PHRQINPT—AN INTERACTIVE COMPUTER PROGRAM FOR CONSTRUCTING INPUT DATA SETS TO THE GEOCHEMICAL SIMULATION PROGRAM PHREEQE

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ABSTRACT

PHRQINPT is a FORTRAN 77 program that facilitates formulation of the input data file to PHREEQE (Parkhurst, Thorstenson, and Plummer, 1980). PHRQINPT runs interactively and contains many features to help the user construct the input data set. This report describes these features and gives instructions on the use and implementation of PHRQINPT. A listing of the program and the two accompanying data sets are given in the Attachments, along with two examples.

INTRODUCTION

After publication of the program PHREEQE (Parkhurst, Thorstenson, and Plummer, 1980)*, it became apparent that construction of the input file to PHREEQE is often tedious and subject to user error. With this in mind, PHRQINPT was written to relieve these problems.

GENERAL FEATURES

PHRQINPT, written in Prime Fortran 77, interactively asks the user at the terminal for values of variables required by PHREEQE (Attachment A describes the input required by PHREEQE as given by Parkhurst, Thorstenson, and Plummer, 1980), explains the meaning and significance of each variable when required, and internally checks to make sure that values entered are valid. In some cases, PHRQINPT automatically assigns values to certain variables, based on values previously entered, and keeps track of additional required information. PHRQINPT contains an editor which allows the user to correct mistakes after each line has been completed.

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*For the reader unfamiliar with PHREEQE, this FORTRAN 77 code is capable of simulating the outcome of real or hypothetical chemical reactions (both reversible and irreversible) under a wide variety of physico-chemical conditions of interest in the earth sciences.

Two data files are used by PHRQINPT. One is a table of pre-constructed MINERALS input cards from which the user may select by mineral number listed on the screen. This mineral list may be displayed using the command LIST during MINERALS input. The other file read by PHRQINPT is the thermodynamic data file of PHREEQE, which provides a list of master species, master elements, their charges and appropriate index numbers. In addition to these two files, the user also can specify an optional reference file. The optional reference file contains an existing PHREEQE input data set that the user may copy and/or modify through PHRQINPT and then write the updated PHREEQE input data set to a different file.

HOW TO USE PHRQINPT

This program was written so that the user should be able to run it with no outside information other than knowledge of the desired geochemical simulation. Basic understanding of the program PHREEQE is helpful, though not necessary. The interested reader is referred to several recent reports (Parkhurst, Thorstenson, Plummer, 1980; Plummer, Parkhurst, and Thorstenson, 1983). For those who are running this program for the first time, the following information should be helpful:

The program will recognize commands in either upper or lower case.

All input values are free-formated. Therefore, numbers do not need to be right justified.

All files are opened within the program. The program will first ask for the output file name and name of a reference file. This reference file name, if given, must be the name of an existing data file previously coded to be read by PHREEQE. The reference file may contain more than one simulation. If one does not wish to use a reference file, simply enter a carriage return.

Caution: When copying directly from a reference file, the program assumes that the reference file is correct and does not check the values of variables.

Help messages are automatically printed whenever the value entered is of the wrong format, not within the correct range, or a '?' is entered. In addition to the help messages, a list of pre-constructed minerals and a list of master elements/species is available at certain locations within the program, which are indicated in the help messages.

The program PHRQINPT stores all values in memory, and does not write them into the output file until the end of the session. Because of this, the PHREEQE data blocks (cf. Attachment A) SOLUTION, ELEMENTS, SPECIES, MINERALS, LOOK MIN, and SUMS can be called more than once. New entries are simply attached to the end of the block. The program also keeps track of entries to make sure that there is no duplication; and recognizes for every master species entered, a master element must also be entered.

At the completion of each card, the user is asked (answer Yes, Y; No, N) whether the values on the card are satisfactory. If the user answers Yes, all values on that card are assumed completely correct and may no longer be changed in the current session. If the user answers No, the program goes into the correction mode by reprinting the values one at a time and asks the user for correct values. Previously correct values are retained by keying a carriage return, after each value appears on the system.

The last keyword command required by PHREEQE is END. If the user entered 'END' and has not entered all required information, the program will inform the user of this fact and will list the remaining required keywords. Until these are entered, the program can not be exited normally.

The order that keyword data blocks are entered is not necessarily the order that is printed in the output file. Instead, PHