to be mixed with solution 2 in a fixed volume system. Equals 1 if solution 2 is to be titrated into solution 1, (VO must be specified), equals 2 if any net stoichiometric reaction is to be added to or removed from solution.

IOPT5 Equals 0 prints summary of titration pH curve (if IOPT4 equals 1). Equals 1 omits summary of pH titration curve.

IOPT6 Equals 0, roots are found by scanning, linear, and parabolic approximation. Equals 1, roots are found by scanning and interval halving. Note that IOPT6 equals 0 is significantly faster than IOPT6 equals 1.

IOPT8 Equals 0 if no phase boundary is to be followed. Equals 1 if one phase boundary is to be followed.

IOPT9 Equals 0 if phase boundary is to be followed at all points in the reaction, (provided IOPT8 equals 1). Equals 1, phase boundary will be followed if solution supersaturates with specified phase (PHAS(I), KPHAS), provided IOPT8 equals 1. Thus, if IOPT9 equals 0, the specified mineral will either dissolve or precipitate in maintaining "equilibrium". If equal to 1, the mineral will precipitate only in maintaining SI=KPHAS.

IOPT10 Equals 0, causes printout of convergence iterations on the phase boundary search (if IOPT8 equals 1). Equals 1 omits print.

NMIX Total number of mixtures to be made if IOPT4 equals 0, or total number of titration additions (of defined solution 2 into solution 1), if IOPT4 equals 1, or total number of additions or removals of a net stoichiometric reaction, if IOPT4 equals 2.

VO Initial volume of solution 1 if IOPT4 equals 1, otherwise leave VO blank. If IOPT4 equals 1, VO must be greater than zero and have the same units as XMIX (I).

CLOSE — Absolute value of SI desired in following phase boundary. Reasonable value is 0.001. Leave blank if IOPT8 is not equal to 1.

HCLOSE — A factor that is multiplied times the absolute value of electrical balance to determine the closure on mass balance. 1.0D-08 is reasonable. If the electrical balance is 1.0D-04, convergence on mass balance would be to 1.0D-12 for HCLOSE of 1.0D-08. All initial solutions converge to 1.0D-15 regardless of the value of HCLOSE. Larger values of HCLOSE decrease the time for convergence on mass balance, and increase the error of the aqueous speciation.

STPSIZ — A factor that is multiplied times the total limiting concentration of species in the phase-boundary mineral in order to determine the step size in searching for the phase boundary. STPSIZ must be greater than 0.0 and less than 1.0. Values of 0.3 to 0.6 are reasonable. Large values of STPSIZ usually increase the speed of convergence on saturation.

COEF (I) — Stoichiometric coefficients of the net reaction being added to or removed from solution. Omit card if IOPT4 is not equal to 2. Order is Ca^{++}, Mg^{++}, Na^{++}, K^{+}, Cl^{-}, SO_4^{--}, CO_3^{--} .

PHAS (I) — Number of moles of each major species in one mole of the mineral for which the phase boundary is to be followed. Order is Ca^{++}, Mg^{++}, Na^{+}, K^{+}, Cl^{-}, SO_4^{--}, and CO_3^{--} .

KPHAS — The log of the equilibrium constant for the mineral PHAS (I) written in terms of mineral = ions, where ions are Ca^{++}, Mg^{++}, Na^{+}, K^{+}, Cl^{-}, SO_4^{--} , and CO_3^{--}.

XMIX (I) — Percent of solution 2 to be mixed with solution 1, if IOPT4 equals 0. If IOPT4 equals 1, XMIX is the volume of solution 2 (same units as VO) to be added to solution 1. If IOPT4 equals 2, XMIX is the total number of moles of the net reaction (COEF (I)) to be added to the solution for each desired point along the proposed reaction path. XMIX (I) is negative if the reaction is to be removed. NMIX values of XMIX (I) are read. If NMIX is zero, omit card 4.

TITLE — General description, identifying information, etc.

TEMP — Temperature in degrees C.

PH — Negative log activity H^+.

DENS — Density of Solution (g/cc).

FLAG — Signal for units of input concentration. 1 equals meq/1, 2 equals mg/1, 3 equals ppm, 4 equals molality.

IHOLD — Signal used to hold a previous end-member solution constant on successive mixing or titrating cases. IHOLD must be zero for the first 2 end-member solutions input. On additional mixing cases, IHOLD may be 0, 1, or 2. If IHOLD equals 0, 2 new end-member solutions are read in. If IHOLD equals 1, the previous defined solution 1 is saved and solution 2 is redefined by input. The opposite is true if IHOLD equals 2.

IOPT7 — Equals 0 if chloride or potassium are to be adjusted in the initial solution for charge balance. Equals 1 if the pH of the initial solution is to be adjusted for charge balance.

CUNITS (7) — Total concentration of carbon in solution.

CUNITS (I) (I=1,6) — Total concentrations of Ca^{++}, Mg^{++}, Na^+, K^+, Cl^-, and SO_4^{--} (in order) in initial solution.

Optional Input

Optional input cards can be used to (1) input the total concentrations of species not included on cards 6 and 7 ("CONC" card (s)); (2) change ΔH_r^o ("DELH" card (s)); (3) change log K at 25°C ("TABL" card (s)); or (4) input a value of log K that overrides all previous values of log K and will not be corrected for temperature ("LOGK" card (s)). n option cards fit in the data stream between card 7 and the blank card 8+n. There is no limit to the number of option cards used. However, the order in which option cards appear must be that as described above (1-4), that is, 1., "CONC", 2., "DELH", 3., "TABL", 4., "LOGK". It is possible to use none, 1, 2, 3, or all 4 types of option cards in a single data set provided the sequencing is that shown above. Information coded on option cards must follow a fixed format:

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

Where WORD is either "CONC", "DELH", "TABL", or "LOGK". INT (I) is the subscripting number in the program and VAL(I) is the appropriate new value. As many as 5 values may be input on each option card. Subscript numbers for reactions in the aqueous model are given in Table 1, and subscript numbers for ions appear in Table 2. If IOPT4 is not equal to 2 and thermodynamic data are overridden with optional input for solution 1, similar appropriate input should follow with solution 2.

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TABLE 1 Thermochemical Data[1]

Reaction	ΔH_r^{o} [2]	$\log K_{(25)}$ [3]
(6) $CaOH^+ = Ca^{++} + OH^-$	-1.19	-1.40
(9) $CaSO_4^o = Ca^{++} + SO_4^{--}$	-1.50	-2.309
(2) $MgOH^+ = Mg^{++} + OH^-$	-2.14	-2.60
(5) $MgSO_4^o = Mg^{++} + SO_4^{--}$	-1.27	-2.238
(12) $NaSO_4^- = Na^+ + SO_4^{--}$	-2.229	-0.226
(16) $Na_2SO_4^o = 2Na^+ + SO_4^{--}$	3.657	-1.512
(11) $NaHCO_3^o = Na^+ + HCO_3^-$	----- [4]	0.250
(10) $NaCO_3^- = Na^+ + CO_3^{--}$	-8.911	-1.268
(14) $Na_2CO_3^o = 2Na^+ + CO_3^{--}$	----- [4]	-0.672
(20) $NaCl^o = Na^+ + Cl^-$	----- [4]	1.602
(21) $KCl^o = K^+ + Cl^-$	----- [4]	1.585
(19) $HCl^o = H^+ + Cl^-$	-18.630	+6.10
(17) $H_2O = H^+ + OH^-$	-13.345	-13.998
(22) $H_2SO_4^o = 2H^+ + SO_4^{--}$	-----4	1.00
(26) $CaMg(CO_3)_2$ dolomite) $= Ca^{++} + Mg^{++} + 2CO_3^{--}$	-8.29	-17.00
(24) $CaCO_3$ (aragonite) $= Ca^{++} + CO_3^{--}$	-2.959	-8.215
(25) $MgCO_3$ (magnesite) $= Mg^{++} + CO_3^{--}$	-6.169	-8.24
(27) $CaSO_4$ (anhydrite) $= Ca^{++} + SO_4^{--}$	-3.769	-4.548

	Analytical Expression
(7) $CaHCO_3^+ = Ca^{++} + HCO_3^-$	$\log K(T)$ [5] = 2.95 - .0133T
(8) $CaCO_3^o = Ca^{++} + CO_3^{--}$	$\log K(T)$ [6] = 27.393 - 4114/T - .05617T
(4) $MgHCO_3^+ = Mg^{++} + HCO_3^-$	$\log K(T)$ [7] = $-2.319 + 1.1056\times10^{-2}T + 2.29812\times10^{-5}T^2$
(3) $MgCO_3^o = Mg^{++} + CO_3^{--}$	$\log K(T)$ [8] = -.991 - .00667T
(18) $H_2CO_3^o = H^+ + HCO_3^-$	$\log K(T)$ [9] = 14.8435 - 0.032786T - 3404.71/T
(1) $HCO_3^- = H^+ + CO_3^{--}$	$\log K(T)$ [10] = 6.498 - 0.02379T - 2902.39/T
(13) $KSO_4 = K^+ + SO_4^{--}$	$\log K(T) = -3.106 + 673.6/T$
(15) $HSO_4^- = H^+ + SO_4^{--}$	$\log K(T) = 5.3505 - 0.0183412T - 557.2461/T$
$CO_2 + H_2O = H_2CO_3^o$	$\log a_{H_2CO_3}$ [9,11] $= P_{CO_2} - 14.0184 + 0.015264T + 2385.73/T$
(23) $CaCO_3$ (calcite) $= Ca^{++} + CO_3^{--}$	$\log K(T)$ [5] = 13.870 - 0.04035T - 3059/T
(28) $CaSO_4$ (gypsum) $= Ca^{++} + SO_4^{--}$	$\log K(T)$ [12] = $-4.6535 + 4.545\times10^{-3}T - 1.01\times10^{-4}T^2$

(footnotes, see next page)

Footnotes to Table 1

1/ Thermochemical data used in the aqueous model, except where noted have been taken from the recent compilation of Truesdell and Jones (1974). Numbers in parentheses indicate appropriate reaction numbers required for optional input of thermochemical data.

2/ Standard enthalpy of reaction (Kcal/mole).

3/ Log of equilibrium constant, K, for the reaction at 25°C.

4/ No value of ΔH_r^o is available. The temperature dependence of log K has been ignored.

5/ Jacobson and Langmuir (1974).

6/ Reardon and Langmuir (1974).

7/ Least squares fit to the data of Siebert (1974).

8/ Siebert (1974).

9/ Harned and Davis (1943).

10/ Harned and Scholes (1941).

11/ Based on the assumption that γH_2CO_3 is unity in CO_2 saturated aqueous solutions. The temperature and ionic strength dependence of γH_2CO_3 in the presence of dissolved solids has been estimated from the solubility of CO_2 in NaCl solutions (Harned and Davis, 1943), and is $\log \gamma H_2CO_3^2 = \frac{I}{T}(a - bI)$ where I is ionic strength, T is temperature in °K, $a = 33.5 - 0.109\theta + 0.0014\theta^2$, and $b = 1.5 + 0.015\theta - 0.004\theta^2$ where θ is temperature in °C.

12/ Wigley (1973).

Table 2--parameters of the Debye-Hückel equation[1]

Major ions[2]	a	b
Ca^{++}(1)	5.0	0.165
Mg^{++}(1)	5.5	.20
Na^{+}(3)	4.0	.075
K^{+}(4)	3.5	.015
Cl^{-}(5)	3.5	.015
SO_4^{--}(6)	5.0	-.04
HCO_3^{-}(7)	5.4	0.0
CO_3^{--}(8)	5.4	0.0

Minor ions[3]	a
OH^{-}(24)	3.5
$MgHCO_3^{+}$(11)	4.0
HSO_4^{-}(22)	4.5
$NaCO_3^{-}$(17), $NaSO_4^{-}$(19), KSO_4^{-}(20)	5.4
$CaOH^{+}$(13), $CaHCO_3^{+}$(14)	6.0
$MgOH^{+}$(9)	6.5
H^{+}(23)	

1/ Numbers in parentheses are the subscript numbers for the ions in MIX2. Subscription for the neutral species is as follows: $MgCO_3^o$(10), $MgSO_4^o$(12), $CaCO_3^o$(15), $CaSO_4^o$(16), $NaHCO_3^o$(18), $Na_2CO_3^o$(21), $Na_2SO_4^o$(25), $H_2CO_3^o$(26), HCl^o(27), $NaCl^o$(28), KCl^o(29), $H_2SO_4^o$(30).

2/ a and b values calculated from experimental mean salt single - ion activity coefficients by Truesdell and Jones (1974).

3/ a values from Kielland (1937); b values set to zero.

TABLE 3

Two test cases are presented below that serve as examples of input data sets for MIX2, and provide output from MIX2 suitable for comparison.

Example 1

The first case is that of mixing sea water with a solution saturated with calcite at a P_{CO_2} of 10^{-2} atmospheres and $10^{\circ}C$. After each mixture is solved, the solubility of calcite in the solution is computed. The $CaHCO_3^+$ ion pair is ignored via the optional "LOGK" card. The input data set provides for 3 mixtures to be computed (10%, 30% and 50% sea water).

Example 2

The second case simulates a proposed closed system reaction path in the Floridian aquifer (based upon the field data of Back and Hanshaw, 1970). It is assumed that the chemical path of the ground water results from the net stoichiometric reaction

$$\text{starting water} + \text{XMIX}\ (Ca_{.873}Mg_{.059}SO_{4\ .093}CO_{3\ .907}) \rightarrow \text{groundwater}$$

$$+ \text{XMOL}\ (Ca_{.98}Mg_{.02}CO_3)$$

where "starting water" is the Polk City analysis of Back and Hanshaw (1970), and XMIX is the moles of the net stoichiometric reaction dissolved. A 2 mole percent magnesian calcite is precipitated at approximately 2-fold saturation (pK=8.2) where XMOL is the number of moles of calcite precipitated along the path. Two points along the proposed reaction path (XMIX = 10^{-3} and 10^{-2} moles) are presented.

List of data cards for example 1

```
      1       3            1.000D-03 1.000D-08 5.000D-01
 1.000D 00                                                    1.000D 00-8.359D 00
 1.000D 01 3.000D 01 5.000D 01
     SOLUTION NUMBER 1
 1.000D 01 7.335D 00 1.000D 00 400  4.86028D-03
 2.16600D-03
LOGK    7-3.00000D 01

   SEA WATER  SOLUTION NUMBER 2  DRYSSEN AND WEDBORG(1974) 35 PPT, CL=19.374PPT
 1.000D 01 8.150D 00 1.000D 00 400  2.36820D-03
 1.06600D-02 5.50800D-02 4.84630D-01 1.05800D-02 5.65720D-01 2.92600D-02
LOGK    7-3.00000D 01
```

List of data cards for example 2

```
000200110    2           1.000D-03 1.000D-08 5.000D-01
 0.273D 00 0.059D 00                                0.093D 00 0.907D 00
 0.980D 00 0.020D 00                                          1.000D 00-8.200D 00
 1.000D-03 1.000D-02
  SIMULATION OF CENTRAL FLORIDA GROUND WATER CHEMISTRY,  START = 1N.
 2.500D 01 8.000D 00 1.000D 00 400  1.27000D-04
 8.40000D-04 2.30000D-04 1.39000D-04 1.30000D-04 2.50000D-04 2.10000D-03
```

DATA

I	NREACT	DH	LOGKTO	LOGKT
1	KHCO3	3.5500	-10.3296	-10.4884
2	KMGOH	2.1400	2.6000	2.5169
3	KMGCO3	0.0580	3.3980	2.8797
4	KMGHCO3	10.3700	0.9280	1.0310
5	KMGSO4	1.2700	2.2380	2.1887
6	KCAOH	1.1900	1.4000	1.3538
7	KCAHCO3	6.3310	1.2600	-30.0000*
8	KCACO3	3.1300	3.2000	3.0410
9	KCASO4	1.5000	2.3090	2.2508
10	KNACO3	8.9110	1.2680	0.9220
11	KNAHCO3	0.0	-0.2500	-0.2500
12	KNASO4	2.2290	0.2260	0.1395
13	KKSO4	3.0820	0.8470	0.7271
14	KNA2CO3	0.0	0.6720	0.6720
15	KHSO4	4.9100	1.9870	1.8109
16	KNA2SO4	-3.6570	1.5120	1.6540
17	KW	13.3450	-13.9980	-14.5162
18	KH2CO3	1.9760	-6.3510	-6.4642
19	KHCL	18.6300	-6.1000	-6.8234
20	KNACL	0.0	-1.6020	-1.6020
21	KKCL	0.0	-1.5850	-1.5850
22	KH2SO4	0.0	-1.0000	-1.0000
23	CALCITE	-3.1900	-8.4100	-8.3586
24	ARAGONIT	-2.9590	-8.2150	-8.1001
25	MAGNESIT	-6.1690	-8.2400	-8.0005
26	DOLOMITE	-8.2900	-17.0000	-16.6781
27	ANHYDRIT	-3.7690	-4.5480	-4.4017
28	GYPSUM	0.2610	-4.7590	-4.7691
29	BRUCITE	0.8500	-11.4100	-11.4430
30	HUNTITE	-25.7600	-30.5100	-29.5098

I	NSPEC	Z	DHA	GFW
1	CA++	2.	5.0	40.0800
2	MG++	2.	5.5	24.3120
3	NA+	1.	4.0	22.9898
4	K+	1.	3.5	39.1020
5	CL-	-1.	3.5	35.4530
6	SO4--	-2.	5.0	96.0616
7	HCO3-	-1.	5.4	61.0173
8	CO3--	-2.	5.4	60.0094
9	MGOH+	1.	6.5	41.3194
10	MGCO3	0.	0.0	84.3214
11	MGHCO3+	1.	4.0	85.3293
12	MGSO4	0.	0.0	120.3736
13	CAOH+	1.	6.0	57.0874
14	CAHCO3+	1.	6.0	101.0973
15	CACO3	0.	0.0	100.0890
16	CASO4	0.	0.0	136.1416
17	NACO3-	-1.	5.4	82.9992
18	NAHCO3	0.	0.0	83.9909
19	NASO4-	-1.	5.4	119.0514
20	KSO4-	-1.	5.4	135.1636
21	NA2CO3	0.	0.0	105.9890
22	HSO4-	-1.	4.5	97.0696
23	H+	1.	9.0	1.0080
24	OH-	-1.	3.5	17.0074
25	NA2SO4	0.	0.0	142.0412
26	H2CO3	0.	0.0	62.0253
27	HCL	0.	0.0	36.4610
28	NACL	0.	0.0	58.4428
29	KCL	0.	0.0	74.5550
30	H2SO4	0.	0.0	98.0775

* DENOTES VALUES CHANGED IN INPUT

SOLUTION NUMBER 1

********** SOLUTION NUMBER 1 **********

TEMPERATURE = 10.00 DEGREES C PH = 7.335 ANALYTICAL EPMCAT = 4.3 ANALYTICAL EPMAN = 4.9

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.216600D-02	-2.6643	0.868133D-01
MGTOT	2.	0.0	0.0	0.0
NATOT	1.	0.0	0.0	0.0
KTOT	1.	0.0	0.0	0.0
CLTOT	-1.	0.0	0.0	0.0
SO4TOT	-2.	0.0	0.0	0.0
CO2TOT	-1.	0.486028D-02	-2.3133	0.296561D 00

--- CONVERGENCE ITERATIONS ---

ITERATION	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	ELECTRICAL BALANCE	N MODEL
1	-0.405058D-15	0.0	0.0	-0.1902923017002310D-05	6
2	-0.405058D-15	0.0	0.0	-0.2534392682736184D-08	6
3	-0.405058D-15	0.0	0.0	0.1897854459901889D-05	6
4	-0.405058D-15	0.0	0.0	-0.1521011901777524D-15	6

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	4.33	4.32	PH 7.335	ACTIVITY H2O = 0.9999
EPMAN	4.86	4.32		PCO2 = 0.100004D-01
IONIC STRENGTH = 0.648944D-02			TEMPERATURE	LOG PCO2 = -2.0000
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.485549D-02
CLTOT = 0.0				CO2TOT = 0.486028D-02
KTOT = 0.190546D-05				ELECT = -0.152101D-15
				ALKALINITY = 4.334 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.86588D 02	0.21612D-02	-2.6653	0.15621D-02	-2.8063	0.72279D 00	-0.1410
4	K+	1.	0.74479D-01	0.19055D-05	-5.7200	0.17511D-05	-5.7567	0.91897D 00	-0.0367
7	HCO3-	-1.	0.26328D 03	0.43166D-02	-2.3649	0.39806D-02	-2.4000	0.92217D 00	-0.0352
8	CO3--	-2.	0.23194D 00	0.38666D-05	-5.4127	0.27962D-05	-5.5534	0.72318D 00	-0.1408
13	CAOH+	1.	0.14367D-03	0.25176D-08	-8.5990	0.23242D-08	-8.6337	0.92319D 00	-0.0347
14	CAHCO3+	1.	0.68067D-30	0.67354D-35	-35.1716	0.62181D-35	-35.2063	0.92319D 00	-0.0347
15	CACO3	0.	0.47955D 00	0.47931D-05	-5.3194	0.48003D-05	-5.3187	0.10015D 01	0.0006
23	H+	1.	0.50210D-04	0.49830D-07	-7.3025	0.46238D-07	-7.3350	0.92791D 00	-0.0325
24	OH-	-1.	0.12191D-02	0.71709D-07	-7.1444	0.65845D-07	-7.1812	0.91876D 00	-0.0368
26	HPCO3	0.	0.33174D 02	0.53506D-03	-3.2716	0.53598D-03	-3.2709	0.10017D 01	0.0007

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.4368D-08	0.4379D-08	-8.3597	-8.3586	0.9974D 00	-0.00113
24	ARAGONIT	0.4368D-08	0.7941D-08	-8.3597	-8.1001	0.5500D 00	-0.25961
25	MAGNESIT	0.0	0.9989D-08	-100.0000	-8.0005	0.1000D-49	-100.00000
26	DOLOMITE	0.0	0.2098D-16	-100.0000	-16.6781	0.1000D-49	-100.00000
28	GYPSUM	0.0	0.1702D-04	-100.0000	-4.7691	0.1000D-49	-100.00000

SEA WATER SOLUTION NUMBER 2 DRYSSEN AND WEDBORG(1974) 35 PPT. CL=19.374PPT

********** SOLUTION NUMBER 2 **********

TEMPERATURE = 10.00 DEGREES C PH = 8.150 ANALYTICAL EPMCAT = 626.7 ANALYTICAL EPMAN = 626.6

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.106600D-01	-1.9722	0.427253D 00
MGTOT	2.	0.550800D-01	-1.2590	0.133910D 01
NATOT	1.	0.484630D 00	-0.3146	0.111415D 02
KTOT	1.	0.105800D-01	-1.9755	0.413699D 00
CLTOT	-1.	0.565720D 00	-0.2474	0.200565D 02
SO4TOT	-2.	0.292600D-01	-1.5337	0.281076D 01
CO2TOT	-1.	0.236820D-02	-2.6256	0.144501D 00

--- CONVERGENCE ITERATIONS ---

ITERATION	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	ELECTRICAL BALANCE	N MODEL
1	0.182009D-13	0.110955D-12	0.133782D-12	-0.165582401244894 3D-04	12
2	0.339897D-16	0.303577D-16	-0.693889D-16	-0.617191847954614 5D-11	15
3	0.180886D-13	0.111621D-12	0.126843D-12	0.165582270183933 6D-04	12
4	0.335561D-16	0.277556D-16	-0.138778D-16	0.273269372396488 3D-16	15

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	626.69	591.38	PH 8.150	ACTIVITY H2O = 0.9808
EPMAN	626.61	591.38		PCO2 = 0.457076D-03
IONIC STRENGTH = 0.663643D 00			TEMPERATURE	LOG PCO2 = -3.3400
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.179090D-02
CLTOT = 0.565720D 00				CO2TOT = 0.236820D-02
KTOT = 0.105966D-01				ELECT = 0.273269D-16
				ALKALINITY = 2.464 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.37659D 03	0.97501D-02	-2.0110	0.25158D-02	-2.5993	0.25802D 00	-0.5883
2	MG++	2.	0.11744D 04	0.50127D-01	-1.2999	0.14881D-01	-1.8274	0.29687D 00	-0.5274
3	NA+	1.	0.10211D 05	0.46090D 00	-0.3364	0.32843D 00	-0.4836	0.71258D 00	-0.1472
4	K+	1.	0.39281D 03	0.10425D-01	-1.9819	0.65692D-02	-2.1825	0.63017D 00	-0.2005
5	CL-	-1.	0.19241D 05	0.56317D 00	-0.2494	0.35489D 00	-0.4499	0.63017D 00	-0.2005
6	SO4--	-2.	0.11443D 04	0.12362D-01	-1.9079	0.23318D-02	-2.6323	0.18863D 00	-0.7244
7	HCO3-	-1.	0.10260D 03	0.17449D-02	-2.7582	0.11883D-02	-2.9251	0.68101D 00	-0.1668
8	CO3--	-2.	0.14658D 01	0.25347D-04	-4.5961	0.54519D-05	-5.2635	0.21509D 00	-0.6674
9	MGOH+	1.	0.11588D 00	0.29101D-05	-5.5361	0.20651D-05	-5.6850	0.70965D 00	-0.1490
10	MGCO3	0.	0.42890D 01	0.52782D-04	-4.2775	0.61497D-04	-4.2111	0.11651D 01	0.0664
11	MGHCO3+	1.	0.24576D 02	0.29888D-03	-3.5245	0.18991D-03	-3.7214	0.63542D 00	-0.1969
12	MGSO4	0.	0.53346D 03	0.45988D-02	-2.3374	0.53581D-02	-2.2710	0.11651D 01	0.0664
13	CAOH+	1.	0.18921D-02	0.34393D-07	-7.4635	0.23982D-07	-7.6201	0.69729D 00	-0.1566
14	CAHCO3+	1.	0.41768D-30	0.42873D-35	-35.3678	0.29894D-35	-35.5244	0.69729D 00	-0.1566
15	CACO3	0.	0.12478D 01	0.12937D-04	-4.8882	0.15073D-04	-4.8218	0.11651D 01	0.0664
16	CASO4	0.	0.11767D 03	0.89692D-03	-3.0472	0.10450D-02	-2.9809	0.11651D 01	0.0664
17	NACO3-	-1.	0.17572D 01	0.21970D-04	-4.6582	0.14962D-04	-4.8250	0.68101D 00	-0.1668
18	NAHCO3	0.	0.15246D 02	0.18836D-03	-3.7250	0.21946D-03	-3.6586	0.11651D 01	0.0664
19	NASO4-	-1.	0.17786D 03	0.15503D-02	-2.8096	0.10558D-02	-2.9764	0.68101D 00	-0.1668
20	KSO4-	-1.	0.15630D 02	0.12000D-03	-3.9208	0.81722D-04	-4.0877	0.68101D 00	-0.1668
21	NA2CO3	0.	0.24224D 00	0.23717D-05	-5.6249	0.27633D-05	-5.5586	0.11651D 01	0.0664
22	HSO4-	-1.	0.15299D-03	0.16355D-08	-8.7863	0.10682D-08	-8.9714	0.65310D 00	-0.1850
23	H+	1.	0.90608D-05	0.93278D-08	-8.0302	0.70795D-08	-8.1500	0.75897D 00	-0.1198
24	OH-	-1.	0.11233D-01	0.68535D-06	-6.1641	0.42210D-06	-6.3746	0.61589D 00	-0.2105
25	NA2SO4	0.	0.13321D 04	0.97321D-02	-2.0118	0.11339D-01	-1.9454	0.11651D 01	0.0664
26	H2CO3	0.	0.12354D 01	0.20668D-04	-4.6847	0.24497D-04	-4.6109	0.11853D 01	0.0738
27	HCL	0.	0.11379D-10	0.32385D-15	-15.4897	0.37732D-15	-15.4233	0.11651D 01	0.0664
28	NACL	0.	0.14087D 03	0.25013D-02	-2.6018	0.29143D-02	-2.5355	0.11651D 01	0.0664
29	KCL	0.	0.37381D 01	0.52029D-04	-4.2838	0.60619D-04	-4.2174	0.11651D 01	0.0664
30	H2SO4	0.	0.94804D-15	0.10031D-19	-19.9987	0.11687D-19	-19.9323	0.11651D 01	0.0664

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.1372D-07	0.4379D-08	-7.8628	-8.3586	0.3132D 01	0.49580
24	ARAGONIT	0.1372D-07	0.7941D-08	-7.8628	-8.1001	0.1727D 01	0.23732
25	MAGNESIT	0.8113D-07	0.9989D-08	-7.0908	-8.0005	0.8122D 01	0.90964
26	DOLOMITE	0.1113D-14	0.2098D-16	-14.9536	-16.6781	0.5303D 02	1.72450
28	GYPSUM	0.5866D-05	0.1702D-04	-5.2316	-4.7691	0.3447D 00	-0.46250

********** MIXTURE NUMBER 1 CONTAINING 90.00 PERCENT OF SOLUTION 1 AND 10.00 PERCENT OF SOLUTION 2 **********

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES	TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O

CATOT	2.	0.301540D-02	-2.5207	0.120857D 00
MGTOT	2.	0.550800D-02	-2.2590	0.133910D 00
NATOT	1.	0.484630D-01	-1.3146	0.111415D 01
KTOT	1.	0.106137D-02	-2.9741	0.415017D-01
CLTOT	-1.	0.565720D-01	-1.2474	0.200565D 01
SO4TOT	-2.	0.292600D-02	-2.5337	0.281076D 00
CO2TOT	-1.	0.461107D-02	-2.3913	0.247814D 00

--- CONVERGENCE ITERATIONS ---

NSTEP	IPH	PH	ELECTRICAL BALANCE	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	1	7.335000	-0.498345D-04	-0.326128D-14	-0.742212D-13	0.632879D-13	8
1	2	7.135000	0.171219D-03	0.410653D-12	-0.954410D-13	0.509913D-13	8
1	3	7.289912	-0.629836D-05	-0.642281D-14	-0.830304D-14	0.509705D-13	9
1	4	7.283620	0.486138D-07	-0.967108D-15	-0.565411D-16	-0.170870D-15	10

----DESCRIPTION OF SOLUTION ----

ANALYTICAL	COMPUTED	PH	
EPMCAT 66.57	65.11	7.284	ACTIVITY H2O = 0.9979
EPMAN 67.04	65.11		PCO2 = 0.904967D-02
IONIC STRENGTH = 0.752782D-01		TEMPERATURE	LOG PCO2 = -2.0434
DENSITY = 1.0000		10.00 DEG C	UNCOMPLEX CO2 = 0.443784D-02
CLTOT = 0.565720D-01			CO2TOT = 0.461107D-02
KTOT = 0.106137D-02			ELECT = 0.486138D-07
			ALKALINITY = 4.147 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.10863D 03	0.28125D-02	-2.5509	0.12116D-02	-2.9166	0.43080D 00	-0.3657
2	MG++	2.	0.11908D 03	0.50825D-02	-2.2939	0.22611D-02	-2.6457	0.44489D 00	-0.3517
3	NA+	1.	0.10670D 04	0.48164D-01	-1.3173	0.38600D-01	-1.4124	0.80330D 00	-0.0951
4	K+	1.	0.39763D 02	0.10552D-02	-2.9767	0.83229D-03	-3.0797	0.78872D 00	-0.1031
5	CL-	-1.	0.19313D 04	0.56529D-01	-1.2477	0.44586D-01	-1.3508	0.78872D 00	-0.1031
6	SO4--	-2.	0.21027D 03	0.22715D-02	-2.6437	0.94439D-03	-3.0248	0.41576D 00	-0.3812
7	HCO3-	-1.	0.23271D 03	0.39577D-02	-2.4026	0.32003D-02	-2.4948	0.80862D 00	-0.0923
8	CO3--	-2.	0.27014D 00	0.46714D-05	-5.3305	0.19972D-05	-5.6996	0.42754D 00	-0.3690
9	MGOH+	1.	0.21105D-02	0.53003D-07	-7.2757	0.43430D-07	-7.3622	0.81939D 00	-0.0865
10	MGCO3	0.	0.27338D 00	0.33644D-05	-5.4731	0.34232D-05	-5.4656	0.10175D 01	0.0075
11	MGHCO3+	1.	0.80596D 01	0.98014D-04	-4.0087	0.77718D-04	-4.1095	0.79292D 00	-0.1008
12	MGSO4	0.	0.37592D 02	0.32407D-03	-3.4894	0.32974D-03	-3.4818	0.10175D 01	0.0075
13	CAOH+	1.	0.10795D-03	0.19622D-08	-8.7073	0.15985D-08	-8.7963	0.81465D 00	-0.0890
14	CAHCO3+	1.	0.46371D-30	0.47597D-35	-35.3224	0.38774D-35	-35.4115	0.81465D 00	-0.0890
15	CACO3	0.	0.25209D 00	0.26137D-05	-5.5828	0.26593D-05	-5.5752	0.10175D 01	0.0075
16	CASO4	0.	0.26282D 02	0.20033D-03	-3.6983	0.20383D-03	-3.6907	0.10175D 01	0.0075
17	NACO3-	-1.	0.63867D-01	0.79851D-06	-6.0977	0.64569D-06	-6.1900	0.80862D 00	-0.0923

18	NAHCO3	0.	0.55388D 01	0.68432D-04	-4.1647	0.69628D-04	-4.1572	0.10175D 01	0.0075
19	NAS04-	-1.	0.71468D 01	0.62295D-04	-4.2055	0.50373D-04	-4.2978	0.80862D 00	-0.0923
20	KS04-	-1.	0.67546D 00	0.51858D-05	-5.2852	0.41933D-05	-5.3774	0.80862D 00	-0.0923
21	NA2CO3	0.	0.14102D-02	0.13807D-07	-7.8599	0.14048D-07	-7.8524	0.10175D 01	0.0075
22	HS04-	-1.	0.37243D-03	0.39814D-08	-8.4000	0.31804D-08	-8.4975	0.79881D 00	-0.0976
23	H+	1.	0.60194D-04	0.61968D-07	-7.2078	0.52045D-07	-7.2836	0.83987D 00	-0.0758
24	OH-	-1.	0.12171D-02	0.74260D-07	-7.1292	0.58419D-07	-7.2334	0.78668D 00	-0.1042
25	NA2S04	0.	0.85734D 01	0.62635D-04	-4.2032	0.63730D-04	-4.1957	0.10175D 01	0.0075
26	H2CO3	0.	0.28420D 02	0.47547D-03	-3.3229	0.48503D-03	-3.3142	0.10201D 01	0.0086
27	HCL	0.	0.12034D-10	0.34250D-15	-15.4653	0.34849D-15	-15.4578	0.10175D 01	0.0075
28	NACL	0.	0.23874D 01	0.42390D-04	-4.3727	0.43131D-04	-4.3652	0.10175D 01	0.0075
29	KCL	0.	0.68131D-01	0.94829D-06	-6.0231	0.96487D-06	-6.0155	0.10175D 01	0.0075
30	H2S04	0.	0.23762D-13	0.25141D-18	-18.5996	0.25581D-18	-18.5921	0.10175D 01	0.0075

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.2420D-08	0.4379D-08	-8.6162	-8.3586	0.5526D 00	-0.25762
24	ARAGONIT	0.2420D-08	0.7941D-08	-8.6162	-8.1001	0.3047D 00	-0.51610
25	MAGNESIT	0.4516D-08	0.9989D-08	-8.3452	-8.0005	0.4521D 00	-0.34478
26	DOLOMITE	0.1093D-16	0.2098D-16	-16.9615	-16.6781	0.5208D 00	-0.28334
28	GYPSUM	0.1144D-05	0.1702D-04	-5.9415	-4.7691	0.6724D-01	-1.17236

---CONVERGENCE ON PHASE BOUNDARY---				---CONVERGENCE ON MASS AND PH---						
ITER	MOLES	SI	PH	IPH	PH	ELECT	S1-C02TOT	S2-S04TOT	S3-CLTOT	N MODEL
1	0.151D-02	-0.257D 00	0.728D 01							
				1	7.284	0.166D-02	0.989D-12	0.611D-11	0.139D-10	7
				2	8.284	0.930D-03	0.262D-11	0.842D-11	0.424D-11	7
				3	9.284	-0.357D-03	0.780D-13	0.284D-13	-0.175D-11	9
				4	9.006	0.213D-03	0.956D-12	0.101D-11	0.502D-12	8
				5	9.141	-0.363D-04	-0.365D-13	-0.493D-13	0.271D-13	9
				6	9.125	-0.436D-05	-0.303D-14	-0.130D-13	0.238D-13	11
				7	9.122	0.841D-08	-0.379D-15	-0.296D-15	-0.222D-15	11
2	0.187D-03	0.181D 01	0.912D 01							
				1	9.122	-0.104D-02	0.284D-12	0.883D-11	0.206D-11	8
				2	8.122	-0.290D-03	0.901D-12	-0.115D-12	0.270D-11	8
				3	7.122	0.401D-03	0.463D-12	0.356D-11	0.258D-11	7
				4	7.703	-0.110D-03	0.604D-12	-0.107D-12	0.569D-13	8
				5	7.501	0.147D-04	-0.717D-14	-0.102D-12	0.556D-13	8
				6	7.522	-0.810D-06	-0.512D-16	-0.218D-15	-0.326D-14	10
				7	7.521	0.237D-08	-0.243D-16	-0.752D-16	-0.185D-15	10
3	0.161D-03	0.413D-01	0.752D 01							
				1	7.521	-0.280D-04	-0.712D-14	-0.100D-12	0.552D-13	8
				2	7.321	0.138D-03	0.489D-12	-0.104D-12	0.544D-13	8
				3	7.488	-0.385D-05	-0.812D-14	-0.925D-14	-0.321D-14	9
				4	7.482	0.213D-07	-0.226D-16	-0.733D-16	-0.189D-15	10
4	0.164D-03	-0.575D-02	0.748D 01							
				1	7.482	0.350D-05	-0.810D-14	-0.926D-14	-0.322D-14	9
				2	7.682	-0.123D-03	0.588D-12	-0.106D-12	0.563D-13	8
				3	7.488	-0.593D-06	-0.121D-14	-0.636D-16	-0.322D-14	10
				4	7.487	0.468D-09	-0.243D-16	-0.738D-16	-0.181D-15	10

THE PHASE BOUNDARY HAS BEEN FOUND
0.16411D-03 MOLES OF CA(1.000)MG(0.0)NA(0.0)K(0.0)CL(0.0)SO4(0.0)CO3(1.000) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.317951D-02	-2.5280	0.118834D 00
MGTOT	2.	0.550800D-02	-2.2945	0.123393D 00
NATOT	1.	0.484630D-01	-1.3173	0.110717D 01
KTOT	1.	0.106137D-02	-2.9766	0.412629D-01
CLTOT	-1.	0.565720D-01	-1.2477	0.200411D 01
SO4TOT	-2.	0.292600D-02	-2.6449	0.217585D 00
CO2TOT	-1.	0.477518D-02	-2.3709	0.259733D 00

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	66.57	65.40	PH 7.487	ACTIVITY H2O = 0.9979
EPMAN	67.04	65.40		PCO2 = 0.608901D-02
IONIC STRENGTH = 0.757137D-01			TEMPERATURE	LOG PCO2 = -2.2155
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.456464D-02
CLTOT = 0.565720D-01				CO2TOT = 0.477518D-02
KTOT = 0.106137D-02				ELECT = 0.468061D-09
				ALKALINITY = 4.475 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.114520 03	0.29649D-02	-2.5280	0.12753D-02	-2.8944	0.43012D 00	-0.3664
2	MG++	2.	0.11891D 03	0.50754D-02	-2.2945	0.22547D-02	-2.6469	0.44425D 00	-0.3524
3	NA+	1.	0.10669D 04	0.48159D-01	-1.3173	0.38670D-01	-1.4126	0.80296D 00	-0.0953
4	K+	1.	0.39764D 02	0.10553D-02	-2.9766	0.83188D-03	-3.0799	0.78832D 00	-0.1033
5	CL-	-1.	0.19313D 04	0.56529D-01	-1.2477	0.44563D-01	-1.3510	0.78832D 00	-0.1033
6	SO4--	-2.	0.20968D 03	0.22651D-02	-2.6449	0.94005D-03	-3.0269	0.41502D 00	-0.3819
7	HCO3-	-1.	0.25030D 03	0.42567D-02	-2.3709	0.34406D-02	-2.4634	0.80829D 00	-0.0924
8	CO3--	-2.	0.46484D 00	0.80383D-05	-5.0948	0.34310D-05	-5.4646	0.42684D 00	-0.3697
9	MGOH+	1.	0.33639D-02	0.84482D-07	-7.0732	0.69198D-07	-7.1599	0.81909D 00	-0.0867
10	MGCO3	0.	0.46827D 00	0.57627D-05	-5.2394	0.58641D-05	-5.2318	0.10176D 01	0.0076
11	MGHCO3+	1.	0.86447D 01	0.10513D-03	-3.9783	0.83319D-04	-4.0793	0.79253D 00	-0.1010
12	MGSO4	0.	0.37310D 02	0.32163D-03	-3.4926	0.32729D-03	-3.4851	0.10176D 01	0.0076
13	CAOH+	1.	0.18162D-03	0.33013D-08	-8.4813	0.26884D-08	-8.5705	0.81433D 00	-0.0892
14	CAHCO3+	1.	0.52494D-30	0.53882D-35	-35.2686	0.43878D-35	-35.3578	0.81433D 00	-0.0892
15	CACO3	0.	0.45578D 00	0.47254D-05	-5.3256	0.48085D-05	-5.3180	0.10176D 01	0.0076
16	CASO4	0.	0.27533D 02	0.20986D-03	-3.6781	0.21355D-03	-3.6705	0.10176D 01	0.0076
17	NACO3-	-1.	0.10971D 00	0.13716D-05	-5.8628	0.11086D-05	-5.9552	0.80829D 00	-0.0924
18	NAHCO3	0.	0.59512D 01	0.73526D-04	-4.1336	0.74819D-04	-4.1260	0.10176D 01	0.0076

19 NAS04-	-1.	0.711330 01	0.62002D-04	-4.2076	0.50116D-04	-4.3000	0.80829D 00	-0.0924
20 KS04-	-1.	0.672300 00	0.51615D-05	-5.2872	0.41720D-05	-5.3797	0.80829D 00	-0.0924
21 NA2C03	0.	0.24199D-02	0.23692D-07	-7.6254	0.24109D-07	-7.6178	0.10176D 01	0.0076
22 HS04-	-1.	0.23211D-03	0.24814D-08	-8.6053	0.19812D-08	-8.7031	0.79845D 00	-0.0978
23 H+	1.	0.37682D-04	0.38793D-07	-7.4113	0.32572D-07	-7.4872	0.83964D 00	-0.0759
24 OH-	-1.	0.19458D-02	0.11872D-06	-6.9255	0.93345D-07	-7.0299	0.78626D 00	-0.1044
25 NA2S04	0.	0.85244D 01	0.62276D-04	-4.2057	0.63371D-04	-4.1981	0.10176D 01	0.0076
26 H2C03	0.	0.19120D 02	0.31988D-03	-3.4950	0.32635D-03	-3.4863	0.10202D 01	0.0087
27 HCL	0.	0.75268D-11	0.21422D-15	-15.6691	0.21799D-15	-15.6616	0.10176D 01	0.0076
28 NACL	0.	0.23847D 01	0.42342D-04	-4.3732	0.43087D-04	-4.3657	0.10176D 01	0.0076
29 KCL	0.	0.68056D-01	0.94725D-06	-6.0235	0.96391D-06	-6.0160	0.10176D 01	0.0076
30 H2S04	0.	0.92630D-14	0.98007D-19	-19.0087	0.99731D-19	-19.0012	0.10176D 01	0.0076

PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23 CALCITE	0.4375D-08	0.4379D-08	-8.3590	-8.3586	0.9991D 00	-0.00039
24 ARAGONIT	0.4375D-08	0.7941D-08	-8.3590	-8.1001	0.5510D 00	-0.25887
25 MAGNESIT	0.7736D-08	0.9989D-08	-8.1115	-8.0005	0.7744D 00	-0.11101
26 DOLOMITE	0.3385D-16	0.2098D-16	-16.4705	-16.6781	0.1613D 01	0.20766
28 GYPSUM	0.1199D-05	0.1702D-04	-5.9212	-4.7691	0.7045D-01	-1.15211

********** MIXTURE NUMBER 2 CONTAINING 70.00 PERCENT OF SOLUTION 1 AND 30.00 PERCENT OF SOLUTION 2 **********

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.471420D-02	-2.3266	0.188945D 00
MGTOT	2.	0.165240D-01	-1.7819	0.401731D 00
NATOT	1.	0.145389D 00	-0.8375	0.334246D 01
KTOT	1.	0.318030D-02	-2.4975	0.124356D 00
CLTOT	-1.	0.169716D 00	-0.7703	0.601694D 01
S04TOT	-2.	0.877800D-02	-2.0566	0.843229D 00
C02TOT	-1.	0.411266D-02	-2.4256	0.228995D 00

--- CONVERGENCE ITERATIONS ---

NSTEP	IPH	PH	ELECTRICAL BALANCE	S1-C02TOT	S2-S04TOT	S3-CLTOT	N MODEL
2	1	7.487161	-0.129669D-03	-0.782941D-13	-0.893799D-12	-0.385109D-12	9
2	2	7.287161	0.6363170-05	-0.281025D-15	-0.115324D-13	-0.368872D-13	11
2	3	7.296516	-0.106552D-05	-0.170090D-14	-0.100987D-13	-0.152656D-15	10
2	4	7.295163	0.157004D-08	0.111022D-15	0.154390D-15	-0.138778D-16	12

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	191.05	184.88	PH	ACTIVITY H2O = 0.9941
EPMAN	191.38	184.88	7.295	PCO2 = 0.699595D-02
IONIC STRENGTH = 0.210037D 00			TEMPERATURE	LOG PCO2 = -2.1552
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.375955D-02
CLTOT = 0.169716D 00				CO2TOT = 0.411266D-02
KTOT = 0.318030D-02				ELECT = 0.157004D-08
				ALKALINITY = 3.774 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.166240 03	0.430400-02	-2.3661	0.139740-02	-2.8547	0.32469D 00	-0.4885
2	MG++	2.	0.351510 03	0.150030-01	-1.8238	0.520560-02	-2.2835	0.34696D 00	-0.4597
3	NA+	1.	0.316630 04	0.142920 00	-0.8449	0.106610 00	-0.9722	0.74596D 00	-0.1273
4	K+	1.	0.118550 03	0.314610-02	-2.5022	0.224320-02	-2.6491	0.71301D 00	-0.1469
5	CL-	-1.	0.578760 04	0.169400 00	-0.7711	0.120780 00	-0.9180	0.71301D 00	-0.1469
6	SO4--	-2.	0.541360 03	0.584800-02	-2.2330	0.171960-02	-2.7646	0.29404D 00	-0.5316
7	HCO3-	-1.	0.199890 03	0.339950-02	-2.4686	0.254060-02	-2.5951	0.74736D 00	-0.1265
8	CO3--	-2.	0.301820 00	0.521920-05	-5.2824	0.162830-05	-5.7883	0.31198D 00	-0.5059
9	MGOH+	1.	0.531850-02	0.133570-06	-6.8743	0.102280-06	-6.9902	0.76574D 00	-0.1159
10	MGCO3	0.	0.497440 00	0.612180-05	-5.2131	0.642510-05	-5.1921	0.10496D 01	0.0210
11	MGHCO3+	1.	0.162360 02	0.197450-03	-3.7045	0.142040-03	-3.8476	0.71939D 00	-0.1430
12	MGSO4	0.	0.152770 03	0.131700-02	-2.8804	0.138220-02	-2.8594	0.10496D 01	0.0210
13	CAOH+	1.	0.136930-03	0.248900-08	-8.6040	0.188600-08	-8.7245	0.75773D 00	-0.1205
14	CAHCO3+	1.	0.456490-30	0.468560-35	-35.3292	0.355040-35	-35.4497	0.75773D 00	-0.1205
15	CACO3	0.	0.229810 00	0.238260-05	-5.6230	0.250060-05	-5.6019	0.10496D 01	0.0210
16	CASO4	0.	0.535080 02	0.407850-03	-3.3895	0.428060-03	-3.3685	0.10496D 01	0.0210
17	NACO3-	-1.	0.155240 00	0.194090-05	-5.7120	0.145050-05	-5.8385	0.74736D 00	-0.1265
18	NAHCO3	0.	0.117460 02	0.145130-03	-3.8383	0.152320-03	-3.8173	0.10496D 01	0.0210
19	NASO4-	-1.	0.387970 02	0.338170-03	-3.4709	0.252740-03	-3.5973	0.74736D 00	-0.1265
20	KSO4-	-1.	0.358640 01	0.275340-04	-4.5601	0.205780-04	-4.6866	0.74736D 00	-0.1265
21	NA2CO3	0.	0.846290-02	0.828580-07	-7.0817	0.869630-07	-7.0607	0.10496D 01	0.0210
22	HSO4-	-1.	0.722530-03	0.772400-08	-8.1122	0.563900-08	-8.2488	0.73006D 00	-0.1366
23	H+	1.	0.616120-04	0.634280-07	-7.1977	0.506800-07	-7.2952	0.79902D 00	-0.0974
24	OH-	-1.	0.138370-02	0.844250-07	-7.0735	0.597610-07	-7.2236	0.70785D 00	-0.1501
25	NA2SO4	0.	0.114910 03	0.839490-03	-3.0760	0.881080-03	-3.0550	0.10496D 01	0.0210
26	H2CO3	0.	0.212100 02	0.354850-03	-3.4500	0.374950-03	-3.4260	0.10566D 01	0.0239
27	HCL	0.	0.307760-10	0.875920-15	-15.0575	0.919320-15	-15.0365	0.10496D 01	0.0210
28	NACL	0.	0.172770 02	0.306770-03	-3.5132	0.321970-03	-3.4922	0.10496D 01	0.0210
29	KCL	0.	0.482250 00	0.671220-05	-5.1731	0.704480-05	-5.1521	0.10496D 01	0.0210
30	H2SO4	0.	0.397720-13	0.420810-18	-18.3759	0.441660-18	-18.3549	0.10496D 01	0.0210

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.2275D-08	0.4379D-08	-8.6429	-8.3586	0.5196D 00	-0.28435
24	ARAGONIT	0.2275D-08	0.7941D-08	-8.6429	-8.1001	0.2865D 00	-0.54283
25	MAGNESIT	0.8476D-08	0.9989D-08	-8.0718	-8.0005	0.8485D 00	-0.07133
26	DOLOMITE	0.1929D-16	0.2098D-16	-16.7147	-16.6781	0.9191D 00	-0.03662
28	GYPSUM	0.2403D-05	0.1702D-04	-5.6192	-4.7691	0.1412D 00	-0.85012

---CONVERGENCE ON PHASE BOUNDARY---				---CONVERGENCE ON MASS AND PH---						
ITER	MOLES	SI	PH	IPH	PH	ELECT	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	0.206D-02	-0.284D 00	0.730D 01							
				1	7.295	0.222D-02	0.210D-10	-0.916D-11	0.708D-11	8
				2	8.295	0.151D-02	-0.276D-12	-0.883D-11	0.806D-11	8
				3	9.295	-0.175D-03	-0.148D-11	-0.171D-12	-0.356D-12	10
				4	9.191	0.124D-03	-0.116D-11	-0.826D-13	-0.455D-12	10
				5	9.238	-0.731D-05	0.222D-14	0.896D-14	-0.522D-14	11
				6	9.236	-0.326D-06	0.284D-14	0.151D-14	0.569D-15	12
2	0.271D-03	0.187D 01	0.924D 01							
				1	9.236	-0.125D-02	0.659D-12	-0.318D-11	-0.348D-12	8
				2	8.236	-0.178D-03	-0.229D-12	-0.101D-11	-0.408D-12	9
				3	7.236	0.346D-03	-0.658D-13	-0.937D-12	-0.397D-12	9
				4	7.896	-0.393D-04	-0.136D-12	-0.131D-13	-0.264D-15	10
				5	7.809	-0.444D-05	-0.224D-14	-0.116D-13	-0.394D-13	10
				6	7.798	0.144D-06	0.159D-15	0.173D-15	-0.694D-16	12
				7	7.799	-0.498D-09	0.158D-15	0.173D-15	-0.555D-16	12
3	0.108D-03	0.293D 00	0.780D 01							
				1	7.799	-0.166D-03	-0.110D-12	-0.926D-12	-0.390D-12	9
				2	7.599	-0.769D-04	-0.879D-13	-0.103D-13	-0.388D-12	10
				3	7.399	0.397D-04	-0.725D-13	-0.100D-13	-0.388D-12	10
				4	7.467	-0.417D-05	-0.225D-14	-0.143D-13	-0.378D-13	10
				5	7.460	0.228D-07	0.123D-15	0.160D-15	-0.139D-16	12
4	0.151D-03	-0.873D-01	0.746D 01							
				1	7.460	0.451D-04	-0.778D-13	-0.102D-13	-0.390D-12	10
				2	7.660	-0.624D-04	-0.958D-13	-0.106D-13	-0.391D-12	10
				3	7.544	-0.385D-05	-0.236D-14	-0.147D-13	-0.381D-13	10
				4	7.537	0.157D-07	0.130D-15	0.164D-15	-0.278D-16	12
5	0.150D-03	0.147D-02	0.754D 01							
				1	7.537	-0.706D-06	-0.182D-14	0.314D-14	-0.139D-16	11
				2	7.337	0.129D-03	-0.682D-13	-0.917D-12	-0.390D-12	9
				3	7.536	-0.106D-06	0.130D-15	0.162D-15	-0.139D-16	12

THE PHASE BOUNDARY HAS BEEN FOUND
0.14989D-03 MOLES OF CA(1.000)MG(0.0)NA(0.0)K(0.0)CL(0.0)SO4(0.0)CO3(1.000) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.486409D-02	-2.3526	0.177943D 00
MGTOT	2.	0.165240D-01	-1.8243	0.364386D 00
NATOT	1.	0.145389D 00	-0.8449	0.328546D 01
KTOT	1.	0.318030D-02	-2.5022	0.123019D 00
CLTOT	-1.	0.169716D 00	-0.7711	0.600583D 01
SO4TOT	-2.	0.877800D-02	-2.2334	0.561229D 00
CO2TOT	-1.	0.426255D-02	-2.4381	0.222534D 00

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	191.05	185.12	PH 7.535	ACTIVITY H2O = 0.9941
EPMAN	191.38	185.12		PCO2 = 0.431421D-02
IONIC STRENGTH = 0.210403D 00			TEMPERATURE	LOG PCO2 = -2.3651
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.387561D-02
CLTOT = 0.169716D 00				CO2TOT = 0.426255D-02
KTOT = 0.318030D-02				ELECT = -0.105624D-06
				ALKALINITY = 4.073 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.17148D 03	0.44397D-02	-2.3526	0.14409D-02	-2.8414	0.32454D 00	-0.4887
2	MG++	2.	0.35115D 03	0.14988D-01	-1.8243	0.51983D-02	-2.2841	0.34683D 00	-0.4599
3	NA+	1.	0.31661D 04	0.14291D 00	-0.8449	0.10659D 00	-0.9723	0.74587D 00	-0.1273
4	K+	1.	0.11855D 03	0.31461D-02	-2.5022	0.22428D-02	-2.6492	0.71287D 00	-0.1470
5	CL-	-1.	0.57876D 04	0.16940D 00	-0.7711	0.12076D 00	-0.9181	0.71287D 00	-0.1470
6	SO4--	-2.	0.54084D 03	0.58424D-02	-2.2334	0.17168D-02	-2.7653	0.29386D 00	-0.5319
7	HCO3-	-1.	0.21445D 03	0.36471D-02	-2.4381	0.27253D-02	-2.5646	0.74726D 00	-0.1265
8	CO3--	-2.	0.56348D 00	0.97439D-05	-5.0113	0.30382D-05	-5.5174	0.31180D 00	-0.5061
9	MGOH+	1.	0.92394D-02	0.23204D-06	-6.6344	0.17766D-06	-6.7504	0.76565D 00	-0.1160
10	MGCO3	0.	0.92678D 00	0.11405D-04	-4.9429	0.11972D-04	-4.9218	0.10496D 01	0.0210
11	MGHCO3+	1.	0.17395D 02	0.21154D-03	-3.6746	0.15215D-03	-3.8177	0.71926D 00	-0.1431
12	MGSO4	0.	0.15230D 03	0.13129D-02	-2.8818	0.13781D-02	-2.8607	0.10496D 01	0.0210
13	CAOH+	1.	0.24561D-03	0.44646D-08	-8.3502	0.33825D-08	-8.4708	0.75763D 00	-0.1205
14	CAHCO3+	1.	0.50494D-30	0.51829D-35	-35.2854	0.39247D-35	-35.4060	0.75763D 00	-0.1205
15	CACO3	0.	0.44207D 00	0.45833D-05	-5.3388	0.48108D-05	-5.3178	0.10496D 01	0.0210
16	CASO4	0.	0.55078D 02	0.41982D-03	-3.3769	0.44066D-03	-3.3559	0.10496D 01	0.0210
17	NACO3-	-1.	0.28965D 00	0.36213D-05	-5.4411	0.27061D-05	-5.5677	0.74726D 00	-0.1265
18	NAHCO3	0.	0.12597D 02	0.15563D-03	-3.8079	0.16336D-03	-3.7869	0.10496D 01	0.0210

19 NAS04-	-1.	0.387340 02	0.337620-03	-3.4716	0.252290-03	-3.5981	0.74726D 00	-0.1265
20 KS04-	-1.	0.358060 01	0.274900-04	-4.5608	0.205420-04	-4.6874	0.74726D 00	-0.1265
21 NA2C03	0.	0.157840-01	0.154540-06	-6.8110	0.162210-06	-6.7899	0.10496D 01	0.0210
22 HS04-	-1.	0.417880-03	0.443410-08	-8.3532	0.323660-08	-8.4899	0.72994D 00	-0.1367
23 H+	1.	0.354230-04	0.364670-07	-7.4381	0.291350-07	-7.5356	0.79895D 00	-0.0975
24 OH-	-1.	0.240730-02	0.146880-06	-6.8330	0.103950-06	-6.9832	0.70771D 00	-0.1501
25 NA2S04	0.	0.114680 03	0.837790-03	-3.0769	0.879380-03	-3.0558	0.10496D 01	0.0210
26 H2C03	0.	0.130780 02	0.218810-03	-3.6599	0.231220-03	-3.6360	0.10567D 01	0.0240
27 HCL	0.	0.176880-10	0.503420-15	-15.2981	0.528410-15	-15.2770	0.10496D 01	0.0210
28 NACL	0.	0.172690 02	0.306630-03	-3.5134	0.321450-03	-3.4923	0.10496D 01	0.0210
29 KCL	0.	0.482040 00	0.670930-05	-5.1733	0.704240-05	-5.1523	0.10496D 01	0.0210
30 H2S04	0.	0.131230-13	0.138840-18	-18.8575	0.145740-18	-18.8364	0.10496D 01	0.0210

PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23 CALCITE	0.437800-08	0.437900-08	-8.3588	-8.3586	0.9996D 00	-0.00018
24 ARAGONIT	0.437800-08	0.794100-08	-8.3588	-8.1001	0.5512D 00	-0.25866
25 MAGNESIT	0.157900-07	0.998900-08	-7.8015	-8.0005	0.1581D 01	0.19894
26 DOLOMITE	0.691400-16	0.209800-16	-16.1603	-16.6781	0.3295D 01	0.51782
28 GYPSUM	0.247400-05	0.170200-04	-5.6067	-4.7691	0.1454D 00	-0.83752

********** MIXTURE NUMBER 3 CONTAINING 50.00 PERCENT OF SOLUTION 1 AND 50.00 PERCENT OF SOLUTION 2 **********

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.641300D-02	-2.1929	0.257033D 00
MGTOT	2.	0.275400D-01	-1.5600	0.669552D 00
NATOT	1.	0.242315D 00	-0.6156	0.557077D 01
KTOT	1.	0.529923D-02	-2.2758	0.207211D 00
CLTOT	-1.	0.282860D 00	-0.5484	0.100282D 02
S04TOT	-2.	0.146300D-01	-1.8348	0.140538D 01
C02TOT	-1.	0.361424D-02	-2.4778	0.203068D 00

--- CONVERGENCE ITERATIONS ---

NSTEP	IPH	PH	ELECTRICAL BALANCE	S1-C02TOT	S2-S04TOT	S3-CLTOT	N MODEL
3	1	7.535387	-0.801586D-04	-0.191813D-12	-0.174938D-13	-0.526412D-12	10
3	2	7.335387	0.226614D-04	-0.109322D-12	-0.196588D-13	-0.319189D-15	10
3	3	7.379467	-0.281400D-05	-0.147178D-13	-0.228012D-13	-0.388578D-15	10
3	4	7.374421	0.114486D-07	0.173472D-17	-0.152656D-15	0.138778D-15	13

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED			
EPMCAT	315.52	302.69	PH		ACTIVITY H2O = 0.9903
EPMAN	315.73	302.69	7.374		PCO2 = 0.4801130-02
IONIC STRENGTH =	0.3419400 00		TEMPERATURE		LOG PCO2 = -2.3187
DENSITY =	1.0000		10.00 DEG C		UNCOMPLEX CO2 = 0.3154520-02
CLTOT =	0.2828600 00				CO2TOT = 0.3614240-02
KTOT =	0.5299230-02				ELECT = 0.1144860-07
					ALKALINITY = 3.400 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.22541D 03	0.5836ID-02	-2.2339	0.16806D-02	-2.7745	0.28797D 00	-0.5406
2	MG++	2.	0.58433D 03	0.2494ID-01	-1.6031	0.7871OD-02	-2.1040	0.31558D 00	-0.5009
3	NA+	1.	0.52207D 04	0.23565D 00	-0.6277	0.170A0D 00	-0.7675	0.72481D 00	-0.1398
4	K+	1.	0.19702D 03	0.5228ID-02	-2.2816	0.35369D-02	-2.4514	0.67647D 00	-0.1698
5	CL-	-1.	0.96376D 04	0.28209D 00	-0.5496	0.190A2D 00	-0.7194	0.67647D 00	-0.1698
6	SO4--	-2.	0.7A387D 03	0.846780-02	-2.0722	0.20750D-02	-2.6830	0.24505D 00	-0.6107
7	HCO3-	-1.	0.17129D 03	0.29131D-02	-2.5356	0.20927D-02	-2.6793	0.71836D 00	-0.1437
8	CO3--	-2.	0.34955D 00	0.60446D-05	-5.2186	0.16097D-05	-5.7933	0.26630D 00	-0.5746
9	MGOH+	1.	0.99360D-02	0.24953D-06	-6.6029	0.18490D-06	-6.7331	0.74098D 00	-0.1302
10	MGCO3	0.	0.72131D 00	0.88768D-05	-5.0517	0.96039D-05	-5.0176	0.10819D 01	0.0342
11	MGHCO3+	1.	0.21290D 02	0.25891D-03	-3.5868	0.17690D-03	-3.7523	0.68325D 00	-0.1654
12	MGSO4	0.	0.27040D 03	0.23310D-02	-2.6325	0.25220D-02	-2.5983	0.10819D 01	0.0342
13	CAOH+	1.	0.20404D-03	0.37090D-08	-8.4307	0.27119D-08	-8.5667	0.73116D 00	-0.1360
14	CAHCO3+	1.	0.46862D-30	0.48101D-35	-35.3178	0.35170D-35	-35.4538	0.73116D 00	-0.1360
15	CACO3	0.	0.26505D 00	0.27479D-05	-5.5610	0.29730D-05	-5.5268	0.10819D 01	0.0342
16	CASO4	0.	0.75332D 02	0.57419D-03	-3.2409	0.62123D-03	-3.2067	0.10819D 01	0.0342
17	NACO3-	-1.	0.25579D 00	0.31980D-05	-5.4951	0.22974D-05	-5.6388	0.71836D 00	-0.1437
18	NAHCO3	0.	0.15037D 02	0.18578D-03	-3.7310	0.20100D-03	-3.6968	0.10819D 01	0.0342
19	NASO4-	-1.	0.78033D 02	0.680170-03	-3.1674	0.48861D-03	-3.3110	0.71836D 00	-0.1437
20	KSO4-	-1.	0.70994D 01	0.54505D-04	-4.2636	0.39154D-04	-4.4072	0.71836D 00	-0.1437
21	NA2CO3	0.	0.20831D-01	0.203950-06	-6.6905	0.220660-06	-6.6563	0.10819D 01	0.0342
22	HSO4-	-1.	0.76119D-03	0.813730-08	-8.0895	0.566960-08	-8.2464	0.69674D 00	-0.1569
23	H+	1.	0.52518D-04	0.54065D-07	-7.2671	0.42226D-07	-7.3744	0.78102D 00	-0.1073
24	OH-	-1.	0.17517D-02	0.106880-06	-6.9711	0.714500-07	-7.1460	0.66852D 00	-0.1749
25	NA2SO4	0.	0.34526D 03	0.252230-02	-2.5982	0.272900-02	-2.5640	0.10819D 01	0.0342
26	H2CO3	0.	0.14070D 02	0.23539D-03	-3.6282	0.25732D-03	-3.5895	0.10932D 01	0.0387
27	HCL	0.	0.39300D-10	0.11185D-14	-14.9514	0.12101D-14	-14.9172	0.10819D 01	0.0342
28	NACL	0.	0.42422D 02	0.753230-03	-3.1231	0.814930-03	-3.0889	0.10819D 01	0.0342
29	KCL	0.	0.11654D 01	0.162200-04	-4.7899	0.175490-04	-4.7557	0.10819D 01	0.0342
30	H2SO4	0.	0.323210-13	0.341970-18	-18.4660	0.369980-18	-18.4318	0.10819D 01	0.0342

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.2705D-08	0.4379D-08	-8.5678	-8.3586	0.6177D 00	-0.20920
24	ARAGONIT	0.2705D-08	0.7941D-08	-8.5678	-8.1001	0.3407D 00	-0.46768
25	MAGNESIT	0.1267D-07	0.9989D-08	-7.8972	-8.0005	0.1268D 01	0.10324
26	DOLOMITE	0.3428D-16	0.2098D-16	-16.4650	-16.6781	0.1633D 01	0.21310
28	GYPSUM	0.3487D-05	0.1702D-04	-5.4575	-4.7691	0.2049D 00	-0.68837

---CONVERGENCE ON PHASE BOUNDARY--- ITER	MOLES	SI	PH
1	0.181D-02	-0.209D 00	0.737D 01
2	0.193D-03	0.175D 01	0.918D 01
3	0.555D-04	0.300D 00	0.783D 01
4	0.880D-04	-0.805D-01	0.749D 01
5	0.873D-04	0.169D-02	0.756D 01

IPH	PH	---CONVERGENCE ON MASS AND PH--- ELECT	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	7.374	0.191D-02	-0.114D-12	-0.110D-10	-0.525D-11	9
2	8.374	0.130D-02	-0.201D-11	-0.120D-10	-0.538D-11	9
3	9.374	-0.553D-03	-0.177D-11	-0.759D-12	-0.550D-11	10
4	9.075	0.259D-03	-0.137D-12	-0.399D-12	-0.934D-12	10
5	9.194	-0.391D-04	-0.180D-12	0.108D-12	-0.179D-13	11
6	9.181	-0.338D-05	0.171D-13	0.863D-14	-0.167D-13	12
7	9.180	0.353D-08	0.121D-16	-0.193D-15	0.458D-15	13
1	9.180	-0.113D-02	-0.548D-11	-0.256D-12	-0.530D-11	10
2	8.180	-0.129D-03	-0.896D-12	-0.382D-13	-0.554D-12	10
3	7.180	0.340D-03	-0.753D-13	-0.173D-13	-0.533D-12	10
4	7.904	-0.247D-04	-0.207D-13	-0.689D-13	-0.155D-14	10
5	7.843	-0.307D-05	-0.185D-13	0.301D-14	0.196D-14	12
6	7.834	0.532D-07	0.159D-15	-0.186D-15	0.125D-15	13
1	7.835	-0.138D-03	-0.383D-12	-0.249D-13	-0.534D-12	10
2	7.635	-0.645D-04	-0.234D-12	-0.214D-13	-0.530D-12	10
3	7.435	0.260D-04	-0.141D-12	-0.214D-13	-0.361D-15	10
4	7.492	-0.259D-05	-0.154D-13	-0.248D-13	-0.430D-15	10
5	7.487	0.620D-08	0.134D-15	-0.179D-15	0.153D-15	13
1	7.487	0.338D-04	-0.162D-12	-0.223D-13	-0.402D-15	10
2	7.687	-0.516D-04	-0.268D-12	-0.251D-13	-0.583D-15	10
3	7.566	-0.253D-05	-0.145D-13	0.256D-14	0.260D-14	12
4	7.560	0.177D-08	0.139D-15	-0.179D-15	0.125D-15	13
1	7.560	-0.665D-06	0.122D-14	0.257D-14	0.261D-14	12
2	7.360	0.101D-03	-0.117D-12	-0.182D-13	-0.529D-12	10
3	7.559	-0.899D-07	0.139D-15	-0.181D-15	0.153D-15	13
4	7.559	0.768D-11	0.139D-15	-0.183D-15	0.971D-16	13

THE PHASE BOUNDARY HAS BEEN FOUND
0.87328D-04 MOLES OF CA(1.000)MG(0.0)NA(0.0)K(0.0)CL(0.0)SO4(0.0)CO3(1.000) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.650033D-02	-2.2281	0.237048D 00
MGTOT	2.	0.275400D-01	-1.6033	0.606025D 00
NATOT	1.	0.242315D 00	-0.6277	0.541734D 01
KTOT	1.	0.529923D-02	-2.2816	0.204446D 00
CLTOT	-1.	0.282860D 00	-0.5496	0.100010D 02
SO4TOT	-2.	0.146300D-01	-2.0724	0.813194D 00
CO2TOT	-1.	0.370157D-02	-2.5167	0.185659D 00

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	315.52	302.82	PH	ACTIVITY H2O = 0.9903
EPMAN	315.73	302.82	7.559	PCO2 = 0.328141D-02
IONIC STRENGTH = 0.342139D 00			TEMPERATURE	LOG PCO2 = -2.4839
DENSITY = 1.0000			10.00 DEG C	UNCOMPLEX CO2 = 0.321326D-02
CLTOT = 0.282860D 00				CO2TOT = 0.370157D-02
KTOT = 0.529923D-02				ELECT = 0.767682D-11
				ALKALINITY = 3.575 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.228440 03	0.591440-02	-2.2281	0.170300-02	-2.7688	0.287940 00	-0.5407
2	MG++	2.	0.584010 03	0.249270-01	-1.6033	0.786580-02	-2.1043	0.315560 00	-0.5009
3	NA+	1.	0.522050 04	0.235640 00	-0.6277	0.170790 00	-0.7675	0.724790 00	-0.1398
4	K+	1.	0.197020 03	0.522850-02	-2.2816	0.353670-02	-2.4514	0.676420 00	-0.1698
5	CL-	-1.	0.963760 04	0.282090 00	-0.5496	0.190810 00	-0.7194	0.676420 00	-0.1698
6	SO4--	-2.	0.783650 03	0.846530-02	-2.0724	0.207400-02	-2.6832	0.245000 00	-0.6108
7	HCO3-	-1.	0.178910 03	0.304270-02	-2.5167	0.218570-02	-2.6604	0.718330 00	-0.1437
8	CO3--	-2.	0.558030 00	0.964960-05	-5.0155	0.256920-05	-5.5902	0.266250 00	-0.5747
9	MGOH+	1.	0.151750-01	0.381100-06	-6.4190	0.282370-06	-6.5492	0.740950 00	-0.1302
10	MGCO3	0.	0.115050 01	0.141580-04	-4.8490	0.153190-04	-4.8148	0.108200 01	0.0342
11	MGHCO3+	1.	0.222230 02	0.270260-03	-3.5682	0.184650-03	-3.7337	0.683210 00	-0.1654
12	MGSO4	0.	0.270070 03	0.232820-02	-2.6330	0.251900-02	-2.5988	0.108200 01	0.0342
13	CAOH+	1.	0.315970-03	0.574350-08	-8.2408	0.419430-08	-8.3768	0.731130 00	-0.1360
14	CAHCO3+	1.	0.495980-30	0.509100-35	-35.2932	0.372220-35	-35.4292	0.731130 00	-0.1360
15	CACO3	0.	0.428640 00	0.444410-05	-5.3522	0.480840-05	-5.3180	0.108200 01	0.0342
16	CASO4	0.	0.762900 02	0.581500-03	-3.2354	0.629170-03	-3.2012	0.108200 01	0.0342
17	NACO3-	-1.	0.408270 00	0.510440-05	-5.2921	0.366660-05	-5.4357	0.718330 00	-0.1437
18	NAHCO3	0.	0.157040 02	0.194020-03	-3.7122	0.209920-03	-3.6779	0.108200 01	0.0342

19 NAS04-	-1.	0.77993D 02	0.67982D-03	-3.1676	0.48833D-03	-3.3113	0.71833D 00	-0.1437
20 KS04-	-1.	0.70957D 01	0.54477D-04	-4.2638	0.39132D-04	-4.4075	0.71833D 00	-0.1437
21 NA2C03	0.	0.33244D-01	0.32548D-06	-6.4875	0.35215D-06	-6.4533	0.10820D 01	0.0342
22 HS04-	-1.	0.49788D-03	0.53224D-08	-8.2739	0.37082D-08	-8.4308	0.69670D 00	-0.1570
23 H+	1.	0.34367D-04	0.35380D-07	-7.4512	0.27632D-07	-7.5586	0.78100D 00	-0.1074
24 OH-	-1.	0.26770D-02	0.16334D-06	-6.7869	0.10919D-06	-6.9618	0.66848D 00	-0.1749
25 NA2S04	0.	0.34503D 03	0.25207D-02	-2.5985	0.27273D-02	-2.5643	0.10820D 01	0.0342
26 H2C03	0.	0.96156D 01	0.16087D-03	-3.7935	0.17587D-03	-3.7548	0.10932D 01	0.0387
27 HCL	0.	0.25714D-10	0.73184D-15	-15.1356	0.79183D-15	-15.1014	0.10820D 01	0.0342
28 NACL	0.	0.42415D 02	0.75311D-03	-3.1231	0.81484D-03	-3.0889	0.10820D 01	0.0342
29 KCL	0.	0.11652D 01	0.16218D-04	-4.7900	0.17547D-04	-4.7558	0.10820D 01	0.0342
30 H2S04	0.	0.13832D-13	0.14635D-18	-18.8346	0.15835D-18	-18.8004	0.10820D 01	0.0342

PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23 CALCITE	0.4375D-08	0.4379D-08	-8.3590	-8.3586	0.9991D 00	-0.00040
24 ARAGONIT	0.4375D-08	0.7941D-08	-8.3590	-8.1001	0.5510D 00	-0.25888
25 MAGNESIT	0.2021D-07	0.9989D-08	-7.6944	-8.0005	0.2023D 01	0.30602
26 DOLOMITE	0.8842D-16	0.2098D-16	-16.0534	-16.6781	0.4214D 01	0.62467
28 GYPSUM	0.3532D-05	0.1702D-04	-5.4520	-4.7691	0.2076D 00	-0.68286

SIMULATION OF CENTRAL FLORIDA GROUND WATER CHEMISTRY. START = 1N.

********** SOLUTION NUMBER 1 **********

TEMPERATURE = 25.00 DEGREES C PH = 8.000 ANALYTICAL EPMCAT = 2.4 ANALYTICAL EPMAN = 2.7

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.8400000D-03	-3.0757	0.3366720-01
MGTOT	2.	0.2300000D-03	-3.6383	0.5591760-02
NATOT	1.	0.1390000D-03	-3.8570	0.3195580-02
KTOT	1.	0.1300000D-03	-3.8861	0.5083260-02
CLTOT	-1.	0.1270000D-03	-3.8962	0.4502530-02
SO4TOT	-2.	0.2500000D-03	-3.6021	0.2401540-01
CO2TOT	-1.	0.2100000D-02	-2.6778	0.1281360 00

--- CONVERGENCE ITERATIONS ---

ITERATION	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	ELECTRICAL BALANCE	N MODEL
1	-0.172666D-11	-0.192198D-11	0.206212D-11	-0.2973900508305249D-03	5
2	-0.452112D-16	-0.794720D-16	-0.805359D-17	-0.4037034184918647D-07	8
3	-0.159701D-11	-0.177764D-11	-0.747277D-13	0.2973098836565740-03	5
4	-0.452654D-16	-0.795262D-16	-0.814507D-17	-0.3837498776458310D-13	8
5	-0.451570D-16	-0.795604D-16	-0.808747D-17	-0.3523657060577889D-18	8

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED
EPMCAT	2.41	2.62
EPMAN	2.73	2.62

IONIC STRENGTH = 0.3870210-02
DENSITY = 1.0000
CLTOT = 0.1270000-03
KTOT = 0.1274300-03

PH
8.000

TEMPERATURE
25.00 DEG C

ACTIVITY H2O = 0.9999
PCO2 = 0.1240460-02
LOG PCO2 = -2.9064
UNCOMPLEX CO2 = 0.2073910-02
CO2TOT = 0.2100000-02
ELECT = -0.3523660-18
ALKALINITY = 2.079 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.319820 02	0.79812D-03	-3.0979	0.61289D-03	-3.2126	0.76791D 00	-0.1147
2	MG++	2.	0.533600 01	0.21953D-03	-3.6585	0.16904D-03	-3.7720	0.77002D 00	-0.1135
3	NA+	1.	0.319030 01	0.13880D-03	-3.8576	0.12981D-03	-3.8867	0.93522D 00	-0.0291
4	K+	1.	0.166900 02	0.42692D-03	-3.3697	0.39879D-03	-3.3993	0.93412D 00	-0.0296
5	CL-	-1.	0.450160 01	0.12700D-03	-3.8962	0.11863D-03	-3.9258	0.93412D 00	-0.0296
6	SO4--	-2.	0.214290 02	0.22312D-03	-3.6515	0.17102D-03	-3.7669	0.76651D 00	-0.1155
7	HCO3-	-1.	0.123230 03	0.20200D-02	-2.6947	0.18912D-02	-2.7233	0.93622D 00	-0.0286
8	CO3--	-2.	0.691470 00	0.11525D-04	-4.9384	0.88545D-05	-5.0528	0.76828D 00	-0.1145
9	MGOH+	1.	0.297910-02	0.72113D-07	-7.1420	0.67602D-07	-7.1700	0.93745D 00	-0.0281
10	MGCO3	0.	0.120320 00	0.14272D-05	-5.8455	0.14285D-05	-5.8451	0.10009D 01	0.0004
11	MGHCO3+	1.	0.339360 00	0.39779D-05	-5.4003	0.37177D-05	-5.4297	0.93459D 00	-0.0294
12	MGSO4	0.	0.601310 00	0.49964D-05	-5.3013	0.50008D-05	-5.3010	0.10009D 01	0.0004
13	CAOH+	1.	0.942130-03	0.16507D-07	-7.7823	0.15465D-07	-7.8107	0.93690D 00	-0.0283
14	CAHCO3+	1.	0.129600 01	0.12822D-04	-4.8921	0.12013D-04	-4.9204	0.93690D 00	-0.0283
15	CACO3	0.	0.771010 00	0.77049D-05	-5.1132	0.77117D-05	-5.1128	0.10009D 01	0.0004
16	CASO4	0.	0.290370 01	0.21333D-04	-4.6710	0.21352D-04	-4.6706	0.10009D 01	0.0004
17	NACO3-	-1.	0.188830-02	0.22755D-07	-7.6429	0.21304D-07	-7.6715	0.93622D 00	-0.0286
18	NAHCO3	0.	0.115820-01	0.13792D-06	-6.8604	0.13805D-06	-6.8600	0.10009D 01	0.0004
19	NASO4-	-1.	0.474920-02	0.39900D-07	-7.3990	0.37355D-07	-7.4276	0.93622D 00	-0.0286
20	KSO4-	-1.	0.691830-01	0.51195D-06	-6.2908	0.47930D-06	-6.3194	0.93622D 00	-0.0286
21	NA2CO3	0.	0.742240-07	0.70045D-12	-12.1546	0.70107D-12	-12.1542	0.10009D 01	0.0004
22	HSO4-	-1.	0.172270-04	0.17751D-09	-9.7508	0.16600D-09	-9.7799	0.93519D 00	-0.0291
23	H+	1.	0.107200-04	0.10638D-07	-7.9732	0.10000D-07	-8.0000	0.94007D 00	-0.0268
24	OH-	-1.	0.182480-01	0.10755D-05	-5.9684	0.10045D-05	-5.9980	0.93399D 00	-0.0297
25	NA2SO4	0.	0.132920-04	0.93597D-10	-10.0287	0.93681D-10	-10.0284	0.10009D 01	0.0004
26	H2CO3	0.	0.262950 01	0.42403D-04	-4.3726	0.42443D-04	-4.3722	0.10009D 01	0.0004
27	HCL	0.	0.343200-13	0.94148D-18	-18.0262	0.94232D-18	-18.0258	0.10009D 01	0.0004
28	NACL	0.	0.222780-04	0.38469D-09	-9.4149	0.38503D-09	-9.4145	0.10009D 01	0.0004
29	KCL	0.	0.916100-04	0.12290D-08	-8.9104	0.12301D-08	-8.9101	0.10009D 01	0.0004
30	H2SO4	0.	0.167550-15	0.17087D-20	-20.7673	0.17102D-20	-20.7669	0.10009D 01	0.0004

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.54270-08	0.37990-08	-8.2655	-8.4203	0.14290 01	0.15489
24	ARAGONIT	0.54270-08	0.60950-08	-8.2655	-8.2150	0.89030 00	-0.05046
25	MAGNESIT	0.14970-08	0.57540-08	-8.8248	-8.2400	0.2601D 00	-0.58485
26	DOLOMITE	0.81230-17	0.10000-16	-17.0903	-17.0000	0.8123D 00	-0.09030
28	GYPSUM	0.10460-06	0.17460-04	-6.9796	-4.7590	0.60180-02	-2.22057

0.10000D-02 MOLES OF CA(0.873)MG(0.059)NA(0.0)K(0.0)CL(0.0)SO4(0.093)CO3(0.907) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.171300D-02	-2.7662	0.686570D-01
MGTOT	2.	0.289000D-03	-3.5391	0.702617D-02
NATOT	1.	0.139000D-03	-3.8570	0.319558D-02
KTOT	1.	0.427430D-03	-3.3691	0.167134D-01
CLTOT	-1.	0.127000D-03	-3.8962	0.450253D-02
SO4TOT	-2.	0.343000D-03	-3.4647	0.329491D-01
CO2TOT	-1.	0.300700D-02	-2.5335	0.178634D 00

--- CONVERGENCE ITERATIONS ---

NSTEP	IPH	PH	ELECTRICAL BALANCE	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	1	8.000000	0.768559D-03	0.196051D-11	0.271112D-11	0.741850D-11	6
1	2	8.200000	0.722899D-03	0.271597D-11	0.301152D-11	-0.529259D-13	6
1	3	9.200000	0.228942D-03	0.100483D-12	0.172586D-11	0.120899D-11	9
1	4	10.200000	-0.131742D-02	0.476169D-11	-0.117551D-11	0.125415D-11	10
1	5	9.346052	0.716201D-04	-0.207753D-12	0.122335D-12	-0.135285D-12	10
1	6	9.411977	-0.547877D-05	-0.432624D-13	-0.355529D-13	-0.282870D-13	11
1	7	9.407499	0.102517D-06	-0.726849D-15	-0.694974D-16	-0.550680D-15	12

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED
EPMCAT	4.57	3.69
EPMAN	3.82	3.69

IONIC STRENGTH = 0.587025D-02
DENSITY = 1.0000
CLTOT = 0.127000D-03
KTOT = 0.427430D-03

PH = 9.408

TEMPERATURE = 25.00 DEG C

ACTIVITY H2O = 0.9999
PCO2 = 0.534981D-04
LOG PCO2 = -4.2717
UNCOMPLEX CO2 = 0.260090D-02
CO2TOT = 0.300700D-02
ELECT = 0.102517D-06
ALKALINITY = 3.757 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.525320 02	0.131090D-02	-2.8824	0.95390D-03	-3.0205	0.72764D 00	-0.1381
2	MG++	2.	0.35720D 01	0.14353D-03	-3.8283	0.17194D-03	-3.7646	0.73057D 00	-0.1363
3	NA+	1.	0.31757D 01	0.13816D-03	-3.8596	0.12743D-03	-3.8947	0.92232D 00	-0.0351
4	K+	1.	0.166850 02	0.426790-03	-3.3698	0.39295D-03	-3.4057	0.92070D 00	-0.0359
5	CL-	-1.	0.450160 01	0.12700D-03	-3.8962	0.11693D-03	-3.9321	0.92070D 00	-0.0359

6	SO4--	-2.	0.282840 02	0.29450D-03	-3.5309	0.21370D-03	-3.6702	0.72563D 00	-0.1393
7	HCO3-	-1.	0.13766D 03	0.22565D-02	-2.6466	0.20844D-02	-2.6810	0.92373D 00	-0.0345
8	CO3--	-2.	0.205530 02	0.36256D-03	-3.4653	0.24941D-03	-3.6031	0.72809D 00	-0.1378
9	MGOH+	1.	0.78441D-01	0.18988D-05	-5.7215	0.17573D-05	-5.7552	0.92548D 00	-0.0336
10	MGCO3	0.	0.34458D 01	0.40874D-04	-4.3886	0.40929D-04	-4.3880	0.10014D 01	0.0006
11	MGHCO3+	1.	0.38592D 00	0.45236D-05	-5.3445	0.41680D-05	-5.3801	0.92139D 00	-0.0356
12	MGSO4	0.	0.76390D 00	0.63474D-05	-5.1974	0.63560D-05	-5.1968	0.10014D 01	0.0006
13	CAOH+	1.	0.37968D-01	0.66522D-06	-6.1770	0.61512D-06	-6.2110	0.92469D 00	-0.0340
14	CAHCO3+	1.	0.22525D 01	0.22285D-04	-4.6520	0.20607D-04	-4.6860	0.92469D 00	-0.0340
15	CACO3	0.	0.33786D 02	0.33763D-03	-3.4716	0.33809D-03	-3.4710	0.10014D 01	0.0006
16	CASO4	0.	0.56444D 01	0.41468D-04	-4.3823	0.41524D-04	-4.3817	0.10014D 01	0.0006
17	NACO3-	-1.	0.52921D-01	0.93774D-06	-6.1954	0.58910D-06	-6.2298	0.92373D 00	-0.0345
18	NAHCO3	0.	0.12526D-01	0.14917D-06	-6.8263	0.14937D-06	-6.8257	0.10014D 01	0.0006
19	NASO4-	-1.	0.59043D-02	0.49605D-07	-7.3045	0.43821D-07	-7.3589	0.92373D 00	-0.0345
20	KSO4-	-1.	0.86330D-01	0.63884D-06	-6.1946	0.59012D-06	-6.2291	0.92373D 00	-0.0345
21	NA2CO3	0.	0.20140D-05	0.19005D-10	-10.7211	0.19031D-10	-10.7205	0.10014D 01	0.0006
22	HSO4-	-1.	0.85410D-06	0.88006D-11	-11.0555	0.81163D-11	-11.0906	0.92224D 00	-0.0352
23	H+	1.	0.42441D-06	0.42112D-09	-9.3756	0.39129D-09	-9.4075	0.92916D 00	-0.0319
24	OH-	-1.	0.47422D 00	0.27889D-04	-4.5546	0.25672D-04	-4.5905	0.92051D 00	-0.0360
25	NA2SO4	0.	0.15999D-04	0.11266D-09	-9.9482	0.11281D-09	-9.9477	0.10014D 01	0.0006
26	H2CO3	0.	0.11335D 00	0.18278D-05	-5.7381	0.18305D-05	-5.7374	0.10014D 01	0.0006
27	HCL	0.	0.13230D-14	0.46294D-19	-19.4402	0.46343D-19	-19.4396	0.10014D 01	0.0006
28	NACL	0.	0.21739D-04	0.37205D-09	-9.4294	0.37256D-09	-9.4288	0.10014D 01	0.0006
29	KCL	0.	0.88931D-04	0.11931D-08	-8.9233	0.11947D-08	-8.9227	0.10014D 01	0.0006
30	H2SO4	0.	0.32040D-18	0.32675D-23	-23.4858	0.32719D-23	-23.4852	0.10014D 01	0.0006

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.23790D-06	0.37990D-08	-6.6236	-8.4203	0.62630 02	1.79677
24	ARAGONIT	0.23790D-06	0.60950D-08	-6.6236	-8.2150	0.39030 02	1.59142
25	MAGNESIT	0.42890D-07	0.57540D-08	-7.3677	-8.2400	0.74530 01	0.87231
26	DOLOMITE	0.10200D-13	0.10000D-16	-13.9913	-17.0000	0.10200 04	3.00873
28	GYPSUM	0.20380D-06	0.17420D-04	-6.6907	-4.7590	0.11700D-01	-1.93170

ITER	---CONVERGENCE ON PHASE BOUNDARY--- MOLES	SI	PH	IPH	PH	---CONVERGENCE ON MASS AND PH--- ELECT	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	-0.8740D-03	0.1560 01	0.9410 01							
				1	9.408	-0.5730D-03	0.1720D-11	0.1570D-11	0.8350D-12	8
				2	8.408	-0.1640D-03	0.2880D-12	0.4080D-12	0.4630D-13	6
				3	7.408	0.3090D-04	0.7500D-13	0.2730D-12	-0.1490D-12	6
				4	7.466	-0.1820D-04	0.9910D-13	0.3920D-14	-0.1390D-12	7
				5	7.500	0.6020D-06	0.1600D-14	0.4330D-14	-0.5120D-14	7
				6	7.502	0.1040D-07	-0.2840D-16	-0.1140D-15	0.1800D-16	8
2	-0.6380D-03	-0.5780 00	0.7500 01							
				1	7.502	0.2480D-03	-0.1300D-11	-0.6060D-12	-0.1840D-12	5
				2	8.502	0.4300D-04	0.2670D-13	0.1360D-12	0.1120D-12	8
				3	9.502	-0.5070D-03	0.3820D-12	0.2930D-11	0.1030D-11	9
				4	8.580	0.2460D-04	-0.1090D-12	0.2160D-12	0.1740D-12	6
				5	8.680	-0.2370D-05	0.1600D-13	0.8840D-14	-0.1560D-13	8
				6	8.672	0.1150D-06	-0.8950D-15	-0.5040D-15	-0.9930D-15	9
				7	8.672	-0.6470D-10	-0.8580D-15	-0.5650D-15	0.1750D-16	9

***** THE PRESENT VALUE OF STPSIZ (0.50) IS TOO LARGE. A VALUE OF 0.17 IS NOW BEING USED. *****

3	-0.9410D-03	0.7170 00	0.8670 01						
				1	8.672	-0.2790D-03	-0.5000D-12	-0.2110D-12	0.1800D-12	6

				2	7.672	-0.1130-03	-0.8330-12	0.2400-12	-0.1190-12	6
				3	8.672	0.4430-03	-0.3870-12	-0.4780-12	-0.1560-12	5
				4	7.469	-0.6050-04	-0.5850-12	-0.5880-12	-0.1350-12	5
				5	7.264	0.1610-04	0.5130-13	0.2670-14	-0.1430-12	7
				6	7.304	-0.1370-05	0.9680-15	0.3080-14	-0.4530-14	7
				7	7.301	0.1020-07	0.9490-15	-0.7760-16	0.1590-16	8
4	-0.8410-03	-0.8390 00	0.7300 01							
				1	7.301	0.1080-03	-0.6370-12	-0.3570-12	-0.1600-12	5
				2	8.301	-0.1150-03	0.3190-12	0.4800-12	-0.1360-14	6
				3	7.786	-0.3400-04	0.1390-12	0.5720-14	-0.1220-12	7
				4	7.621	0.1800-05	0.2220-14	0.5430-14	-0.5480-14	7
				5	7.629	-0.8540-08	-0.4130-16	-0.1470-15	0.1700-16	8
5	-0.7770-03	-0.4250 00	0.7630 01							
				1	7.629	0.6670-04	0.1390-12	0.4060-12	-0.1500-12	6
				2	7.829	0.2340-04	0.1900-12	0.7590-14	-0.1250-12	7
				3	8.029	-0.1030-04	0.8740-14	0.1460-13	-0.8680-13	7
				4	7.968	-0.6140-06	-0.1120-15	-0.2740-15	-0.8990-17	8
				5	7.964	-0.2250-08	-0.1100-15	-0.2740-15	-0.8290-17	8
6	-0.7720-03	-0.4460-01	0.7960 01							
				1	7.964	0.5200-05	0.7050-14	0.1250-13	-0.6740-14	7
				2	8.164	-0.2590-04	0.1570-13	0.2250-13	-0.5040-13	7
				3	7.997	-0.1920-06	-0.1210-15	-0.2880-15	-0.1460-16	8
				4	7.996	-0.7070-09	-0.1210-15	-0.2880-15	-0.1420-16	8
7	-0.7700-03	-0.9160-02	0.8000 01							
				1	7.996	0.1280-05	0.7790-14	-0.3380-15	-0.6860-14	8
				2	8.196	-0.2950-04	0.1830-13	0.2530-13	-0.4000-13	7
				3	8.004	-0.4060-07	-0.1230-15	-0.2910-15	-0.1610-16	8
				4	8.004	-0.4530-10	-0.1230-15	-0.2910-15	-0.1590-16	8

THE PHASE BOUNDARY HAS BEEN FOUND
-0.770250-03 MOLES OF CA(0.980)MG(0.020)NA(0.0)K(0.0)CL(0.0)SO4(0.0)CO3(1.000) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.958155D-03	-3.0448	0.361544D-01
MGTOT	2.	0.273595D-03	-3.5866	0.629812D-02
NATOT	1.	0.139000D-03	-3.8577	0.319044D-02
KTOT	1.	0.427430D-03	-3.3698	0.166866D-01
CLTOT	-1.	0.127000D-03	-3.8962	0.450247D-02
SO4TOT	-2.	0.343000D-03	-3.5189	0.290851D-01
CO2TOT	-1.	0.223675D-02	-2.6679	0.131097D 00

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED		
EPMCAT	4.57	2.91	PH	ACTIVITY H2O = 0.9999
EPMAN	3.82	2.91	8.004	PCO2 = 0.130182D-02
IONIC STRENGTH =	0.438436D-02		TEMPERATURE	LOG PCO2 = -2.8854
DENSITY =	1.0000		25.00 DEG C	UNCOMPLEX CO2 = 0.220553D-02
CLTOT =	0.127000D-03			CO2TOT = 0.223675D-02
KTOT =	0.427430D-03			ELECT = -0.453352D-10
				ALKALINITY = 2.217 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.361470 02	0.90206D-03	-3.0448	0.682240-03	-3.1661	0.75631D 00	-0.1213
2	MG++	2.	0.629680 01	0.25905D-03	-3.5866	0.19653D-03	-3.7066	0.75865D 00	-0.1200
3	NA+	1.	0.319940 01	0.13878D-03	-3.8577	0.12928D-03	-3.8885	0.93156D 00	-0.0308
4	K+	1.	0.166830 02	0.42675D-03	-3.3698	0.39701D-03	-3.4012	0.93033D 00	-0.0314
5	CL-	-1.	0.450160 01	0.12700D-03	-3.8962	0.11815D-03	-3.9276	0.93033D 00	-0.0314
6	SO4--	-2.	0.290790 02	0.30278D-03	-3.5189	0.22852D-03	-3.6411	0.75475D 00	-0.1222
7	HCO3-	-1.	0.131070 03	0.21485D-02	-2.6679	0.20039D-02	-2.6981	0.93268D 00	-0.0303
8	CO3--	-2.	0.751040 00	0.12519D-04	-4.9024	0.94728D-05	-5.0235	0.75671D 00	-0.1211
9	MGOH+	1.	0.350970-02	0.849580-07	-7.0708	0.79354D-07	-7.1004	0.93404D 00	-0.0296
10	MGCO3	0.	0.149640 00	0.17750D-05	-5.7508	0.17768D-05	-5.7504	0.10010D 01	0.0004
11	MGHCO3+	1.	0.419740 00	0.49201D-05	-5.3080	0.45799D-05	-5.3391	0.93086D 00	-0.0311
12	MGSO4	0.	0.934020 00	0.77609D-05	-5.1101	0.77688D-05	-5.1096	0.10010D 01	0.0004
13	CAOH+	1.	0.106280-02	0.18621D-07	-7.7300	0.17381D-07	-7.7599	0.93343D 00	-0.0299
14	CAHCO3+	1.	0.153430 01	0.15179D-04	-4.8187	0.14169D-04	-4.8487	0.93343D 00	-0.0299
15	CACO3	0.	0.916080 00	0.91745D-05	-5.0374	0.91838D-05	-5.0370	0.10010D 01	0.0004
16	CASO4	0.	0.431840 01	0.31726D-04	-4.4986	0.31758D-04	-4.4981	0.10010D 01	0.0004
17	NACO3-	-1.	0.201960-02	0.24338D-07	-7.6137	0.22699D-07	-7.6440	0.93268D 00	-0.0303
18	NAHCO3	0.	0.122210-01	0.14553D-06	-6.8370	0.14568D-06	-6.8366	0.10010D 01	0.0004

19	NAS04-	-1.	0.634400D-07	0.532990D-07	-7.2733	0.497110-07	-7.3035	0.93268D 00	-0.0303
20	KS04-	-1.	0.923800D-01	0.683600D-06	-6.1652	0.637580-06	-6.1955	0.93268D 00	-0.0303
21	NA2C03	0.	0.787530D-07	0.743180D-12	-12.1289	0.743940-12	-12.1285	0.10010D 01	0.0004
22	HS04-	-1.	0.228880D-04	0.235840D-09	-9.6274	0.219690-09	-9.6582	0.93152D 00	-0.0308
23	H+	1.	0.106530D-04	0.105710D-07	-7.9759	0.990440-08	-8.0042	0.93695D 00	-0.0283
24	OH-	-1.	0.185400D-01	0.109040D-05	-5.9624	0.101420-05	-5.9939	0.93018D 00	-0.0314
25	NA2S04	0.	0.176140D-04	0.124030D-09	-9.9065	0.124160-09	-9.9060	0.10010D 01	0.0004
26	H2C03	0.	0.275930D 01	0.444950D-04	-4.3517	0.445430-04	-4.3512	0.10011D 01	0.0005
27	HCL	0.	0.336500D-13	0.928580D-18	-18.0322	0.929520-18	-18.0317	0.10010D 01	0.0004
28	NACL	0.	0.222930D-04	0.381520D-09	-9.4185	0.381910-09	-9.4180	0.10010D 01	0.0004
29	KCL	0.	0.908210D-04	0.121840D-08	-8.9142	0.121970-08	-8.9138	0.10010D 01	0.0004
30	H2S04	0.	0.219590D-15	0.223940D-20	-20.6499	0.224170-20	-20.6494	0.10010D 01	0.0004

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.6463D-08	0.3799D-08	-8.1896	-8.4203	0.1701D 01	0.23076
24	ARAGONIT	0.6493D-08	0.6093D-08	-8.1876	-8.2150	0.1060D 01	0.02541
25	MAGNESIT	0.1892D-08	0.5754D-08	-8.7301	-8.2400	0.3235D 00	-0.49009
26	DOLOMIT	0.1203D-16	0.1000D-16	-16.9197	-17.0000	0.1203D 01	0.08033
28	GYPSUM	0.1559D-06	0.1742D-04	-6.8071	-4.7590	0.8951D-02	-2.04814

0.100000D-01 MOLES OF CA(0.873)MG(0.039)NA(0.0)K(0.0)CL(0.0)SO4(0.093)CO3(0.907) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.9570000D-02	-2.0191	0.383566D 00
MGTOT	2.	0.8200000D-03	-3.0862	0.199358D-01
NATOT	1.	0.1390000D-03	-3.8570	0.319558D-02
KTOT	1.	0.4274300D-03	-3.3691	0.167134D-01
CLTOT	-1.	0.1270000D-03	-3.8962	0.450253D-02
SO4TOT	-2.	0.1180000D-02	-2.9281	0.113353D 00
CO2TOT	-1.	0.1117000D-01	-1.9635	0.663674D 00

--- CONVERGENCE ITERATIONS ---

ISTEP	IPH	PH	ELECTRICAL BALANCE	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
2	1	8.004173	0.7517950-02	0.7460220-11	0.1845220-11	0.2503580-10	8
2	2	8.204173	0.7245370-02	0.3896880-10	0.1807250-10	0.2907430-10	8
2	3	9.204173	0.4166830-02	-0.4042860-10	-0.2198470-10	0.6129340-11	12
2	4	10.204173	-0.1100010-02	0.4621830-12	-0.4575900-11	-0.8708350-12	15
2	5	9.995318	-0.9762300-04	-0.4838010-12	0.1485720-12	-0.6874300-12	17
2	6	9.975443	0.3593090-05	-0.2382120-13	-0.3460500-13	-0.1344120-13	20
2	7	9.976147	-0.1112060-07	0.7303190-15	-0.8158620-16	0.6884510-15	22

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED
EPMCAT	21.35	10.05
EPMAN	13.66	10.05

IONIC STRENGTH = 0.1789550-01
DENSITY = 1.0000
CLTOT = 0.1270000-03
KTOT = 0.4274300-03

PH 9.976
TEMPERATURE 25.00 DEG C

ACTIVITY H2O = 0.9997
PCO2 = 0.2137380-04
LOG PCO2 = -4.6701
UNCOMPLEX CO2 = 0.5776740-02
CO2TOT = 0.1117000-01
ELECT = -0.1112060-07
ALKALINITY = 18.859 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.1704300 03	0.4253200-02	-2.3713	0.2556100-02	-2.5924	0.600990 00	-0.2211
2	MG++	2.	0.1051800 02	0.4327100-03	-3.3638	0.2628200-03	-3.5803	0.607380 00	-0.2165
3	NA+	1.	0.3190900 01	0.1352600-03	-3.8688	0.1186800-03	-3.9256	0.877460 00	-0.0568
4	K+	1.	0.1664900 02	0.4258700-03	-3.3707	0.3718100-03	-3.4297	0.873060 00	-0.0590
5	CL-	-1.	0.4501800 01	0.1270000-03	-3.8962	0.1108800-03	-3.9552	0.873060 00	-0.0590

6	SO4--	-2.	0.847070D 02	0.88198D-03	-3.0545	0.52560D-03	-3.2793	0.59593D 00	-0.2248
7	HCO3-	-1.	0.21368D 03	0.35027D-02	-2.4556	0.30844D-02	-2.5108	0.88059D 00	-0.0552
8	CO3--	-2.	0.13039D 03	0.42733D-02	-2.6433	0.13670D-02	-2.8642	0.60131D 00	-0.2209
9	MGOH+	1.	0.40439D 00	0.11241D-04	-4.9492	0.99466D-05	-5.0023	0.88481D 00	-0.0531
10	MGCO3	0.	0.26787D 02	0.34147D-03	-3.4666	0.34288D-03	-3.4649	0.10041D 01	0.0018
11	MGHCO3+	1.	0.91942D 00	0.10777D-04	-4.9675	0.94274D-05	-5.0256	0.87475D 00	-0.0581
12	MGSO4	0.	0.28639D 01	0.23797D-04	-4.6235	0.23895D-04	-4.6217	0.10041D 01	0.0018
13	CAOH+	1.	0.39456D 00	0.69130D-05	-5.1603	0.61037D-05	-5.2144	0.88293D 00	-0.0541
14	CAHCO3+	1.	0.93341D 01	0.92545D-04	-4.0336	0.81711D-04	-4.0877	0.88293D 00	-0.0541
15	CACO3	0.	0.49462D 03	0.49448D-02	-2.3058	0.49653D-02	-2.3041	0.10041D 01	0.0018
16	CASO4	0.	0.37097D 02	0.42755D-03	-3.5646	0.27367D-03	-3.5628	0.10041D 01	0.0018
17	NACO3-	-1.	0.28833D 00	0.34149D-05	-5.4666	0.30071D-05	-5.5218	0.88059D 00	-0.0552
18	NAHCO3	0.	0.17216D-01	0.20501D-06	-6.6882	0.20586D-06	-6.6864	0.10041D 01	0.0018
19	NASO4-	-1.	0.14188D-01	0.11920D-06	-6.9237	0.10497D-06	-6.9790	0.88059D 00	-0.0552
20	KSO4-	-1.	0.21076D 00	0.15596D-05	-5.8070	0.13734D-05	-5.8622	0.88059D 00	-0.0552
21	NA2CO3	0.	0.95484D-05	0.90107D-10	-10.0452	0.90479D-10	-10.0435	0.10041D 01	0.0018
22	HSO4-	-1.	0.59650D-06	0.61464D-11	-11.2214	0.53897D-11	-11.2684	0.87690D 00	-0.0571
23	H+	1.	0.11918D-06	0.11825D-09	-9.9272	0.10565D-09	-9.9761	0.89338D 00	-0.0490
24	OH-	-1.	0.18526D 01	0.10895D-03	-3.9628	0.95064D-04	-4.0220	0.87252D 00	-0.0592
25	NA2SO4	0.	0.34034D-04	0.23969D-09	-9.6203	0.24068D-09	-9.6186	0.10041D 01	0.0018
26	H2CO3	0.	0.45154D-01	0.72814D-06	-6.1378	0.73132D-06	-6.1359	0.10044D 01	0.0019
27	HCL	0.	0.33779D-15	0.92663D-20	-20.0331	0.93046D-20	-20.0313	0.10041D 01	0.0018
28	NACL	0.	0.19147D-04	0.32768D-09	-9.4846	0.32903D-09	-9.4828	0.10041D 01	0.0018
29	KCL	0.	0.79573D-04	0.10675D-08	-8.9716	0.10719D-08	-8.9698	0.10041D 01	0.0018
30	H2SO4	0.	0.57286D-19	0.58421D-24	-24.2334	0.58662D-24	-24.2316	0.10041D 01	0.0018

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.34940D-05	0.37990D-08	-5.4567	-8.4203	0.91980 03	2.96368
24	ARAGONIT	0.34940D-05	0.60950D-08	-5.4567	-8.2150	0.57320 03	2.75833
25	MAGNESIT	0.35930D-06	0.57540D-08	-6.4446	-8.2400	0.62430 02	1.79542
26	DOLOMITE	0.12350D-11	0.16000D-16	-11.9012	-17.0000	0.12550 06	5.09875
28	GYPSUM	0.13430D-05	0.17420D-04	-5.8718	-4.7590	0.77130D-01	-1.11277

---CONVERGENCE ON PHASE BOUNDARY---				---CONVERGENCE ON MASS AND PH---					
ITER	MOLES	SI	PH	IPH	PH	ELECT	S1-CO2TOT	S2-SO4TOT	S3-CLTOT	N MODEL
1	-0.4880D-02	0.2720 01	0.9980 01							
				1	9.976	-0.1160D-02	0.5930D-11	0.4680D-11	0.4040D-11	13
				2	8.976	0.1750D-02	-0.3860D-11	0.6070D-11	0.2230D-11	10
				3	9.577	0.1610D-03	-0.1460D-11	-0.2020D-12	-0.1040D-11	13
				4	9.631	-0.1190D-04	0.1220D-13	-0.2930D-13	-0.4420D-13	15
				5	9.627	-0.1530D-06	0.1820D-16	0.1520D-14	0.3410D-15	18
2	-0.7320D-02	0.2240 01	0.9630 01							
				1	9.627	-0.1110D-02	0.5210D-11	0.1150D-11	0.2220D-11	10
				2	8.627	0.1350D-03	-0.3140D-13	-0.5390D-13	0.2230D-12	9
				3	8.736	0.6800D-04	-0.1390D-13	-0.3540D-13	0.4500D-12	9
				4	8.840	-0.8130D-05	0.6180D-13	0.2250D-13	-0.1320D-13	9
				5	8.829	0.3840D-06	-0.2900D-14	-0.2350D-14	0.8520D-16	11
				6	8.829	-0.3560D-09	0.1110D-15	0.1120D-15	0.8460D-16	12
3	-0.8540D-02	0.1310 01	0.8830 01							
				1	8.829	-0.1050D-02	0.3090D-11	0.4610D-11	0.3460D-12	7
				2	7.829	-0.8010D-03	0.8150D-12	0.1360D-11	-0.3160D-12	7
				3	6.829	-0.2490D-03	0.2860D-12	0.1360D-11	-0.4070D-12	7
				4	5.829	0.1120D-02	0.1260D-12	0.2040D-11	-0.4840D-12	7
				5	6.647	-0.3090D-04	0.2670D-12	0.3460D-13	-0.4350D-13	8
				6	6.622	0.2270D-05	0.3840D-14	-0.1520D-14	-0.9200D-15	9
				7	6.624	-0.1790D-07	-0.6050D-16	-0.1320D-15	-0.9190D-15	10
4	-0.7910D-02	-0.1420 01	0.6620 01							

			1	6.624	0.8350-03	0.2360-11	0.4990-11	-0.6780-12	7
			2	7.624	-0.9080-04	0.8310-12	0.8030-13	-0.5610-12	8
			3	7.526	-0.5120-04	0.2300-13	0.9110-13	-0.6660-13	8
			4	7.406	0.6740-05	0.2030-13	-0.7920-14	-0.6680-13	9
			5	7.420	-0.4020-06	-0.9850-15	-0.5520-15	-0.1300-14	10
			6	7.419	0.5280-09	-0.9850-15	-0.5520-15	0.1220-15	10
5	-0.7800-02	-0.2360 00	0.7420 01						
			1	7.419	0.1140-03	0.8570-12	0.8800-13	-0.6320-12	8
			2	7.619	0.2160-04	0.3020-13	0.1070-12	-0.7100-13	8
			3	7.819	-0.4610-04	0.3890-13	0.1230-12	-0.7130-13	8
			4	7.683	-0.2040-05	-0.1630-14	-0.1070-13	-0.1460-14	9
			5	7.677	0.4350-08	-0.1620-15	-0.7850-15	0.1410-15	10
6	-0.7830-02	0.6890-01	0.7680 01						
			1	7.677	-0.2520-04	0.3080-13	0.1070-12	-0.7000-13	8
			2	7.477	0.5780-04	0.2560-13	0.9920-13	-0.1360-14	8
			3	7.616	-0.2740-05	-0.1400-14	-0.9830-14	-0.1400-14	9
			4	7.609	0.1430-07	-0.1400-15	-0.7200-15	0.1360-15	10
7	-0.7820-02	-0.6970-02	0.7610 01						
			1	7.609	0.3030-05	0.2740-13	-0.1010-13	-0.1400-14	9
			2	7.809	-0.6510-04	0.3690-13	0.1180-12	-0.5330-12	8
			3	7.618	-0.4340-06	-0.1540-14	-0.6940-15	-0.1410-14	10
			4	7.617	0.2630-09	-0.1420-15	-0.7280-15	0.1370-15	10

THE PHASE BOUNDARY HAS BEEN FOUND
-0.78234D-02 MOLES OF CA(0.980)MG(0.020)NA(0.0)K(0.0)CL(0.0)SO4(0.0)CO3(1.000) HAVE BEEN ADDED TO SOLUTION NO. 1

--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---

SPECIES		TOTAL MOLALITY	LOG TOTAL MOLALITY	TOTAL GRAMS/KGM H2O
CATOT	2.	0.190310D-02	-2.7701	0.680484D-01
MGTOT	2.	0.663533D-03	-3.2229	0.145511D-01
NATOT	1.	0.139000D-03	-3.8581	0.318704D-02
KTOT	1.	0.427430D-03	-3.3712	0.166358D-01
CLTOT	-1.	0.127000D-03	-3.8962	0.450248D-02
SO4TOT	-2.	0.118000D-02	-3.0124	0.933525D-01
CO2TOT	-1.	0.334663D-02	-2.5058	0.190403D 00

----DESCRIPTION OF SOLUTION ----

	ANALYTICAL	COMPUTED
EPMCAT	21.35	5.21
EPMAN	13.66	5.21

IONIC STRENGTH = 0.848581D-02
DENSITY = 1.0000
CLTOT = 0.127000D-03
KTOT = 0.427430D-03

PH
7.617

TEMPERATURE
25.00 DEG C

ACTIVITY H2O = 0.9999
PCO2 = 0.450380D-02
LOG PCO2 = -2.3464
UNCOMPLEX CO2 = 0.328226D-02
CO2TOT = 0.334663D-02
ELECT = 0.262815D-09
ALKALINITY = 3.213 MEQ/LITRE

DISTRIBUTION OF SPECIES

I	SPECIES		PPM	MOLALITY	LOG MOL	ACTIVITY	LOG ACT	ACT. COEFF.	LOG A COF
1	CA++	2.	0.680350 02	0.169780-02	-2.7701	0.116900-02	-2.9322	0.68852D 00	-0.1621
2	MG++	2.	0.145480 02	0.598510-03	-3.2229	0.413390-03	-3.3826	0.69236D 00	-0.1597
3	NA+	1.	0.319640 01	0.138630-03	-3.8581	0.126040-03	-3.8995	0.90920D 00	-0.0413
4	K+	1.	0.166320 02	0.425450-03	-3.3712	0.385850-03	-3.4136	0.90694D 00	-0.0424
5	CL-	-1.	0.450160 01	0.127000-03	-3.8962	0.115180-03	-3.9386	0.90694D 00	-0.0424
6	SO4--	-2.	0.933330 02	0.971800-03	-3.0124	0.666430-03	-3.1762	0.68577D 00	-0.1638
7	HCO3-	-1.	0.190360 03	0.312050-02	-2.5058	0.284300-02	-2.5462	0.91108D 00	-0.0404
8	CO3--	-2.	0.479930 00	0.799920-05	-5.0970	0.551140-05	-5.2587	0.68900D 00	-0.1618
9	MGOH+	1.	0.310310-02	0.751150-07	-7.1243	0.686130-07	-7.1636	0.91344D 00	-0.0393
10	MGCO3	0.	0.183400 00	0.217550-05	-5.6624	0.217970-05	-5.6616	0.10020D 01	0.0008
11	MGHCO3+	1.	0.128740 01	0.150910-04	-4.8213	0.137010-04	-4.8633	0.90787D 00	-0.0420
12	MGSO4	0.	0.573790 01	0.476770-04	-4.3217	0.477710-04	-4.3208	0.10020D 01	0.0008
13	CAOH+	1.	0.763970-03	0.133850-07	-7.8734	0.122120-07	-7.9132	0.91238D 00	-0.0398
14	CAHCO3+	1.	0.381580 01	0.377520-04	-4.4231	0.344440-04	-4.4629	0.91238D 00	-0.0398
15	CACO3	0.	0.914380 00	0.913750-05	-5.0392	0.915540-05	-5.0383	0.10020D 01	0.0008
16	CASO4	0.	0.215580 02	0.158380-03	-3.8003	0.158690-03	-3.7994	0.10020D 01	0.0008
17	NACO3-	-1.	0.117280-02	0.141330-07	-7.8498	0.128760-07	-7.8902	0.91108D 00	-0.0404
18	NAHCO3	0.	0.168880-01	0.201110-06	-6.6966	0.201510-06	-6.6957	0.10020D 01	0.0008

19	NAS04-	-1.	0.184650-01	0.155140-06	-6.8093	0.141340-06	-6.8497	0.91108D 00	-0.0404
20	KS04-	-1.	0.268040 00	0.198350-05	-5.7026	0.180710-05	-5.7430	0.91108D 00	-0.0404
21	NA2C03	0.	0.435130-07	0.410620-12	-12.3866	0.411430-12	-12.3857	0.10020D 01	0.0008
22	HS04-	-1.	0.166790-03	0.171860-08	-8.7648	0.156230-08	-8.8062	0.90904D 00	-0.0414
23	H+	1.	0.263030-04	0.262980-07	-7.5801	0.241520-07	-7.6171	0.91837D 00	-0.0370
24	OH-	-1.	0.780000-02	0.458720-06	-6.3385	0.415910-06	-6.3810	0.90667D 00	-0.0425
25	NA2S04	0.	0.488820-04	0.343510-09	-9.4641	0.344180-09	-9.4632	0.10020D 01	0.0008
26	H2C03	0.	0.953040 01	0.153780-03	-3.8131	0.154100-03	-3.8122	0.10021D 01	0.0009
27	HCL	0.	0.803930-13	0.220530-17	-17.6565	0.220970-17	-17.6557	0.10020D 01	0.0008
28	NACL	0.	0.211080-04	0.362280-09	-9.4410	0.362990-09	-9.4401	0.10020D 01	0.0008
29	KCL	0.	0.859040-04	0.115330-08	-8.9380	0.115560-08	-8.9372	0.10020D 01	0.0008
30	H2S04	0.	0.380440-14	0.387970-19	-19.4112	0.388730-19	-19.4103	0.10020D 01	0.0008

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT
23	CALCITE	0.844D-08	0.379D-08	-8.1909	-8.4203	0.169D 01	0.22942
24	ARAGONIT	0.844D-08	0.609D-08	-8.1909	-8.2150	0.105D 01	0.02407
25	MAGNESIT	0.226D-08	0.575D-08	-8.6413	-8.2400	0.396D 00	-0.40133
26	DOLOMITE	0.147D-16	0.100D-16	-16.8323	-17.0000	0.147D 01	0.16774
28	GYPSUM	0.779D-06	0.174D-04	-6.1084	-4.7590	0.447D-01	-1.34944

TABLE 4 PROGRAM LISTING

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C     PROGRAM MIX2                                                          AA  10
C     WRITTEN BY L.N. PLUMMER, D. PARKHURST, AND D.R. KOSIUR.               AA  20
C     COMPLETED SEPTEMBER 1975.                                             AA  30
C                                                                           AA  40
C     *** DESCRIPTION OF INPUT ***                                          AA  50
C                                                                           AA  60
C     CARD 1  IOPT1,IOPT2,IOPT3,IOPT4,IOPT5,IOPT6,IOPT8,IOPT9,IOPT10,       AA  70
C             NMIX,V0,CLOSE,HCLOSE,STPSIZ  (9I1,I5,4D10.3)                  AA  80
C       IOPT1  = 0 PRINTS THERMOCHEMICAL DATA, = 1 OMITS PRINT OF           AA  90
C                OF THERMOCHEMICAL DATA.                                    AA 100
C       IOPT2  = 0 PRINTS CONVERGENENCE ITERATIONS ON CHLORIDE, = 1 TO      AA 110
C                OMIT PRINT.                                                AA 120
C       IOPT3  = 0 PRINTS CONVERGENCE ITERATIONS ON PH, = 1 TO OMIT PRT.    AA 130
C       IOPT4  = 0 IF SOLUTION 1 IS TO BE MIXED WITH SOLUTION 2 IN A        AA 140
C                FIXED VOLUME SYSTEM.  = 1 IF SOLUTION 2 IS TO BE           AA 150
C                TITRATED INTO SOLUTION 1, V0 MUST BE SPECIFIED, =2 IF      AA 160
C                ANY NET STOICHIOMETRIC REACTION IS TO BE ADDED TO OR       AA 170
C                REMOVED FROM SOLUTION.                                     AA 180
C       IOPT5  = 0 PRINTS SUMMARY OF TITRATION PH CURVE (IF IOPT4=1).       AA 190
C                = 1 OMITS SUMMARY OF PH TITRATION CURVE.                   AA 200
C       IOPT6  = 0 ROOTS ARE FOUND BY SCANNING,LINEAR, AND PARABOLIC        AA 210
C                APPROXIMATION.                                             AA 220
C              = 1 ROOTS ARE FOUND BY SCANNING AND INTERVAL HALVING.        AA 230
C                NOTE THAT IOPT6=0 IS SIGNIFICANTLY FASTER THAN IOPT6=1.    AA 240
C       IOPT8  = 0 IF NO PHASE BOUNDARY IS TO BE FOLLOWED.  = 1 IF ONE      AA 250
C                PHASE BOUNDARY IS TO BE FOLLOWED.                          AA 260
C       IOPT9  = 0, PHASE BOUNDARY WILL BE FOLLOWED AT ALL TIMES (OPEN      AA 270
C                SYSTEM OR HCH), PROVIDED IOPT8=1.  =1, PHASE BOUNDARY      AA 280
C                WILL BE FOLLOWED IF SOLUTION SUPERSATURATES WITH           AA 290
C                SPECIFIED PHASE (PHAS(I),KPHAS), PROVIDED IOPT8=1.         AA 300
C                THUS, IF IOPT9=0, THE SPECIFIED MINERAL WILL EITHER        AA 310
C                DISSOLVE OR PRECIPITATE IN MAINTAINING EQUILIBRIUM.  IFAA 320
C                EQUAL TO 1, THE MINERAL WILL PRECIPITATE ONLY IN           AA 330
C                MAINTAINING SI=KPHAS.                                      AA 340
C       IOPT10 = 0 PRINTS CONVERGENCE ITERATIONS ON PHASE BOUNDARY          AA 350
C                SEARCH (IF IOPT8=1).  =1 OMITS PRINT.                      AA 360
C       NMIX   = TOTAL NUMBER OF MIXTURES TO BE MADE OR TOTAL NUMBER OF     AA 370
C                TITRATION ADDITIONS (OF DEFINED SOLN. 1 AND SOLN. 2),      AA 380
C                OR TOTAL NUMBER OF ADDITIONS OR REMOVALS OF A NET          AA 390
C                STOICHIOMETRIC REACTION IF IOPT4=2.                        AA 400
C       V0     = INITIAL VOLUME OF SYSTEM IF IOPT4 = 1, OTHERWISE LEAVE     AA 410
C                V0 BLANK.  IF IOPT4=1, V0 MUST BE GREATER THAN ZERO ANDAA 420
C                HAVE THE SAME UNITS AS XMIX(I).                            AA 430
C       CLOSE  = ABSOLUTE VALUE OF SI DESIRED IN FOLLOWING PHASE            AA 440
C                BOUNDARY.  REASONABLE VALUE IS 0.001.  LEAVE BLANK IF      AA 450
C                IOPT8 NE. 1.                                               AA 460
C       HCLOSE = FACTOR THAT IS MULTIPLIED TIMES THE ELECTRICAL BALANCE     AA 470
C                TO DETERMINE THE CLOSURE ON MASS BALANCE.  1.0D-08 IS      AA 480
C                 REASONABLE.  IF THE ELECTRICAL BALANCE IS 1.0D-04,        AA 490
C                 CONVERGENCE ON MASS BALANCE WOULD BE TO 1.0D-12 FOR       AA 500
C                 HCOLSE OF 1.0D-08.  ALL INITIAL SOLUTIONS CONVERGE TO     AA 510
C                 1.0D-15 REGARDLESS OF THE VALUE OF HCLOSE.  LARGER        AA 520
C                 VALUES OF HCLOSE DECREASE THE TIME FOR CONVERGENCE ON     AA 530
C                 MASS BALANCE, AND INCREASE THE ERROR ON SPECIATION.       AA 540
C       STPSIZ = FACTOR THAT IS MULTIPLIED TIMES THE TOTAL LIMITING         AA 550
C                CONCENTRATION OF SPECIES IN THE PHASE-BOUNDARY MINERAL     AA 560
C                INORDER TO DETERMINE THE STEP SIZE IN SEARCHING FOR THEAA 570
C                PHASE BOUNDARY.  STPSIZ MUST BE GREATER THAN 0.0 AND       AA 580
C                LESS THAN 1.0.  VALUES OF 0.5 TO 0.9 ARE REASONABLE.       AA 590
C                LARGER VALUES OF STPSIZ USUALLY INCREASE THE SPEED OF      AA 600
C                CONVERGENCE ON SATURATION.                                 AA 610
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C     CARD 2  COEF(I),I=1,7     (8D10.3)                                  AA  620
C       COEF(I)= STOICHIOMETRIC COEFFICIENTS OF THE NET REACTION          AA  630
C                BEING ADDED TO OR REMOVED FROM SOLUTION.  OMIT CARD 2    AA  640
C                IF IOPT4 NE. 2.  ORDER IS CA,MG,NA,K,CL,SO4,CO3.         AA  650
C     CARD 3  (PHAS(I),I=1,7),KPHAS     (8D10.3)                         AA  660
C       PHAS(I)= STOICHIOMETRIC COEFFICIENTS OF THE MINERAL FOR           AA  670
C                WHICH THE PHASE BOUNDARY IS TO BE FOLLOWED.  ORDER IS    AA  680
C                CA,MG,NA,K,CL,SO4,CO3.  OMIT CARD 3 IF IOPT8 NE.1        AA  690
C       KPHAS  = THE LOG OF THE EQUILIBRIUM CONSTANT FOR THE MINERAL      AA  700
C                PHAS(1), WRITTEN IN TERMS OF MINERAL = IONS, WHERE       AA  710
C                IONS ARE CA++,MG++,NA+,K+,CL-,SO4--, AND CO3--.          AA  720
C     CARD 4  XMIX(I) I=1,NMIX      (8D10.3)                            AA  730
C       XMIX(I)= PERCENT OF SOLUTION 2 TO BE MIXED WITH SOLUTION 1, IF    AA  740
C                IOPT4=0.  IF IOPT4=1, XMIX IS THE VOLUME OF SOLUTION 2   AA  750
C                (SAME UNITS AS V0) TO BE ADDED TO SOLUTION 1. IF IOPT4   AA  760
C                =2, XMIX IS THE TOTAL NUMBER OF MOLES OF THE NET         AA  770
C                REACTION (COEF(I)) TO BE ADDED TO THE SOLUTION, FOR      AA  780
C                EACH DESIRED POINT ALONG THE PROPOSED REACTION PATH.     AA  790
C                XMIX(I) IS NEGATIVE IF THE REACTION IS TO BE REMOVED.    AA  800
C                NMIX VALUES OF XMIX(I) ARE READ.  IF NMIX IS ZERO, OMITAA  810
C                CARD 4.                                                  AA  820
C     CARD 5  TITLE     (20A4)                                            AA  830
C     CARD 6  TEMP,PH,DENS,FLAG,IHOLD,IOPT7,CUNITS(5).                    AA  840
C             (3D10.3,1X,3I1,1X,D12.5)                                    AA  850
C       TEMP    = TEMPERATURE IN DEGREES C.  THE TEMPERATURE OF MIXTURES  AA  860
C                 IS ESTIMATED LINEARLY FROM THE END MEMBER TEMPERATURES  AA  870
C                 AND ALL CONSTANTS AND THERMODYNAMIC DATA ARE RECOMPUTEDAA  880
C                 IF TEMP OF SOLN 1.NE.TEMP OF SOLN 2.                    AA  890
C       PH      = NEGATIVE LOG ACTIVITY H+.                               AA  900
C       DENS    = DENSITY OF SOLUTION (G/CC)                              AA  910
C       FLAG    = SIGNAL FOR UNITS OF INPUT CONCENTRATION.  1=MEQ/L,      AA  920
C                 2=MG/L, 3=PPM, 4=MOLALITY.                              AA  930
C       IHOLD   = SIGNAL USED TO HOLD A PREVIOUS ENDMEMBER SOLUTION       AA  940
C                 CONSTANT ON SUCCESSIVE MIXING OR TITRATING CASES.       AA  950
C                 IHOLD MUST BE ZERO FOR THE FIRST 2 ENDMEMBER SOLUTIONS  AA  960
C                 INPUT.  ON ADDITIONAL MIXING CASES, IHOLD MAY BE 0,1,ORAA  970
C                 2.  IF IHOLD=0, 2 NEW ENDMEMBER SOLUTIONS ARE READ IN.  AA  980
C                 IF IHOLD=1, THE PREVIOUS DEFINED SOLUTION 1 IS SAVED    AA  990
C                 AND SOLUTION 2 IS REDEFINED BY INPUT.  THE OPPOSITE IS  AA 1000
C                 TRUE IF IHOLD=2.                                        AA 1010
C       IOPT7   = 0 IF CHLORIDE OR POTASSIUM ARE TO BE ADDED TO THE       AA 1020
C                  INITIAL SOLUTION FOR CHARGE BALANCE.  = 1 IF THE PH    AA 1030
C                  OF THE INITIAL SOLUTION IS TO BE ADJUSTED FOR CHARGE   AA 1040
C                  BALANCE.                                               AA 1050
C       CUNITS(5)  = TOTAL CONCENTRATION OF CHLORIDE IN SOLUTION.         AA 1060
C     CARD 7  CUNITS(1), CUNITS(2), CUNITS(3), CUNITS(4), CUNITS(6),      AA 1070
C             CUNITS(7)   (6D12.5)   TOTAL CONCENTRATIONS OF CA,MG,NA,    AA 1080
C             K,SO4,AND CO2 (IN ORDER) IN INITIAL SOLUTION.               AA 1090
C     CARD 8  BLANK CARD                                                  AA 1100
C     CARD 9 - 12 REPEAT CARDS 5 - 8 FOR SOLUTION 2,IF IOPT4=0 OR 1.      AA 1110
C                                                                         AA 1120
C      FOR ADDITIONAL CASES, REPEAT CARDS 1-12 IF IHOLD=0, OR 1-8 IF      AA 1130
C      IHOLD = 1 OR 2.                                                    AA 1140
C     ... OPTIONAL INPUT ...       (A4,1X,5(I3,D12.5))                   AA 1150
C     ADDITIONAL INPUT IS OPTIONAL AND APPEARS BETWEEN CARDS 7 AND 8 ANDAA 1160
C     (IF IHOLD=0) CARDS 11 AND 12.                                       AA 1170
C     THE CONCENTRATIONS OF INDIVIDUAL IONS AND ION PAIRS CAN BE INPUT    AA 1180
C     ON OPTIONAL CONC CARDS.  THESE VALUES ARE SUMMED WITH THE PREVIOUSAA 1190
C     READ CUNITS(1)-CUNITS(7) VALUES.  THIS PRECEDURE IS USEFUL          AA 1200
C     PARTICULARLY FOR THE CARBONATE SPECIES.                             AA 1210
C     THERMODYNAMIC DATA IN THE PROGRAM MAY BE CHANGED ON APPROPRIATE     AA 1220
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C     OPTION CARDS.  DELH CARDS ARE USED TO CHANGE DELTA H OF REACTION.  AA 1230
C     TABL CARDS CAN CHANGE LOG K OF REACTION AT 25 DEGREES C, AND LOGK  AA 1240
C     CARDS CAN CHANGE TEMPERATURE CORRECTED LOG K VALUES.  SEE THE      AA 1250
C     WRITEUP FOR INFORMATION ON OPTIONAL INPUT.                         AA 1260
C     IF OPTIONAL THERMODYNAMIC DATA ARE INPUT FOR SOLUTION 1, THE SAME  AA 1270
C     OPTIONAL DATA MUST BE READ FOR SOLUTION 2.                         AA 1280
C     THE LAST CARD IN THE DATA STREAM FOR EACH SOLUTION DEFINED MUST    AA 1290
C     BE BLANK, WHETHER OPTION CARDS ARE USED OR NOT.                    AA 1300
C                                                                        AA 1310
      IMPLICIT REAL*8(A-H,O-Z)                                           AA 1320
      INTEGER D,E,DD,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),SIG3,SIAA 1330
     1G4,SIG5,SIG6,RBIT                                                  AA 1340
      DOUBLE PRECISION K1(30),LOGKT(30),LOGKTO(30),LH20,MUHALF,MU,KW,KPHAA 1350
     1AS,M1(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)            AA 1360
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100), X4AA 1370
     1(8)                                                                AA 1380
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLM1(30),XLAA 1390
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH20,MU,MUHALF,KW,CLTOT,PH,ELECTAA 1400
     2,M1,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,AA 1410
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH20,AA 1420
     4C1,C1SAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSEAA 1430
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,1HOLD,IOPT1,IAA 1440
     6OPT2,IOPT3,NSTEP,IMIX,RBIT,N1,ICHECK,IDAT,IOPT7,1TEMP,ISIG(9),ITERAA 1450
      IDAT=0                                                             AA 1460
      D=30                                                               AA 1470
      E=30                                                               AA 1480
      DD=D+1                                                             AA 1490
   10 CONTINUE                                                           AA 1500
      READ (5,660,END=600) IOPT1,IOPT2,IOPT3,IOPT4,IOPT5,IOPT6,IOPT8,IOPAA 1510
     1T9,IOPT10,NMIX,V0,CLOSE,HCLOSE,STPSIZ                              AA 1520
      STPSAV=STPSIZ                                                      AA 1530
      ITEMP=0                                                            AA 1540
      NSTEP=0                                                            AA 1550
      IPH=0                                                              AA 1560
      IMIX=0                                                             AA 1570
      NNMIX=NMIX                                                         AA 1580
      IF (IOPT4.EQ.2) GO TO 20                                           AA 1590
      GO TO 30                                                           AA 1600
   20 CONTINUE                                                           AA 1610
      READ 670, (COEF(I),I=1,7)                                          AA 1620
   30 CONTINUE                                                           AA 1630
      IF (IOPT8.EQ.1) GO TO 40                                           AA 1640
      GO TO 50                                                           AA 1650
   40 CONTINUE                                                           AA 1660
      READ 670, (PHAS(I),I=1,7),KPHAS                                    AA 1670
   50 CONTINUE                                                           AA 1680
      IF (NMIX.EQ.0) GO TO 60                                            AA 1690
      READ 670, (XMIX(I),I=1,NMIX)                                       AA 1700
   60 CONTINUE                                                           AA 1710
      CALL PREP                                                          AA 1720
      CALL SET                                                           AA 1730
      CALL SET1(SIG1,SIG2,SIG3)                                          AA 1740
      CALL SET1(SIG4,SIG5,SIG6)                                          AA 1750
      XMOL=0D0                                                           AA 1760
      ILOOK=0                                                            AA 1770
      IPASS=0                                                            AA 1780
      IPHAS=0                                                            AA 1790
      DO 70 I=1,9                                                        AA 1800
      ISIG(I)=0                                                          AA 1810
   70 CONTINUE                                                           AA 1820
   80 CONTINUE                                                           AA 1830
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C     BEGIN MASS BALANCE LOOP                                                  AA 1840
      CALL MODEL                                                               AA 1850
      IF (N1.LE.4) ICHECK=1                                                    AA 1860
      IF (N1.GT.80) GO TO 90                                                   AA 1870
      IF (ITER.EQ.50) GO TO 110                                                AA 1880
      IF (ICHECK.EQ.1) GO TO 80                                                AA 1890
   90 ITER=ITER+1                                                              AA 1900
      DO 100 I=1,9                                                             AA 1910
      ISIG(I)=0                                                                AA 1920
  100 CONTINUE                                                                 AA 1930
      IF (NSTEP.NE.0) GO TO 220                                                AA 1940
      IF (NSTEP.EQ.0.AND.IPASS.EQ.1) GO TO 220                                 AA 1950
C     BEGIN CHARGE BALANCE LOOP ON INITIAL SOLUTION.                           AA 1960
      IF (ELECT.GT.0.0D0.AND.ITER.EQ.1) IBALNC=0                               AA 1970
      IF (ELECT.LT.0.0D0.AND.ITER.EQ.1) IBALNC=1                               AA 1980
      IF (IOPT2.EQ.1) GO TO 120                                                AA 1990
  110 PRINT 690, ITER,TEST1,TEST2,TEST3,ELECT,N1                               AA 2000
      IF (ITER.GE.50) GO TO 590                                                AA 2010
  120 CONTINUE                                                                 AA 2020
      IF (DABS(ELECT).LT.1.D-15) GO TO 290                                     AA 2030
      IF (IOPT7.EQ.1) GO TO 150                                                AA 2040
      IF (SIG1.EQ.0.AND.SIG2.EQ.0) XINT=DABS(ELECT)                            AA 2050
      IF (IBALNC.EQ.1) GO TO 180                                               AA 2060
      IF (IOPT6.EQ.1) GO TO 130                                                AA 2070
      IF (SIG3.GE.1) GO TO 140                                                 AA 2080
  130 CONTINUE                                                                 AA 2090
      CALL ZERO(CLTOT,ELECT,XINT,SIG1,SIG2,SIG3,IOPT6,0,P1,P2,SAVP,E1,E2AA 2100
     1)                                                                        AA 2110
      GO TO 210                                                                AA 2120
  140 CALL PARBOL(SIG3,P1,E1,P2,E2,PMID,EMID,CLTOT,ELECT)                      AA 2130
      GO TO 210                                                                AA 2140
  150 CONTINUE                                                                 AA 2150
      IF (SIG1.EQ.0.AND.SIG2.EQ.0) XINT=0.5D0                                  AA 2160
      IF (IOPT6.EQ.1) GO TO 160                                                AA 2170
      IF (SIG3.GE.1) GO TO 170                                                 AA 2180
  160 CONTINUE                                                                 AA 2190
      CALL ZERO(PH,ELECT,XINT,SIG1,SIG2,SIG3,IOPT6,0,P1,P2,SAVP,E1,E2)         AA 2200
      GO TO 210                                                                AA 2210
  170 CALL PARBOL(SIG3,P1,E1,P2,E2,PMID,EMID,PH,ELECT)                         AA 2220
      GO TO 210                                                                AA 2230
  180 CONTINUE                                                                 AA 2240
      IF (IOPT6.EQ.1) GO TO 190                                                AA 2250
      IF (SIG3.GE.1) GO TO 200                                                 AA 2260
  190 CONTINUE                                                                 AA 2270
      CALL ZERO(KTOT,ELECT,XINT,SIG1,SIG2,SIG3,IOPT6,1,P1,P2,SAVP,E1,E2)AA 2280
      GO TO 210                                                                AA 2290
  200 CALL PARBOL(SIG3,P1,E1,P2,E2,PMID,EMID,KTOT,ELECT)                       AA 2300
  210 CONTINUE                                                                 AA 2310
      ISAV=ITER                                                                AA 2320
      CALL SET                                                                 AA 2330
      ITER=ISAV                                                                AA 2340
      GO TO 80                                                                 AA 2350
  220 CONTINUE                                                                 AA 2360
C     FIND PH FOLLOWING REACTION PROGRESS.                                     AA 2370
      ELECT=0.D0                                                               AA 2380
      DO 230 I=1,D                                                             AA 2390
      ELECT=ELECT+Z(I)*MI(I)                                                   AA 2400
  230 CONTINUE                                                                 AA 2410
      IPH=IPH+1                                                                AA 2420
      IF (IPH.GE.50) GO TO 600                                                 AA 2430
      IF (ILOOK.EQ.1.OR.IPASS.EQ.1) GO TO 240                                  AA 2440
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      IF (IOPT3.EQ.0) PRINT 700, NSTEP,IPH,PH,ELECT,TEST1,TEST2,TEST3,N1AA 2450
      GO TO 250                                                         AA 2460
  240 IF (IOPT10.EQ.0) PRINT 620, IPH,PH,ELECT,TEST1,TEST2,TEST3,N1     AA 2470
  250 CONTINUE                                                          AA 2480
      IF (DABS(ELECT).LT.1.D-15) GO TO 290                              AA 2490
      XINT=0.2D0                                                        AA 2500
      IF (IPH.GE.2.AND.SIG3.EQ.0) XINT=1.D0                             AA 2510
      IF (IPASS.EQ.1) XINT=1.D0                                         AA 2520
      IF (IPASS.EQ.1.AND.SIG6.GE.2) XINT=0.2D0                          AA 2530
      SAVPH=PH                                                          AA 2540
      IF (IOPT6.EQ.1) GO TO 260                                         AA 2550
      IF (SIG3.GE.1) GO TO 270                                          AA 2560
  260 CONTINUE                                                          AA 2570
      CALL ZERO(PH,ELECT,XINT,SIG1,SIG2,SIG3,IOPT6,0,P1,P2,SAVP,E1,E2)  AA 2580
      GO TO 280                                                         AA 2590
  270 CALL PARBOL(SIG3,P1,E1,P2,E2,PMID,EMID,PH,ELECT)                  AA 2600
  280 CONTINUE                                                          AA 2610
      IF (DABS(SAVPH-PH).LE.2.0D-04) GO TO 290                          AA 2620
      CALL SET                                                          AA 2630
      GO TO 80                                                          AA 2640
  290 CONTINUE                                                          AA 2650
      ITER=0                                                            AA 2660
      IPH=0                                                             AA 2670
C     END OF MASS AND CHARGE BALANCE LOOPS.                             AA 2680
      IF (IPASS.EQ.1.OR.ILOOK.EQ.1) GO TO 320                           AA 2690
      IF (NSTEP.NE.0) DUM1(NSTEP)=PH                                    AA 2700
      CALL PRINT                                                        AA 2710
      IF (IHOLD.EQ.2.OR.IMIX.EQ.1) GO TO 300                            AA 2720
      IF (IHOLD.EQ.1.OR.IMIX.EQ.2) GO TO 310                            AA 2730
      GO TO 320                                                         AA 2740
  300 CALL SAVE(X1,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)          AA 2750
      PHSAVE=PH                                                         AA 2760
      GO TO 320                                                         AA 2770
  310 CALL SAVE(X2,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)          AA 2780
      IF (DABS(T1-T2).GT.0.001D0) ITEMP=1                               AA 2790
  320 CONTINUE                                                          AA 2800
      IF (IOPT8.EQ.1) GO TO 330                                         AA 2810
      GO TO 500                                                         AA 2820
  330 CONTINUE                                                          AA 2830
      IF (NSTEP.EQ.0.AND.NMIX.NE.0) GO TO 500                           AA 2840
C     BEGIN PHASE BOUNDARY SEARCH.                                      AA 2850
      IF (IPHAS.EQ.0) GO TO 340                                         AA 2860
      GO TO 350                                                         AA 2870
  340 CONTINUE                                                          AA 2880
      IF (IOPT10.EQ.0) PRINT 630                                        AA 2890
      CALL SET1(SIG4,SIG5,SIG6)                                         AA 2900
      CALL SAVE(X3,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)          AA 2910
  350 CONTINUE                                                          AA 2920
      ITER=0                                                            AA 2930
      N1=0                                                              AA 2940
      SUM=0D0                                                           AA 2950
      ILOOK=0                                                           AA 2960
      DO 360 I=1,6                                                      AA 2970
      VALU(I)=0.D0                                                      AA 2980
      IF (ALFA(I).GT.0.D0) VALU(I)=PHAS(I)*DLOG10(ALFA(I))              AA 2990
      IF (PHAS(I).NE.0.0D0.AND.ALFA(I).LE.0.0D0) ILOOK=1                AA 3000
      SUM=SUM+VALU(I)                                                   AA 3010
  360 CONTINUE                                                          AA 3020
      VALU(7)=0.D0                                                      AA 3030
      IF (ALFA(8).GT.0.D0) VALU(7)=PHAS(7)*DLOG10(ALFA(8))              AA 3040
      IF (PHAS(7).NE.0.0D0.AND.ALFA(7).LE.0.0D0) ILOOK=1                AA 3050
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      SUM=SUM+VALU(7)                                                   AA 3060
      IF (SUM.EQ.0.0D0.OR.ILOOK.EQ.1) SUM=-1.0D1+KPHAS                  AA 3070
      SI=SUM-KPHAS                                                      AA 3080
      CALL SAVE(X4,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)          AA 3090
      IF (DABS(SI).LT.CLOSE) GO TO 460                                  AA 3100
      IF (IPHAS.GT.0) GO TO 370                                         AA 3110
      IF (SI.LT.0.0D0.AND.IOPT9.EQ.1) GO TO 500                         AA 3120
  370 CONTINUE                                                          AA 3130
      IF (ILOOK.EQ.1) GO TO 430                                         AA 3140
      IF (SIG6.EQ.5) GO TO 380                                          AA 3150
      GO TO 390                                                         AA 3160
  380 CONTINUE                                                          AA 3170
      IF (SI1*SIMID.LT.0.0D0) XMOL=(XMOL1+XMID)/2.0D0                   AA 3180
      IF (SI2*SIMID.LT.0.0D0) XMOL=(XMOL2+XMID)/2.0D0                   AA 3190
      PRESTP=STPSIZ                                                     AA 3200
      STPSIZ=STPSIZ/3.0D0                                               AA 3210
      PRINT 610, PRESTP,STPSIZ                                          AA 3220
      CALL SET1(SIG4,SIG5,SIG6)                                         AA 3230
  390 CONTINUE                                                          AA 3240
      IF (SIG6.GT.0) GO TO 410                                          AA 3250
      DO 400 I=1,7                                                      AA 3260
      XNT(I)=100.D0                                                     AA 3270
      IF (PHAS(I).GT.0.D0) XNT(I)=X4(I)/PHAS(I)                         AA 3280
  400 CONTINUE                                                          AA 3290
      SIZE=DMIN1(XNT(1),XNT(2),XNT(3),XNT(4),XNT(5),XNT(6),XNT(7))      AA 3300
      SIZE=SIZE*STPSIZ                                                  AA 3310
  410 CONTINUE                                                          AA 3320
      IF (IOPT6.EQ.1) GO TO 420                                         AA 3330
      IF (SIG6.GE.1) GO TO 440                                          AA 3340
  420 CONTINUE                                                          AA 3350
      CALL ZERO(XMOL,SI,SIZE,SIG4,SIG5,SIG6,IOPT6,1,XMOL1,XMOL2,SAVML,SIAA 3360
     11,SI2)                                                            AA 3370
      IPASS=1                                                           AA 3380
      CALL STEP(CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,X3,X2,XMIX,NSAA 3390
     1TEP,2,V0,T1,T2,TEMP,PHAS,XMOL,IOPT8,IPASS)                        AA 3400
      GO TO 450                                                         AA 3410
  430 CONTINUE                                                          AA 3420
      XMOL=1.0D-03                                                      AA 3430
      IPASS=1                                                           AA 3440
      CALL STEP(CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,X3,X2,XMIX,NSAA 3450
     1TEP,2,V0,T1,T2,TEMP,PHAS,XMOL,IOPT8,IPASS)                        AA 3460
      IPASS=0                                                           AA 3470
      GO TO 450                                                         AA 3480
  440 CONTINUE                                                          AA 3490
      CALL PARBOL(SIG6,XMOL1,SI1,XMOL2,SI2,XMID,SIMID,XMOL,SI)          AA 3500
      IF (XMOL.LT.XMOL1.OR.XMOL.GT.XMOL2) GO TO 380                     AA 3510
      CALL STEP(CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,X3,X2,XMIX,NSAA 3520
     1TEP,2,V0,T1,T2,TEMP,PHAS,XMOL,IOPT8,IPASS)                        AA 3530
  450 CONTINUE                                                          AA 3540
      NSTEP=NSTEP-1                                                     AA 3550
      IPHAS=IPHAS+1                                                     AA 3560
      IF (IOPT10.EQ.0) PRINT 640, IPHAS,XMOL,SI,PH                      AA 3570
      IF (IPHAS.GT.30) PRINT 810                                        AA 3580
      IF (IPHAS.GT.30) GO TO 470                                        AA 3590
      IPH=0                                                             AA 3600
      CALL SET                                                          AA 3610
      CALL SET1(SIG1,SIG2,SIG3)                                         AA 3620
      GO TO 80                                                          AA 3630
  460 PRINT 650                                                         AA 3640
  470 PRINT 800, XMOL,(PHAS(I),I=1,7)                                   AA 3650
      CALL SET1(SIG1,SIG2,SIG3)                                         AA 3660
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      ITER=0                                                                AA 3670
      N1=0                                                                  AA 3680
      IPASS=0                                                               AA 3690
C     END OF PHASE BOUNDARY LOOP.                                           AA 3700
      DO 480 I=1,7                                                          AA 3710
      GRAMS(I)=MI(I)*GFW(I)                                                 AA 3720
      XLMI(I)=0D0                                                           AA 3730
      IF (MI(I).GT.0D0) XLMI(I)=DLOG10(MI(I))                               AA 3740
  480 CONTINUE                                                              AA 3750
      PRINT 770                                                             AA 3760
      CALL SAVE(X3,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)              AA 3770
      DO 490 I=1,7                                                          AA 3780
      PRINT 780, NTOT(I),Z(I),X3(I),XLMI(I),GRAMS(I)                        AA 3790
  490 CONTINUE                                                              AA 3800
      CALL PRINT                                                            AA 3810
  500 CONTINUE                                                              AA 3820
      STPSIZ=STPSAV                                                         AA 3830
      IPHAS=0                                                               AA 3840
      IHOLD=0                                                               AA 3850
      IF (IOPT4.EQ.2.AND.IMIX.EQ.1) IMIX=0                                  AA 3860
      IF (IOPT4.EQ.2) GO TO 530                                             AA 3870
      IF (IMIX.EQ.1.AND.NMIX.GT.0) GO TO 60                                 AA 3880
      IF (IMIX.EQ.2) IMIX=0                                                 AA 3890
      IF (NSTEP.EQ.NMIX.AND.IOPT4.EQ.1) GO TO 510                           AA 3900
      GO TO 530                                                             AA 3910
  510 CONTINUE                                                              AA 3920
      IF (IOPT4.EQ.0.OR.IOPT5.EQ.1) GO TO 10                                AA 3930
      PRINT 710, V0                                                         AA 3940
      VDUM=0.0D0                                                            AA 3950
      PRINT 720, VDUM,PHSAVE                                                AA 3960
      DO 520 I=1,NNMIX                                                      AA 3970
      PRINT 720, AMIX(I),DUM1(I)                                            AA 3980
  520 CONTINUE                                                              AA 3990
      GO TO 10                                                              AA 4000
  530 CONTINUE                                                              AA 4010
      IF (NSTEP.EQ.NMIX) GO TO 10                                           AA 4020
C     COMPUTE MASS COMPOSITION FOR DESIRED REACTION PROGRESS.               AA 4030
      CALL STEP(CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,X1,X2,XMIX,NSAA 4040
     1TEP,IOPT4,V0,T1,T2,TEMP,COEF,XMOL,IOPT8,0)                            AA 4050
      XMOL=0.0D0                                                            AA 4060
      IF (ITEMP.EQ.1.AND.IOPT4.NE.2) GO TO 540                              AA 4070
      GO TO 550                                                             AA 4080
  540 CALL PREP                                                             AA 4090
  550 CONTINUE                                                              AA 4100
      AMIX=1.D2-XMIX(NSTEP)                                                 AA 4110
      PRINT 680                                                             AA 4120
      IF (IOPT4.EQ.0) PRINT 740, NSTEP,AMIX,XMIX(NSTEP)                     AA 4130
      IF (IOPT4.EQ.1) PRINT 750, NSTEP,V0,XMIX(NSTEP)                       AA 4140
      IF (IOPT4.EQ.2) PRINT 790                                             AA 4150
      IF (IOPT4.EQ.2) PRINT 800, XMIX(NSTEP),(COEF(I),I=1,7)                AA 4160
      IF (NSTEP.EQ.1) PH=PHSAVE                                             AA 4170
      CALL SET1(SIG1,SIG2,SIG3)                                             AA 4180
      CALL SET                                                              AA 4190
      EPMCAT=(NATOT+KTOT+2.D0*(CATOT+MGTOT))*1D3                            AA 4200
      EPMAN=(CLTOT+CO2TOT+2.D0*SO4TOT)*1D3                                  AA 4210
      DO 560 I=1,7                                                          AA 4220
      GRAMS(I)=MI(I)*GFW(I)                                                 AA 4230
      XLMI(I)=0D0                                                           AA 4240
      IF (MI(I).GT.0D0) XLMI(I)=DLOG10(MI(I))                               AA 4250
  560 CONTINUE                                                              AA 4260
      CALL SAVE(X3,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)              AA 4270
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      PRINT 770                                                          AA 4280
      DO 570 I=1,7                                                       AA 4290
      PRINT 780, NTOT(I),Z(I),X3(I),XLMI(I),GRAMS(I)                     AA 4300
  570 CONTINUE                                                           AA 4310
      IF (IOPT3.EQ.1) GO TO 580                                          AA 4320
      PRINT 730                                                          AA 4330
  580 CONTINUE                                                           AA 4340
      IF (IOPT3.EQ.1) PRINT 680                                          AA 4350
      IPASS=0                                                            AA 4360
C     RETURN TO MASS AND CHARGE BALANCE LOOPS                            AA 4370
      GO TO 80                                                           AA 4380
  590 PRINT 760, N1,ITER                                                 AA 4390
  600 CONTINUE                                                           AA 4400
C     END OF PROGRAM                                                     AA 4410
      STOP                                                               AA 4420
C                                                                        AA 4430
C                                                                        AA 4440
  610 FORMAT (//,10X,'***** THE PRESENT VALUE OF STPSIZ (',F5.2,') IS TOAA 4450
     1O LARGE.  A VALUE OF ',F5.2,' IS NOW BEING USED. *****',//)        AA 4460
  620 FORMAT (48X,I2,2A,F6.3,4(2X,D10.3),3X,I3)                          AA 4470
  630 FORMAT (///,7X,'---CONVERGENCE ON PHASE BOUNDARY---',23X,'---CONVEAA 4480
     1RGENCE ON MASS AND PH---',/,5X,'ITER',4X,'MOLES',9X,'SI',10X,'PH',AA 4490
     27X,'IPH',3X,'PH',7X,'ELECT',5X,'S1-CO2TOT',3X,'S2-SO4TOT',3X,'S3-CAA 4500
     3LTOT',2X,'N MODEL')                                                AA 4510
  640 FORMAT (5X,I3,3(2A,D10.3))                                         AA 4520
  650 FORMAT (/,1H1,10X,'THE PHASE BOUNDARY HAS BEEN FOUND')             AA 4530
  660 FORMAT (911,I5,4D10.3)                                             AA 4540
  670 FORMAT (8D10.3)                                                    AA 4550
  680 FORMAT (//)                                                        AA 4560
  690 FORMAT (1H ,23X,I3,5X,3(E13.6,3X),3X,E23.16,1X,I4)                 AA 4570
  700 FORMAT (20X,I4,2X,I4,2X,F10.6,2X,E13.6,3X,3(E13.6,2X),1X,I4)       AA 4580
  710 FORMAT ('1'//10X,'TITRATION OF SOLUTION 1 BY SOLUTION 2'//10X,'INIAA 4590
     1TIAL VOLUME = ',F7.3,' ML'//15X,'V(ML)    PH'//)                   AA 4600
  720 FORMAT (15X,F7.3,4X,F7.3)                                          AA 4610
  730 FORMAT (//,45X,'--- CONVERGENCE ITERATIONS ---',//,21X,'NSTEP',2X,AA 4620
     1'IPH',5X,'PH',4X,'ELECTRICAL BALANCE  S1-CO2TOT',5X,'S2-SO4TOT',7XAA 4630
     2,'S3-CLTOT',5X,'N MODEL',/)                                        AA 4640
  740 FORMAT (///,5X,'********** MIXTURE NUMBER ',I3,' CONTAINING ',F5.2AA 4650
     1,' PERCENT OF SOLUTION 1 AND ',F5.2,' PERCENT OF SOLUTION 2 ******AA 4660
     2****',///)                                                         AA 4670
  750 FORMAT (//10X,'********** MIXTURE NUMBER ',I3,' CONTAINING ',F7.3,AA 4680
     1' ML OF SOLN 1 AND ',F7.3,' ML OF SOLN 2 **********',//)           AA 4690
  760 FORMAT (10X,'N1 = ',I4,5X,'ITER = ',I4,' CALCULATION TERMINATED',/AA 4700
     1)                                                                  AA 4710
  770 FORMAT (40X,'--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---',//,50XAA 4720
     1,'TOTAL',13X,'LOG TOTAL',12X,'TOTAL',/,33X,'SPECIES',8X,'MOLALITY'AA 4730
     2,12X,'MOLALITY',9X,'GRAMS/KGM H2O',/,33X,'--------',8X,'--------',1AA 4740
     32X,'---------',9X,'------------',/)                                AA 4750
  780 FORMAT (1H ,32X,A8,F3.0,3X,E13.6,8X,F9.4,8X,E13.6)                 AA 4760
  790 FORMAT (1H1)                                                       AA 4770
  800 FORMAT (2X,D12.5,' MOLES OF CA(',F5.3,')MG(',F5.3,')NA(',F5.3,')K(AA 4780
     1',F5.3,')CL(',F5.3,')SO4(',F5.3,')CO3(',F5.3,') HAVE BEEN ADDED TOAA 4790
     2 SOLUTION NO. 1',/)                                                AA 4800
  810 FORMAT (//,10X,'UNABLE TO FIND THE PHASE BOUNDARY IN 30 ITERATIONSAA 4810
     1, CALCULATION TERMINATED',/)                                       AA 4820
      END                                                                AA 4830-
      SUBROUTINE PREP                                                    BB   10
      IMPLICIT REAL*8(A-H,O-Z)                                           BB   20
      INTEGER SIGN(2),IDH(30),IKTO(30),IKT(30),RBIT                      BB   30
      INTEGER D,E,DD,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),WORD,CABB   40
     1RD(5),INT(5)                                                       BB   50
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      DOUBLE PRECISION KT(30),LOGKT(30),LOGKTO(30),LH2O,MUHALF,MU,KW,KPHBB   60
     1AS,MI(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)             BB   70
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100), VABB   80
     1L(5)                                                                BB   90
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLMI(30),XLBB  100
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH2O,MU,MUHALF,KW,CLTOT,PH,ELECTBB  110
     2,MI,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,BB  120
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH2O,BB  130
     4C1,C1SAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSEBB  140
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,IHOLD,IOPT1,IBB  150
     6OPT2,IOPT3,NSTEP,IMIX,KBIT,N1,ICHECK,IDAT,IOPT7,ITEMP,ISIG(9),ITERBB  160
      DATA CARD/'CONC','DELH','TABL','LOGK','    '/                      BB  170
      DATA SIGN/' ','*'/                                                 BB  180
      IF (NSTEP.NE.0) GO TO 170                                          BB  190
      C=2.302585092D0                                                    BB  200
      R=1.987190D-03                                                     BB  210
      ISTAR=0                                                            BB  220
      IPRT=0                                                             BB  230
      DO 10 I=1,E                                                        BB  240
      IDH(I)=SIGN(1)                                                     BB  250
      IKTO(I)=SIGN(1)                                                    BB  260
      IKT(I)=SIGN(1)                                                     BB  270
   10 CONTINUE                                                           BB  280
C     READ SOLUTION DATA                                                 BB  290
      READ 360, TITL                                                     BB  300
      IMIX=IMIX+1                                                        BB  310
      DO 20 I=1,D                                                        BB  320
      CUNITS(I)=0D0                                                      BB  330
      ALFA(I)=0D0                                                        BB  340
      MI(I)=0D0                                                          BB  350
      XLMI(I)=0D0                                                        BB  360
   20 CONTINUE                                                           BB  370
      READ 370, TEMP,PH,DENS,FLAG,IHOLD,IOPT7,CUNITS(7)                  BB  380
      READ 380, CUNITS(1),CUNITS(2),CUNITS(3),CUNITS(4),CUNITS(5),CUNITSBB  390
     1(6)                                                                BB  400
C     READ OPTIONAL CONCENTRATION INPUT                                  BB  410
   30 READ 390, WORD,(INT(I),VAL(I),I=1,5)                               BB  420
      IF (WORD.EQ.CARD(5).OR.WORD.NE.CARD(1)) GO TO 50                   BB  430
      DO 40 I=1,5                                                        BB  440
      IF (INT(I).EQ.0) GO TO 40                                          BB  450
      CUNITS(INT(I))=VAL(I)                                              BB  460
   40 CONTINUE                                                           BB  470
      GO TO 30                                                           BB  480
   50 CONTINUE                                                           BB  490
      IF (IHOLD.EQ.1) JHOLD=2                                            BB  500
      IF (IHOLD.EQ.2) JHOLD=1                                            BB  510
      IF (IHOLD.NE.0) IPRT=1                                             BB  520
      IF (IHOLD.NE.0) IMIX=2                                             BB  530
C     CONVERT CONCENTRATION UNITS TO MOLALITY                            BB  540
      IF (FLAG.NE.1) GO TO 70                                            BB  550
      DO 60 I=1,D                                                        BB  560
      IF (Z(I).LT.0D0) Z1=-1.D0*Z(I)                                     BB  570
      IF (Z(I).EQ.0D0) Z1=1.D0                                           BB  580
      IF (Z(I).GT.0D0) Z1=Z(I)                                           BB  590
      CUNITS(I)=CUNITS(I)*GFW(I)/Z1                                      BB  600
   60 CONTINUE                                                           BB  610
      FLAG=2                                                             BB  620
   70 CONTINUE                                                           BB  630
      IF (FLAG.NE.2) GO TO 90                                            BB  640
      DO 80 I=1,D                                                        BB  650
      CUNITS(I)=CUNITS(I)/DENS                                           BB  660
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   80 CONTINUE                                                          BB  670
      FLAG=3                                                            BB  680
   90 CONTINUE                                                          BB  690
      IF (FLAG.NE.3) GO TO 120                                          BB  700
      C1=0D0                                                            BB  710
      DO 100 I=1,D                                                      BB  720
      C1=C1+CUNITS(I)                                                   BB  730
  100 CONTINUE                                                          BB  740
      DO 110 I=1,D                                                      BB  750
      C1SAVE=C1                                                         BB  760
      MI(I)=(CUNITS(I)/(1.0D+03*GFW(I)))*(1D0/(1D0-1.0D-06*C1))         BB  770
      IF (MI(I).GT.0D0) XLMI(I)=DLOG10(MI(I))                           BB  780
      GRAMS(I)=MI(I)*GFW(I)                                             BB  790
  110 CONTINUE                                                          BB  800
      GO TO 140                                                         BB  810
  120 CONTINUE                                                          BB  820
      C1=0D0                                                            BB  830
      IF (FLAG.NE.4) GO TO 280                                          BB  840
      DO 130 I=1,D                                                      BB  850
      MI(I)=CUNITS(I)                                                   BB  860
      C1=C1+MI(I)*GFW(I)*1D3/DENS                                       BB  870
      IF (MI(I).GT.0D0) XLMI(I)=DLOG10(MI(I))                           BB  880
      GRAMS(I)=MI(I)*GFW(I)                                             BB  890
  130 CONTINUE                                                          BB  900
      C1SAVE=C1                                                         BB  910
  140 CONTINUE                                                          BB  920
      EPMCAT=0D0                                                        BB  930
      EPMAN=0D0                                                         BB  940
      DO 160 I=1,D                                                      BB  950
      IF (Z(I).GT.0D0) GO TO 150                                        BB  960
      EPMAN=EPMAN-Z(I)*MI(I)                                            BB  970
      GO TO 160                                                         BB  980
  150 EPMCAT=EPMCAT+Z(I)*MI(I)                                          BB  990
  160 CONTINUE                                                          BB 1000
      EPMAN=EPMAN*1D3                                                   BB 1010
      EPMCAT=EPMCAT*1D3                                                 BB 1020
C     COMPUTE TEMPERATURE DEPENDENCE OF DEBYE-HUCKEL CONSTANTS          BB 1030
  170 T=TEMP+273.16D0                                                   BB 1040
      IF (IMIX.EQ.1.AND.NSTEP.EQ.0) T1=TEMP                             BB 1050
      IF (IMIX.EQ.2.AND.NSTEP.EQ.0) T2=TEMP                             BB 1060
      S1=374.11D0-TEMP                                                  BB 1070
      S2=S1**0.33333D0                                                  BB 1080
      S3=DSQRT((1D0+0.1342489D0*S2-3.946263D-03*S1)/(3.1975D0-.3151548D0BB 1090
     1*S2-1.203374D-3*S1+7.48908D-13*S1**4D0))                          BB 1100
      IF (T.LT.373.16D0) GO TO 180                                      BB 1110
      C1=5321D0/T+233.76D0-T*(T*(8.292D-7*T-1.417D-3)+.9297D0)          BB 1120
      GO TO 190                                                         BB 1130
  180 C1=87.74D0-TEMP*(TEMP*(1.41D-6*TEMP-9.398D-4)+.4008D0)            BB 1140
  190 CONTINUE                                                          BB 1150
      C1=DSQRT(C1*T)                                                    BB 1160
      A=18246.0D02*S3/C1**3D0                                           BB 1170
      B=50.29D0*S3/C1                                                   BB 1180
      IF (NSTEP.NE.0) GO TO 240                                         BB 1190
C     SET TOTAL MOLALITIES OF INPUT SPECIES                             BB 1200
      CO2TOT=MI(7)+MI(26)+MI(8)+MI(10)+MI(11)+MI(14)+MI(15)+MI(17)+MI(18BB 1210
     1)+MI(21)                                                          BB 1220
      CATOT=MI(1)+MI(13)+MI(14)+MI(15)                                  BB 1230
      MGTOT=MI(2)+MI(10)+MI(11)+MI(12)                                  BB 1240
      NATOT=MI(3)+MI(17)+MI(18)+MI(19)+2.D0*MI(21)+2.D0*MI(25)+MI(28)   BB 1250
      KTOT=MI(4)+MI(20)+MI(29)                                          BB 1260
      CLTOT=MI(5)+MI(27)+MI(28)+MI(29)                                  BB 1270
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      SO4TOT=MI(6)+MI(12)+MI(16)+MI(19)+MI(20)+MI(22)+MI(25)+MI(30)      BB 1280
      CALL SAVE(X3,CATOT,MGTOT,NATOT,KTOT,CLTOT,SO4TOT,CO2TOT)          BB 1290
C     SET OPTIONAL DELTA H OF REACTION DATA                             BB 1300
  200 IF (WORD.EQ.CARD(5).OR.WORD.NE.CARD(2)) GO TO 220                 BB 1310
      DO 210 I=1,5                                                      BB 1320
      IF (INT(I).EQ.0) GO TO 210                                        BB 1330
      DH(INT(I))=VAL(I)                                                 BB 1340
      IDH(INT(I))=SIGN(2)                                               BB 1350
      ISTAK=1                                                           BB 1360
  210 CONTINUE                                                          BB 1370
      READ 390, WORD,(INT(I),VAL(I),I=1,5)                              BB 1380
      GO TO 200                                                         BB 1390
C     SET OPTIONAL LOG K (25 DEG) DATA                                  BB 1400
  220 IF (WORD.EQ.CARD(5).OR.WORD.NE.CARD(3)) GO TO 240                 BB 1410
      DO 230 I=1,5                                                      BB 1420
      IF (INT(I).EQ.0) GO TO 230                                        BB 1430
      LOGKTO(INT(I))=VAL(I)                                             BB 1440
      IKTO(INT(I))=SIGN(2)                                              BB 1450
      ISTAK=1                                                           BB 1460
  230 CONTINUE                                                          BB 1470
      READ 390, WORD,(INT(I),VAL(I),I=1,5)                              BB 1480
      GO TO 220                                                         BB 1490
  240 CONTINUE                                                          BB 1500
C     VANT HOFF EQUATION FOR EFFECT OF T ON K                           BB 1510
      C1=(298.16D0-T)/(298.16D0*T*C*R)                                  BB 1520
      DO 250 I=1,E                                                      BB 1530
      LOGKT(I)=LOGKTO(I)-DH(I)*C1                                       BB 1540
      LCHEK(I)=0                                                        BB 1550
      IF (LOGKT(I).LT.-200D0.OR.LOGKT(I).GT.200D0) LCHEK(I)=1           BB 1560
      IF (LCHEK(I).EQ.1) GO TO 250                                      BB 1570
      KT(I)=1D1**LOGKT(I)                                               BB 1580
  250 CONTINUE                                                          BB 1590
C     ANALYTICAL EXPRESSIONS FOR EFFECT OF T ON K                       BB 1600
      C1=DLOG10(T)                                                      BB 1610
      KT(1)=1D1**(6.498D0-0.02379D0*T-2902.39/T)                        BB 1620
      KT(3)=1D1**(.991D0+.00667D0*T)                                    BB 1630
      KT(4)=1D1**(2.319D0-1.1056D-02*T+2.29812D-05*T*T)                 BB 1640
      KT(7)=1D1**(-2.95D0+.0133D0*T)                                    BB 1650
      KT(8)=1D1**(-27.393D0+4114.D0/T+.05617D0*T)                       BB 1660
      KT(13)=1D1**(3.106D0-673.6D0/T)                                   BB 1670
      KT(15)=1D1**(+557.2461D0/T-5.3505D0+0.0183412D0*T)                BB 1680
      KW=KT(17)                                                         BB 1690
      KT(18)=1D1**(14.8435D0-.032786D0*T-3404.72D0/T)                   BB 1700
      KT(23)=1D1**(13.87D0-3059.0D0/T-0.04035D0*T)                      BB 1710
      LOGKT(1)=DLOG10(KT(1))                                            BB 1720
      LOGKT(3)=DLOG10(KT(3))                                            BB 1730
      LOGKT(4)=DLOG10(KT(4))                                            BB 1740
      LOGKT(7)=DLOG10(KT(7))                                            BB 1750
      LOGKT(8)=DLOG10(KT(8))                                            BB 1760
      LOGKT(13)=DLOG10(KT(13))                                          BB 1770
      LOGKT(15)=DLOG10(KT(15))                                          BB 1780
      LOGKT(18)=DLOG10(KT(18))                                          BB 1790
      LOGKT(23)=DLOG10(KT(23))                                          BB 1800
      IF (NSTEP.NE.0) GO TO 350                                         BB 1810
C     INPUT OPTIONAL TEMPERATURE CORRECTED K DATA                       BB 1820
  260 IF (WORD.EQ.CARD(5)) GO TO 300                                    BB 1830
      IF (WORD.NE.CARD(4)) GO TO 290                                    BB 1840
      DO 270 I=1,5                                                      BB 1850
      IF (INT(I).EQ.0) GO TO 270                                        BB 1860
      LOGKT(INT(I))=VAL(I)                                              BB 1870
      KT(INT(I))=1D1**LOGKT(INT(I))                                     BB 1880
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      IKT(INT(I))=SIGN(2)                                                    BB 1890
      ISTAR=1                                                                BB 1900
  270 CONTINUE                                                               BB 1910
      READ 390, WORD,(INT(I),VAL(I),I=1,5)                                   BB 1920
      GO TO 260                                                              BB 1930
  280 PRINT 450                                                              BB 1940
  290 PRINT 460, WORD                                                        BB 1950
      READ 390, WORD,(INT(I),VAL(I),I=1,5)                                   BB 1960
      IF (WORD.EQ.CARD(5)) GO TO 300                                         BB 1970
      GO TO 290                                                              BB 1980
  300 CONTINUE                                                               BB 1990
C     PRINT THERMODYNAMIC DATA AND COMPOSITION OF INPUT SOLUTION             BB 2000
      IF (IDAT.EQ.1.OR.IOPT1.EQ.1) GO TO 330                                 BB 2010
      PRINT 470                                                              BB 2020
      DO 310 I=1,D                                                           BB 2030
      PRINT 480, I,NREACT(I),DH(I),IDH(I),LOGKTO(I),IKTO(I),LOGKT(I),IKTBB 2040
     1(I),I,NSPEC(I),Z(I),DHA(I),GFW(I)                                      BB 2050
  310 CONTINUE                                                               BB 2060
      IF (DD.GT.E) GO TO 330                                                 BB 2070
      DO 320 I=DD,E                                                          BB 2080
      PRINT 490, I,NREACT(I),DH(I),IDH(I),LOGKTO(I),IKTO(I),LOGKT(I),IKTBB 2090
     1(I)                                                                    BB 2100
  320 CONTINUE                                                               BB 2110
  330 CONTINUE                                                               BB 2120
      IF (ISTAR.EQ.1.AND.IOPT1.EQ.0.AND.IDAT.EQ.0) PRINT 500, SIGN(2)        BB 2130
      IDAT=1                                                                 BB 2140
      PRINT 510, TITL                                                        BB 2150
      PRINT 530                                                              BB 2160
      IF (IPRT.EQ.0) PRINT 400, IMIX                                         BB 2170
      IF (IPRT.EQ.1) PRINT 400, JHOLD                                        BB 2180
      IF (IPRT.EQ.1) PRINT 410, IHOLD,JHOLD                                  BB 2190
      PRINT 420, TEMP,PH,EPMCAT,EPMAN                                        BB 2200
      PRINT 430                                                              BB 2210
      DO 340 K=1,7                                                           BB 2220
      PRINT 520, NTOT(K),Z(K),X3(K),XLMI(K),GRAMS(K)                         BB 2230
  340 CONTINUE                                                               BB 2240
      PRINT 530                                                              BB 2250
      IF (IOPT2.EQ.1) GO TO 350                                              BB 2260
      PRINT 530                                                              BB 2270
      PRINT 440                                                              BB 2280
  350 CONTINUE                                                               BB 2290
      RETURN                                                                 BB 2300
C                                                                            BB 2310
C                                                                            BB 2320
C                                                                            BB 2330
  360 FORMAT (20A4)                                                          BB 2340
  370 FORMAT (3D10.3,1X,3I1,1X,D12.5)                                        BB 2350
  380 FORMAT (6D12.5)                                                        BB 2360
  390 FORMAT (A4,1X,5(I3,D12.5))                                             BB 2370
  400 FORMAT (//5X,'********** SOLUTION NUMBER ',I1,' **********'//)        BB 2380
  410 FORMAT (//,5X,'SOLUTION NUMBER',I2,' IS BEING HELD CONSTANT AND SOBB 2390
     1LUTION NUMBER',I2,' IS BEING CHANGED',//)                              BB 2400
  420 FORMAT (15X,'TEMPERATURE = ',F6.2,' DEGREES C     PH = ',F6.3,'     BB 2410
     1ANALYTICAL EPMCAT = ',F7.1,'     ANALYTICAL EPMAN = ',F7.1,//)        BB 2420
  430 FORMAT (40X,'--- TOTAL CONCENTRATIONS OF INPUT SPECIES ---',//,50XBB 2430
     1,'TOTAL',13X,'LOG TOTAL',12X,'TOTAL',/,33X,'SPECIES',8X,'MOLALITY'BB 2440
     2,12X,'MOLALITY',9X,'GRAMS/KGM H2O',/,33X,'---------',8X,'--------',1BB 2450
     32X,'---------',9X,'------------',/)                                    BB 2460
  440 FORMAT (45X,'--- CONVERGENCE ITERATIONS ---',//,20X,'ITERATION',5XBB 2470
     1,'S1-CO2TOT',6X,'S2-SO4TOT',8X,'S3-CLTOT',11X,'ELECTRICAL BALANCE'BB 2480
     2,4X,'N MODEL',/)                                                       BB 2490
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  450 FORMAT (10X,'CONCENTRATION UNITS UNKNOWN, CHECK FLAG.')                BB 2500
  460 FORMAT (5X,/,'----WARNING---- INPUT ERROR -- OPTION WORD = ',A4,/)BB 2510
  470 FORMAT ('1',//,54X,'----',/,54X,'DATA',/,54X,'----',//,18X,'I',2X,BB 2520
     1'NREACT',9X,'DH',8X,'LOGKTO',6X,'LOGKT',14X,'I',2X,'NSPEC',6X,'Z',BB 2530
     23X,'DHA',6X,'GFW'/)                                                  BB 2540
  480 FORMAT (1H ,15X,I3,2X,A8,3(1X,F10.4,A1),10X,I3,2X,A8,2X,F3.0,2X,F3BB 2550
     1.1,2X,F10.4)                                                         BB 2560
  490 FORMAT (1H ,15X,I3,2X,A8,3(1X,F10.4,A1))                             BB 2570
  500 FORMAT (/,15X,A1,' DENOTES VALUES CHANGED IN INPUT',/)               BB 2580
  510 FORMAT (1H1,(5X,20A4)/)                                              BB 2590
  520 FORMAT (1H ,32X,A8,F3.0,3X,E13.6,6X,F9.4,8X,E13.6)                   BB 2600
  530 FORMAT (//)                                                          BB 2610
      END                                                                  BB 2620-
      SUBROUTINE MODEL                                                     CC   10
      IMPLICIT REAL*8(A-H,O-Z)                                             CC   20
      INTEGER D,E,DD,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),SIG3      CC   30
      INTEGER RBIT,LCO2(9),LSO4(7)                                         CC   40
      DOUBLE PRECISION KT(30),LOGKT(30),LOGKTO(30),LH2O,MUHALF,MU,KW,KPHCC   50
     1AS,MI(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)              CC   60
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100)       CC   70
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLMI(30),XLCC   80
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH2O,MU,MUHALF,KW,CLTOT,PH,ELECTCC   90
     2,MI,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,CC  100
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH2O,CC  110
     4C1,C1SAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSECC  120
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,IHOLD,IOPT1,ICC  130
     6OPT2,IOPT3,NSTEP,IMIX,RBIT,N1,ICHECK,IDAT,IOPT7,ITEMP,ISIG(9),ITERCC  140
      DATA LCO2/20,7,10,11,14,15,17,18,21/                                 CC  150
      DATA LSO4/12,16,19,20,22,25,30/                                      CC  160
C     ACTIVITY OF WATER                                                    CC  170
      C1=0D0                                                               CC  180
      DO 10 I=1,D                                                          CC  190
      C1=C1+MI(I)                                                          CC  200
   10 CONTINUE                                                             CC  210
      AH2O=1D0-1.7D-2*C1                                                   CC  220
      LH2O=DLOG10(AH2O)                                                    CC  230
C     COMPUTE IONIC STRENGTH                                               CC  240
      MU=0D0                                                               CC  250
      DO 20 I=1,D                                                          CC  260
      MU=MU+0.500*MI(I)*Z(I)*Z(I)                                          CC  270
   20 CONTINUE                                                             CC  280
      IF (MU.LT.0.000) MU=0.0D0                                            CC  290
      MUHALF=DSQRT(MU)                                                     CC  300
C     COMPUTE INDIVIDUAL ION ACTIVITY COEFFICIENTS                         CC  310
      C1=-A*4D0*MUHALF                                                     CC  320
      GAMMA(1)=1D1**(C1/(1D0+B*5D0*MUHALF)+0.165D0*MU)                     CC  330
      GAMMA(2)=1D1**(C1/(1D0+B*5.5D0*MUHALF)+0.2D0*MU)                     CC  340
      GAMMA(3)=1D1**(-A*MUHALF/(1D0+B*4D0*MUHALF)+0.075D0*MU)              CC  350
      GAMMA(4)=1D1**(-A*MUHALF/(1D0+B*3.5D0*MUHALF)+0.015D0*MU)            CC  360
      GAMMA(5)=GAMMA(4)                                                    CC  370
      GAMMA(6)=1D1**(C1/(1D0+B*5D0*MUHALF)-0.04D0*MU)                      CC  380
      DO 40 I=7,D                                                          CC  390
      IF (Z(I).EQ.0D0) GO TO 30                                            CC  400
      GAMMA(I)=1D1**(-A*MUHALF*Z(I)*Z(1)/(1D0+DHA(I)*B*MUHALF))            CC  410
      GO TO 40                                                             CC  420
   30 GAMMA(I)=1D1**(0.1D0*MU)                                             CC  430
   40 CONTINUE                                                             CC  440
      GAMMA(26)=1D1**(MU*(170.01/T-.8798+.0013935*T)+MU*MU*(28.81/T-.210CC  450
     18+.0003641*T))                                                       CC  460
C     COMPUTE MOLALITIES AND ACTIVITIES OF IONS IN SOLUTION                CC  470
      DO 50 I=5,8                                                          CC  480
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      ALFA(I)=MI(I)*GAMMA(I)                                                CC  490
   50 CONTINUE                                                              CC  500
      ALFA(24)=AH2O*KW*TENPH                                                CC  510
      MI(24)=ALFA(24)/GAMMA(24)                                             CC  520
      MI(23)=1D0/(TENPH*GAMMA(23))                                          CC  530
C     MAGNESIUM SPECIES                                                     CC  540
      MI(9)=ALFA(24)*KT(2)/GAMMA(9)                                         CC  550
      MI(10)=ALFA(8)*KT(3)/GAMMA(10)                                        CC  560
      MI(11)=ALFA(7)*KT(4)/GAMMA(11)                                        CC  570
      MI(12)=ALFA(6)*KT(5)/GAMMA(12)                                        CC  580
      MI(2)=MGTOT/(1D0+GAMMA(2)*(MI(9)+MI(10)+MI(11)+MI(12)))               CC  590
      ALFA(2)=MI(2)*GAMMA(2)                                                CC  600
      C1=ALFA(2)                                                            CC  610
      DO 60 I=9,12                                                          CC  620
      MI(I)=C1*MI(I)                                                        CC  630
      ALFA(I)=MI(I)*GAMMA(I)                                                CC  640
   60 CONTINUE                                                              CC  650
C     CALCIUM SPECIES                                                       CC  660
      MI(13)=ALFA(24)*KT(6)/GAMMA(13)                                       CC  670
      MI(14)=ALFA(7)*KT(7)/GAMMA(14)                                        CC  680
      MI(15)=ALFA(8)*KT(8)/GAMMA(15)                                        CC  690
      MI(16)=ALFA(6)*KT(9)/GAMMA(16)                                        CC  700
      MI(1)=CATOT/(1D0+GAMMA(1)*(MI(13)+MI(14)+MI(15)+MI(16)))              CC  710
      C1=MI(1)*GAMMA(1)                                                     CC  720
      ALFA(1)=C1                                                            CC  730
      DO 70 I=13,16                                                         CC  740
      MI(I)=C1*MI(I)                                                        CC  750
      ALFA(I)=MI(I)*GAMMA(I)                                                CC  760
   70 CONTINUE                                                              CC  770
C     SODIUM SPECIES                                                        CC  780
      MI(17)=ALFA(8)*KT(10)/GAMMA(17)                                       CC  790
      MI(18)=ALFA(7)*KT(11)/GAMMA(18)                                       CC  800
      MI(19)=ALFA(6)*KT(12)/GAMMA(19)                                       CC  810
      MI(21)=MI(3)*GAMMA(3)*ALFA(8)*KT(14)/GAMMA(21)                        CC  820
      MI(25)=MI(3)*GAMMA(3)*ALFA(6)*KT(16)/GAMMA(25)                        CC  830
      MI(28)=ALFA(5)*KT(20)/GAMMA(28)                                       CC  840
      MI(3)=NATOT/(1D0+GAMMA(3)*(MI(17)+MI(18)+MI(19)+MI(28)+2D0*(MI(21)CC  850
     1+MI(25))))                                                            CC  860
      ALFA(3)=MI(3)*GAMMA(3)                                                CC  870
      C1=ALFA(3)                                                            CC  880
      DO 80 I=1,6                                                           CC  890
      K=LIST1(I)                                                            CC  900
      MI(K)=C1*MI(K)                                                        CC  910
      ALFA(K)=MI(K)*GAMMA(K)                                                CC  920
   80 CONTINUE                                                              CC  930
C     POTASSIUM SPECIES                                                     CC  940
      MI(20)=ALFA(6)*KT(13)/GAMMA(20)                                       CC  950
      MI(29)=ALFA(5)*KT(21)/GAMMA(29)                                       CC  960
      MI(4)=KTOT/(1D0+GAMMA(4)*(MI(20)+MI(29)))                             CC  970
      ALFA(4)=MI(4)*GAMMA(4)                                                CC  980
      C1=ALFA(4)                                                            CC  990
      MI(20)=C1*MI(20)                                                      CC 1000
      ALFA(20)=MI(20)*GAMMA(20)                                             CC 1010
      MI(29)=C1*MI(29)                                                      CC 1020
      ALFA(29)=MI(29)*GAMMA(29)                                             CC 1030
C     COMPUTED MASS OF ANION SPECIES                                        CC 1040
      S1=MI(7)+MI(8)+MI(10)+MI(11)+MI(14)+MI(15)+MI(17)+MI(18)+MI(21)+MICC 1050
     1(26)                                                                  CC 1060
      S2=MI(6)+MI(12)+MI(16)+MI(19)+MI(20)+MI(22)+MI(25)+MI(30)             CC 1070
      S3=MI(5)+MI(27)+MI(28)+MI(29)                                         CC 1080
      TEST1=S1-CO2TOT                                                       CC 1090
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      TEST2=S2-SO4TOT                                                    CC 1100
      TEST3=S3-CLTOT                                                     CC 1110
      ELECT=0D0                                                          CC 1120
      DO 90 I=1,D                                                        CC 1130
      ELECT=ELECT+MI(I)*Z(I)                                             CC 1140
   90 CONTINUE                                                           CC 1150
      XDUM=HCLOSE*DABS(ELECT)                                            CC 1160
      XDUM1=1.D-15                                                       CC 1170
      HCHEK=DMAX1(XDUM,XDUM1)                                            CC 1180
      ICHECK=0                                                           CC 1190
      RBIT=0                                                             CC 1200
C     CHECK MASS BALANCE ON CARBON.                                      CC 1210
      IF (CO2TOT.LE.0.0D0) GO TO 110                                     CC 1220
      IF (DABS(TEST1).GT.HCHEK) RBIT=1                                   CC 1230
      IF (RBIT.EQ.0) GO TO 110                                           CC 1240
      MI(26)=ALFA(23)*ALFA(23)/(GAMMA(26)*KT(18)*KT(1))                  CC 1250
      MI(7)=ALFA(23)/(GAMMA(7)*KT(1))                                    CC 1260
      MI(10)=ALFA(2)*KT(3)/GAMMA(10)                                     CC 1270
      MI(11)=ALFA(2)*ALFA(23)*KT(4)/(GAMMA(11)*KT(1))                    CC 1280
      MI(14)=ALFA(1)*ALFA(23)*KT(7)/(GAMMA(14)*KT(1))                    CC 1290
      MI(15)=ALFA(1)*KT(8)/GAMMA(15)                                     CC 1300
      MI(17)=ALFA(3)*KT(10)/GAMMA(17)                                    CC 1310
      MI(18)=ALFA(3)*ALFA(23)*KT(11)/(GAMMA(18)*KT(1))                   CC 1320
      MI(21)=ALFA(3)*ALFA(3)*KT(14)/GAMMA(21)                            CC 1330
      MI(8)=CO2TOT/(1D0+GAMMA(8)*(MI(26)+MI(7)+MI(10)+MI(11)+MI(14)+MI(1CC 1340
     15)+MI(17)+MI(18)+MI(21)))                                          CC 1350
      ALFA(8)=MI(8)*GAMMA(8)                                             CC 1360
      DO 100 I=1,9                                                       CC 1370
      MI(LCO2(I))=MI(LCO2(I))*ALFA(8)                                    CC 1380
      ALFA(LCO2(I))=MI(LCO2(I))*GAMMA(LCO2(I))                           CC 1390
  100 CONTINUE                                                           CC 1400
      ICHECK=1                                                           CC 1410
      RBIT=0                                                             CC 1420
  110 CONTINUE                                                           CC 1430
C     CHECK MASS BALANCE ON SULFATE.                                     CC 1440
      IF (SO4TOT.LE.0.0D0) GO TO 130                                     CC 1450
      IF (DABS(TEST2).GT.HCHEK) RBIT=1                                   CC 1460
      IF (RBIT.EQ.0) GO TO 130                                           CC 1470
      MI(12)=ALFA(2)*KT(5)/GAMMA(12)                                     CC 1480
      MI(16)=ALFA(1)*KT(9)/GAMMA(16)                                     CC 1490
      MI(19)=ALFA(3)*KT(12)/GAMMA(19)                                    CC 1500
      MI(20)=ALFA(4)*KT(13)/GAMMA(20)                                    CC 1510
      MI(22)=ALFA(23)*KT(15)/GAMMA(22)                                   CC 1520
      MI(25)=ALFA(3)*ALFA(3)*KT(16)/GAMMA(25)                            CC 1530
      MI(30)=ALFA(23)*ALFA(23)*KT(22)/GAMMA(30)                          CC 1540
      MI(6)=SO4TOT/(1D0+GAMMA(6)*(MI(12)+MI(16)+MI(19)+MI(20)+MI(22)+MI(CC 1550
     125)+MI(30)))                                                       CC 1560
      ALFA(6)=MI(6)*GAMMA(6)                                             CC 1570
      DO 120 I=1,7                                                       CC 1580
      MI(LSO4(I))=MI(LSO4(I))*ALFA(6)                                    CC 1590
      ALFA(LSO4(I))=MI(LSO4(I))*GAMMA(LSO4(I))                           CC 1600
  120 CONTINUE                                                           CC 1610
      ICHECK=1                                                           CC 1620
      RBIT=0                                                             CC 1630
  130 CONTINUE                                                           CC 1640
C     CHECK MASS BALANCE ON CHLORIDE.                                    CC 1650
      IF (CLTOT.LE.0.0D0) GO TO 150                                      CC 1660
      IF (DABS(TEST3).GT.HCHEK) RBIT=1                                   CC 1670
      IF (RBIT.EQ.0) GO TO 150                                           CC 1680
      MI(27)=ALFA(23)*KT(19)/GAMMA(27)                                   CC 1690
      MI(28)=ALFA(3)*KT(20)/GAMMA(28)                                    CC 1700
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      MI(29)=ALFA(4)*KT(21)/GAMMA(29)                                    CC 1710
      MI(5)=CLTOT/(1D0+GAMMA(5)*(MI(27)+MI(28)+MI(29)))                  CC 1720
      ALFA(5)=MI(5)*GAMMA(5)                                             CC 1730
      DO 140 I=27,29                                                     CC 1740
      MI(I)=MI(1)*ALFA(5)                                                CC 1750
      ALFA(I)=MI(5)*GAMMA(I)                                             CC 1760
  140 CONTINUE                                                           CC 1770
      ICHECK=1                                                           CC 1780
  150 CONTINUE                                                           CC 1790
      N1=N1+1                                                            CC 1800
      RETURN                                                             CC 1810
      END                                                                CC 1820-
      SUBROUTINE ZERO(PH,ELECT,XINT,SIG1,SIG2,SIG3,IOP5,I,PH1,PH2,SAVPH,DD   10
     1ELECT1,ELECT2)                                                     DD   20
      DOUBLE PRECISION PH,PH1,PH2,SAVPH,ELECT,ELECT1,ELECT2,XINT         DD   30
      INTEGER SIG1,SIG2,SIG3                                             DD   40
      IF (SIG3.GT.0) GO TO 30                                            DD   50
      IF (ELECT.LT.0.0D0) SIG1=1                                         DD   60
      IF (ELECT.GT.0.0D0) SIG2=1                                         DD   70
      IF (ELECT.LT.0.0D0.AND.I.EQ.0) ELECT2=ELECT                        DD   80
      IF (ELECT.LT.0.0D0.AND.I.EQ.1) ELECT1=ELECT                        DD   90
      IF (ELECT.GT.0.0D0.AND.I.EQ.0) ELECT1=ELECT                        DD  100
      IF (ELECT.GT.0.0D0.AND.I.EQ.1) ELECT2=ELECT                        DD  110
      IF (SIG1.EQ.1.AND.SIG2.EQ.1) GO TO 30                              DD  120
      SIG3=0                                                             DD  130
C     SCAN UNTIL ROOT IS CROSSED                                         DD  140
      IF (ELECT.LT.0.0D0.AND.I.EQ.0) GO TO 10                            DD  150
      IF (ELECT.LT.0.0D0.AND.I.EQ.1) GO TO 20                            DD  160
      IF (ELECT.GT.0.0D0.AND.I.EQ.0) GO TO 20                            DD  170
      IF (ELECT.GT.0.0D0.AND.I.EQ.1) GO TO 10                            DD  180
   10 PH2=PH                                                             DD  190
      ELECT2=ELECT                                                       DD  200
      PH=PH2-XINT                                                        DD  210
      PH1=PH                                                             DD  220
      GO TO 100                                                          DD  230
   20 PH1=PH                                                             DD  240
      ELECT1=ELECT                                                       DD  250
      PH=PH1+XINT                                                        DD  260
      PH2=PH                                                             DD  270
      GO TO 100                                                          DD  280
   30 CONTINUE                                                           DD  290
C     LINEAR APPROXIMATION                                               DD  300
      IF (IOP5.NE.0) GO TO 70                                            DD  310
      SIG3=SIG3+1                                                        DD  320
      IF (SIG3.EQ.1) GO TO 60                                            DD  330
      IF (ELECT.LT.0.0D0.AND.I.EQ.0) GO TO 40                            DD  340
      IF (ELECT.GT.0.0D0.AND.I.EQ.1) GO TO 40                            DD  350
      IF (ELECT.GT.0.0D0.AND.I.EQ.0) GO TO 50                            DD  360
      IF (ELECT.LT.0.0D0.AND.I.EQ.1) GO TO 50                            DD  370
      GO TO 100                                                          DD  380
   40 ELECT2=ELECT                                                       DD  390
      PH2=SAVPH                                                          DD  400
      GO TO 60                                                           DD  410
   50 ELECT1=ELECT                                                       DD  420
      PH1=SAVPH                                                          DD  430
   60 PH=PH1-ELECT1*(PH1-PH2)/(ELECT1-ELECT2)                            DD  440
      SAVPH=PH                                                           DD  450
      GO TO 100                                                          DD  460
   70 CONTINUE                                                           DD  470
C     INTERVAL HALVE                                                     DD  480
      IF (ELECT.LT.0.0D0.AND.I.EQ.0) GO TO 80                            DD  490
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      IF (ELECT.GT.0.0D0.AND.I.EQ.1) GO TO 80                          DD  500
      IF (ELECT.GT.0.0D0.AND.I.EQ.0) GO TO 90                          DD  510
      IF (ELECT.LT.0.0D0.AND.I.EQ.1) GO TO 90                          DD  520
      GO TO 100                                                        DD  530
   80 CONTINUE                                                         DD  540
      PH2=PH                                                           DD  550
      XINT=(PH2-PH1)/2.0                                               DD  560
      PH=PH2-XINT                                                      DD  570
      GO TO 100                                                        DD  580
   90 CONTINUE                                                         DD  590
      PH1=PH                                                           DD  600
      XINT=(PH2-PH1)/2.0                                               DD  610
      PH=PH1+XINT                                                      DD  620
  100 CONTINUE                                                         DD  630
      RETURN                                                           DD  640
      END                                                              DD  650-
      SUBROUTINE STEP(CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,C1,C2,XEE   10
     1MIX,NSTEP,IOPT4,V0,T1,T2,TEMP,COEF,XMOL,IOPT8,IPASS)             EE   20
      DOUBLE PRECISION CATOT,MGTOT,CO2TOT,SO4TOT,CLTOT,NATOT,KTOT,C1(8),EE   30
     1C2(8),XMIX(100),XX,V0,T1,T2,TEMP,COEF(7),XMOL,VTOT               EE   40
      NSTEP=NSTEP+1                                                    EE   50
      IF (IOPT4.EQ.1) GO TO 10                                         EE   60
      IF (IOPT4.EQ.2) GO TO 20                                         EE   70
      IF (IOPT8.EQ.1.AND.IPASS.EQ.1) GO TO 30                          EE   80
C     COMPUTE COMPOSITION OF MIXTURES                                  EE   90
      XX=XMIX(NSTEP)/10000                                             EE  100
      CATOT=(1D0-XX)*C1(1)+XX*C2(1)                                    EE  110
      MGTOT=(1D0-XX)*C1(2)+XX*C2(2)                                    EE  120
      NATOT=(1D0-XX)*C1(3)+XX*C2(3)                                    EE  130
      KTOT=(1D0-XX)*C1(4)+XX*C2(4)                                     EE  140
      CLTOT=(1D0-XX)*C1(5)+XX*C2(5)                                    EE  150
      SO4TOT=(1D0-XX)*C1(6)+XX*C2(6)                                   EE  160
      CO2TOT=(1D0-XX)*C1(7)+XX*C2(7)                                   EE  170
      TEMP=(1D0-XX)*T1+XX*T2                                           EE  180
      GO TO 40                                                         EE  190
   10 XX=XMIX(NSTEP)                                                   EE  200
C     COMPUTE COMPOSITION OF TITRATED MIXTURES                         EE  210
      VTOT=V0+XX                                                       EE  220
      CATOT=(C1(1)*V0+C2(1)*XX)/VTOT                                   EE  230
      MGTOT=(C1(2)*V0+C2(2)*XX)/VTOT                                   EE  240
      NATOT=(C1(3)*V0+C2(3)*XX)/VTOT                                   EE  250
      KTOT=(C1(4)*V0+C2(4)*XX)/VTOT                                    EE  260
      CLTOT=(C1(5)*V0+C2(5)*XX)/VTOT                                   EE  270
      SO4TOT=(C1(6)*V0+C2(6)*XX)/VTOT                                  EE  280
      CO2TOT=(C1(7)*V0+C2(7)*XX)/VTOT                                  EE  290
      TEMP=(V0*T1+XX*T2)/VTOT                                          EE  300
      GO TO 40                                                         EE  310
   20 CONTINUE                                                         EE  320
      IF (IOPT8.EQ.1.AND.IPASS.EQ.1) GO TO 30                          EE  330
      XMOL=XMIX(NSTEP)                                                 EE  340
   30 CONTINUE                                                         EE  350
      CATOT=C1(1)+XMOL*(COEF(1))                                       EE  360
      MGTOT=C1(2)+XMOL*(COEF(2))                                       EE  370
      NATOT=C1(3)+XMOL*(COEF(3))                                       EE  380
      KTOT=C1(4)+XMOL*(COEF(4))                                        EE  390
      CLTOT=C1(5)+XMOL*(COEF(5))                                       EE  400
      SO4TOT=C1(6)+XMOL*(COEF(6))                                      EE  410
      CO2TOT=C1(7)+XMOL*(COEF(7))                                      EE  420
   40 RETURN                                                           EE  430
      END                                                              EE  440-
      SUBROUTINE PRINT                                                 FF   10
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      IMPLICIT REAL*8(A-H,O-Z)                                          FF   20
      INTEGER O,E,OO,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),SIG3,SIFF   30
     1G4,SIG5,SIG6,RBIT                                                 FF   40
      DOUBLE PRECISION KT(30),LOGKT(30),LOGKTO(30),LH2O,MUHALF,MU,KW,KPHFF   50
     1AS,MI(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)           FF   60
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100)    FF   70
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLMI(30),XLFF   80
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH2O,MU,MUHALF,KW,CLTOT,PH,ELECTFF   90
     2,MI,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,FF  100
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH2O,FF  110
     4C1,C1SAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSEFF  120
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,IHOLD,IOPT1,IFF  130
     6OPT2,IOPT3,NSTEP,IMIX,RBIT,N1,ICHECK,IDAT,IOPT7,ITEMP,ISIG(9),ITERFF  140
      ALK=MI(7)+MI(9)+MI(11)+MI(13)+MI(14)+MI(18)+MI(21)+MI(24)+2.D0*(MIFF  150
     1(10)+MI(15)+MI(17)+MI(8))-MI(23)                                  FF   160
      ALK=ALK*1.D3                                                      FF   170
      CARBON=MI(7)+MI(8)+MI(26)                                         FF   180
      CEPMAN=0D0                                                        FF   190
      CEPMCT=0D0                                                        FF   200
      DO 20 I=1,O                                                       FF   210
      IF (Z(I).GT.0D0) GO TO 10                                         FF   220
      CEPMAN=CEPMAN-Z(I)*MI(I)                                          FF   230
      GO TO 20                                                          FF   240
10    CEPMCT=CEPMCT+Z(I)*MI(I)                                          FF   250
20    CONTINUE                                                          FF   260
      PCO2=0D0                                                          FF   270
      XLPCO2=-99.9                                                      FF   280
      IF (ALFA(26).GT.0D0) GO TO 30                                     FF   290
      GO TO 40                                                          FF   300
30    PCO2=1D1**(DLOG10(ALFA(26))-2385.73D0/T-1.52640-2*T+14.0184D0)    FF   310
      XLPCO2=DLOG10(PCO2)                                               FF   320
40    CONTINUE                                                          FF   330
      CEPMAN=CEPMAN*1D3                                                 FF   340
      CEPMCT=CEPMCT*1D3                                                 FF   350
      IF (NSTEP.NE.0) DENS=1.D0                                         FF   360
      PRINT 130                                                         FF   370
      PRINT 130                                                         FF   380
      PRINT 140, AH2O,EPMCAT,CEPMCT,PH,PCO2,EPMAN,CEPMAN,XLPCO2,MU,CARBOFF   390
     1N,DENS,TEMP,S1,CLTOT,ELECT,KTOT,ALK                               FF   400
      PRINT 150                                                         FF   410
      DUM=1D1**(-70.D0)                                                 FF   420
      DO 60 I=1,O                                                       FF   430
      CUNITS(I)=0D0                                                     FF   440
      IF (MI(I).LT.DUM) GO TO 50                                        FF   450
      CUNITS(I)=MI(I)*1D3*GFW(I)*(1D0-1.0D-06*C1SAVE)                   FF   460
      XLMI(I)=DLOG10(MI(I))                                             FF   470
      XLALFA(I)=DLOG10(ALFA(I))                                         FF   480
      XLGAM(I)=DLOG10(GAMMA(I))                                         FF   490
      GO TO 60                                                          FF   500
50    CUNITS(I)=0D0                                                     FF   510
      XLMI(I)=-200.D0                                                   FF   520
      XLALFA(I)=-200.D0                                                 FF   530
      XLGAM(I)=0D0                                                      FF   540
60    CONTINUE                                                          FF   550
      DO 90 K=1,O                                                       FF   560
      IF (MI(K).LT.DUM) GO TO 70                                        FF   570
      PRINT 160, K,NSPEC(K),Z(K),CUNITS(K),MI(K),XLMI(K),ALFA(K),XLALFA(FF   580
     1K),GAMMA(K),XLGAM(K)                                              FF   590
70    CONTINUE                                                          FF   600
      IF (MI(K).LT.0D0) GO TO 80                                        FF   610
      GO TO 90                                                          FF   620
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   80 PRINT 170, NSPEC(K),MI(K)                                                    FF  630
   90 CONTINUE                                                                     FF  640
      AP(1)=ALFA(1)*ALFA(8)                                                        FF  650
      AP(2)=AP(1)                                                                  FF  660
      AP(3)=ALFA(2)*ALFA(8)                                                        FF  670
      AP(4)=ALFA(1)*ALFA(2)*ALFA(8)*ALFA(8)                                        FF  680
      AP(5)=ALFA(1)*ALFA(6)                                                        FF  690
      PRINT 180                                                                    FF  700
      DO 120 I=1,5                                                                 FF  710
      K=LIST2(I)                                                                   FF  720
      IF (AP(I).LT.1.D-50) GO TO 100                                               FF  730
      XLIAP=DLOG10(AP(I))                                                          FF  740
      SII=AP(I)/KT(K)                                                              FF  750
      XLSI=DLOG10(SII)                                                             FF  760
      GO TO 110                                                                    FF  770
  100 CONTINUE                                                                     FF  780
      XLIAP=-100.D0                                                                FF  790
      SII=1.0D-50                                                                  FF  800
      XLSI=-100.D0                                                                 FF  810
  110 CONTINUE                                                                     FF  820
      PRINT 190, LIST2(I),NREACT(K),AP(I),KT(K),XLIAP,LOGKT(K),SII,XLSI            FF  830
  120 CONTINUE                                                                     FF  840
      RETURN                                                                       FF  850
C                                                                                  FF  860
C                                                                                  FF  870
C                                                                                  FF  880
  130 FORMAT (//)                                                                  FF  890
  140 FORMAT (//,46X,'----DESCRIPTION OF SOLUTION ----',//,27X,'ANALYTICFF  900
     1AL  COMPUTED',13X,'PH',16X,'ACTIVITY H2O = ',F7.4,/,20X,'EPMCAT  'FF  910
     2,F7.2,4X,F7.2,12X,F6.3,14X,'PCO2 = ',E13.6,/,20X,'EPMAN   ',F7.2,4FF  920
     3X,F7.2,32X,'LOG PCO2 = ',F8.4,/,20X,'IONIC STRENGTH = ',E13.6,6X,'FF  930
     4TEMPERATURE',11X,'UNCOMPLEX CO2 = ',E13.6,/,20X,'DENSITY = ',F8.4,FF  940
     518X,F6.2,1X,'DEG C',10X,'CO2TOT = ',E13.6,/,20X,'CLTOT = ',E13.6,3FF  950
     67X,'ELECT = ',E13.6,/,20X,'KTOT = ',E13.6,38X,'ALKALINITY = ',F10.FF  960
     73,' MEQ/LITRE',/)                                                            FF  970
  150 FORMAT (///,52X,'--------------------',/,52X,'DISTRIBUTION OF SFF  980
     1PECIES',/,52X,'--------------------',//,5X,'I',2X,'SPECIES',10XFF  990
     2,'PPM',11X,'MOLALITY',8X,'LOG MOL',6X,'ACTIVITY',8X,'LOG ACT',5X,'FF 1000
     3ACT. COEFF.',5X,'LOG A COF',/)                                               FF 1010
  160 FORMAT (1H ,3X,I3,1X,A8,F3.0,2X,E12.5,4X,E12.5,4X,F9.4,4X,E12.5,4XFF 1020
     1,F9.4,4X,E12.5,4X,F9.4)                                                      FF 1030
  170 FORMAT (' ',10X,'----- WARNING -----  THE CALCULATED MOLALITY OF',FF 1040
     11X,A8,' IS ',E12.5)                                                          FF 1050
  180 FORMAT (//,11X,'PHASE',9X,'IAP',10X,'KT',8X,'LOG IAP',4X,'LOG KT',FF 1060
     16X,'IAP/KT',4X,'LOG IAP/KT',/)                                               FF 1070
  190 FORMAT (1H ,6X,I3,1X,A8,2(2X,E11.4),2(2X,F9.4),2X,E11.4,2X,F10.5)            FF 1080
      END                                                                          FF 1090-
      SUBROUTINE SET                                                               GG   10
      IMPLICIT REAL*8(A-H,O-Z)                                                     GG   20
      INTEGER D,E,DD,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),SIG3,SIGG   30
     1G4,SIG5,SIG6,RBIT                                                            GG   40
      DOUBLE PRECISION KT(30),LOGKT(30),LOGKTO(30),LH2O,MUHALF,MU,KW,KPHGG   50
     1AS,MI(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)                      GG   60
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100)               GG   70
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLMI(30),XLGG   80
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH2O,MU,MUHALF,KW,CLTOT,PH,ELECTGG   90
     2,MI,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,GG  100
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH2O,GG  110
     4C1,C1SAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSEGG  120
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,IHOLD,IOPT1,IGG  130
     6OPT2,IOPT3,NSTEP,IMIX,RBIT,N1,ICHECK,IDAT,IOPT7,ITEMP,ISIG(9),ITERGG  140
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C       INITIALIZE VALUES FOR MASS BALANCE LOOP.                        GG  150
        ALFA(23)=1D1**(-PH)                                             GG  160
        MI(23)=ALFA(23)                                                 GG  170
        TENPH=1D1**PH                                                   GG  180
        MI(1)=CATOT                                                     GG  190
        MI(2)=MGTOT                                                     GG  200
        MI(3)=NATOT                                                     GG  210
        MI(4)=KTOT                                                      GG  220
        MI(5)=CLTOT                                                     GG  230
        MI(6)=SO4TOT                                                    GG  240
        MI(26)=ALFA(23)*ALFA(23)/(KT(18)*KT(1))                         GG  250
        MI(7)=ALFA(23)/KT(1)                                            GG  260
        MI(8)=CO2TOT/(1.0D0+(MI(26)+MI(7)))                             GG  270
        MI(7)=MI(7)*MI(8)                                               GG  280
        MI(26)=MI(26)*MI(8)                                             GG  290
        ITER=0                                                          GG  300
        KBIT=1                                                          GG  310
        N1=0                                                            GG  320
        RETURN                                                          GG  330
        END                                                             GG  340-
        SUBROUTINE SAVE(X,C1,C2,C3,C4,C5,C6,C7)                         HH   10
        DOUBLE PRECISION X(8),C1,C2,C3,C4,C5,C6,C7                      HH   20
C       SAVE TOTAL CONCENTRATIONS.                                      HH   30
        X(1)=C1                                                         HH   40
        X(2)=C2                                                         HH   50
        X(3)=C3                                                         HH   60
        X(4)=C4                                                         HH   70
        X(5)=C5                                                         HH   80
        X(6)=C6                                                         HH   90
        X(7)=C7                                                         HH  100
        RETURN                                                          HH  110
        END                                                             HH  120-
        SUBROUTINE PARBOL(SIG6,XMOL1,SI1,XMOL2,SI2,XMID,SIMID,XMOL,SI)  II   10
        IMPLICIT REAL*8(A-H,O-Z)                                        II   20
        INTEGER SIG6                                                    II   30
        IF (SIG6.GT.1) GO TO 10                                         II   40
C       SIG6=1                                                          II   50
        XMID=XMOL                                                       II   60
        SIMID=SI                                                        II   70
        GO TO 90                                                        II   80
   10 CONTINUE                                                          II   90
C       SIG6 > 1                                                        II  100
        IF (SI.GE.0.0D0) GO TO 50                                       II  110
C       SI<0                                                            II  120
        IF (SIMID.GE.0.0D0) GO TO 20                                    II  130
C       SIMID<0                                                         II  140
        XMOL1=XMID                                                      II  150
        XMID=XMOL                                                       II  160
        SI1=SIMID                                                       II  170
        SIMID=SI                                                        II  180
        GO TO 90                                                        II  190
   20 CONTINUE                                                          II  200
C       SIMID>0                                                         II  210
        IF (SI2*SI1) 30,30,40                                           II  220
   30 SI1=SI                                                            II  230
        XMOL1=XMOL                                                      II  240
        GO TO 90                                                        II  250
   40 SI2=SIMID                                                         II  260
        XMOL2=XMID                                                      II  270
        SIMID=SI                                                        II  280
        XMID=XMOL                                                       II  290
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      GO TO 90                                                          II  300
   50 CONTINUE                                                          II  310
C     SI>0                                                              II  320
      IF (SIMID.GE.0.0D0) GO TO 80                                      II  330
C     SIMID<0                                                           II  340
      IF (SI2+SI1) 60,60,70                                             II  350
   60 SI1=SIMID                                                         II  360
      XMOL1=XMID                                                        II  370
      SIMID=SI                                                          II  380
      XMID=XMOL                                                         II  390
      GO TO 90                                                          II  400
   70 SI2=SI                                                            II  410
      XMOL2=XMOL                                                        II  420
      GO TO 90                                                          II  430
   80 CONTINUE                                                          II  440
C     SIMID>0                                                           II  450
      XMOL2=XMID                                                        II  460
      XMID=XMOL                                                         II  470
      SI2=SIMID                                                         II  480
      SIMID=SI                                                          II  490
   90 CONTINUE                                                          II  500
C     MAKE XMOL A FUNCTION OF SI.                                       II  510
      X1=SI1                                                            II  520
      X2=SI2                                                            II  530
      X3=SIMID                                                          II  540
      Y1=XMOL1                                                          II  550
      Y2=XMOL2                                                          II  560
      Y3=XMID                                                           II  570
      XX1=X1*X1                                                         II  580
      XX2=X2*X2                                                         II  590
      XX3=X3*X3                                                         II  600
      D1=(XX3*X2*Y1+XX1*X3*Y2+XX2*X1*Y3-XX2*X3*Y1-XX3*X1*Y2-XX1*X2*Y3)/(II  610
     1(X1-X2)*(X2-X3)*(X3-X1))                                          II  620
      XMOL=D1                                                           II  630
      SIG6=SIG6+1                                                       II  640
      RETURN                                                            II  650
      END                                                               II  660-
      SUBROUTINE SET1(I,J,K)                                            JJ   10
C     RESET COUNTERS FOR ROOT FINDING PROCEDURES.                       JJ   20
      I=0                                                               JJ   30
      J=0                                                               JJ   40
      K=0                                                               JJ   50
      RETURN                                                            JJ   60
      END                                                               JJ   70-
      BLOCK DATA                                                        KK   10
C     DATA USED IN PROGRAM                                              KK   20
      IMPLICIT REAL*8(A-H,O-Z)                                          KK   30
      INTEGER D,E,DD,LIST1(6),LCHEK(40),FLAG,SIG1,SIG2,LIST2(10),SIG3,SIKK   40
     1G4,SIG5,SIG6,RBIT                                                 KK   50
      DOUBLE PRECISION KT(30),LOGKT(30),LOGKTO(30),LH2O,MUHALF,MU,KW,KPHKK   60
     1AS,MI(30),MGTOT,KTOT,NATOT,NSPEC(30),NREACT(30),NTOT(7)           KK   70
      DIMENSION COEF(7), PHAS(7), VALU(7), XNT(7), AP(30), DUM1(100)    KK   80
      COMMON /A/ GRAMS(30),CUNITS(30),DH(30),DHA(30),GFW(30),XLMI(30),XLKK   90
     1ALFA(30),XLGAM(30),Z(30),KT,LOGKT,LH2O,MU,MUHALF,KW,CLTOT,PH,ELECTKK  100
     2,MI,GAMMA(30),X1(8),X2(8),CATOT,MGTOT,NATOT,KTOT,XMIX(100),CO2TOT,KK  110
     3SO4TOT,S1,S2,S3,TEST1,TEST2,TEST3,LOGKTO,TEMP,DENS,A,B,TENPH,AH2O,KK  120
     4CL,CLSAVE,EPMAN,EPMCAT,CEPMAN,CEPMCT,T,T1,T2,ALFA(30),NSPEC,HCLOSEKK  130
     5,NTOT,X3(8),NREACT,TITL(20),D,E,DD,LIST1,LCHEK,LIST2,IHOLD,IOPT1,IKK  140
     6OPT2,IOPT3,NSTEP,IMIX,RBIT,N1,ICHECK,IDAT,IOPT7,ITEMP,ISIG(9),ITERKK  150
      DATA NSPEC/4HCA++,4HMG++,3HNA+,2HK+,3HCL-,5HSO4--,5HHCO3-,5HCO3--,KK  160
     15HMGOH+,5HMGCO3,7HMGHCO3+,5HMGSO4,5HCAOH+,7HCAHCO3+,5HCACO3,5HCASOKK  170
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24,6HNACO3-,6HNAHCO3,6HNAS04-,5HKS04-,6HNA2C03,5HHS04-,2HH+,3HOH-,6KK  180
3HNA2S04,5HH2C03,3HHCL,4HNACL,3HKCL,5HH2S04/,NREACT/5HKHC03,5HKMGOHKK  190
4,6HKMGC03,7HKMGHC03,6HKMGS04,5HKCAOH,7HKCAHC03,6HKCAC03,6HKCAS04,6KK  200
5HKNAC03,7HKNAHC03,6HKNAS04,5HKKS04,7HKNA2C03,5HKHS04,7HKNA2S04,2HKKK  210
6W,6HKH2C03,4HKHCL,5HKNACL,4HKKCL,6HKH2S04,7HCALCITE,8HARAGONIT,8HMKK  220
7AGNESIT,8HDOLOMITE,8HANHYDRIT,6HGYPSUM,7HBRUCITE,7HHUNTITE/        KK  230
 DATA Z/2.0D0,2.0D0,1.0D0,1.0D0,-1.0D0,-2.0D0,-1.0D0,-2.0D0,1.0D0,0KK  240
1.0D0,1.0D0,0.0D0,1.0D0,1.0D0,0.0D0,0.0D0,-1.0D0,0.0D0,-1.0D0,-1.0DKK  250
20,0.0D0,-1.0D0,1.0D0,-1.0D0,0.0D0,0.0D0,0.0D0,0.0D0,0.0D0,0.0D0/,DKK  260
3HA/5.0D0,5.5D0,4.0D0,3.5D0,3.5D0,5.0D0,5.4D0,5.4D0,6.5D0,0.0D0,4.0KK  270
4D0,0.0D0,0.0D0,6.0D0,0.0D0,0.0D0,5.4D0,0.0D0,5.4D0,5.4D0,0.0D0,4.5KK  280
5D0,9.0D0,3.5D0,0.0D0,0.0D0,0.0D0,0.0D0,0.0D0,0.0D0/,GFW/40.08D0,24KK  290
6.312D0,22.9898D0,39.102D0,35.453D0,96.0616D0,61.0173D0,60.0094D0,4KK  300
71.3194D0,84.3214D0,65.3293D0,120.3736D0,57.0874D0,101.0973D0,100.0KK  310
889D0,136.1416D0,82.9992D0,83.9909D0,119.0514D0,135.1636D0,105.989KK  320
9DD0,97.0696D0,1.008D0,17.0074D0,142.0412D0,62.0253D0,36.461D0,58.4KK  330
$428D0,74.555D0,98.0775D0/                                          KK  340
 DATA DH/3.55D0,2.14D0,0.058D0,10.37D0,1.27D0,1.19D0,6.331D0,3.13D0KK  350
1,1.50D0,8.911D0,0.0D0,2.229D0,3.082D0,0.00D0,4.91D0,-3.657D0,13.34KK  360
25D0,1.976D0,18.63D0,0.0D0,0.0D0,0.0D0,-3.19D0,-2.959D0,-6.169D0,-8KK  370
3.29D0,-3.769D0,0.261D0,0.85D0,-25.76D0/                            KK  380
 DATA LOGKTO/-10.329D0,2.60D0,3.398D0,0.928D0,2.238D0,1.40D0,1.260KK  390
1D0,3.20D0,2.309D0,1.268D0,-0.25D0,0.226D0,0.847D0,0.672D0,1.987D0KK  400
2,1.512D0,-13.998D0,-6.351D0,-6.10D0,-1.602D0,-1.585D0,-1.00D0,-8.4KK  410
31D0,-8.215D0,-8.240D0,-17.00D0,-4.548D0,-4.759D0,-11.410D0,-30.51KK  420
40D0/                                                               KK  430
 DATA LIST1/17,18,19,21,25,28/                                      KK  440
 DATA LIST2/23,24,25,26,28/                                         KK  450
 DATA NTOT/'CATOT','MGTOT','NATOT','KTOT','CLTOT','S04TOT','C02TOT'KK  460
1/                                                                  KK  470
 END                                                                KK  480-
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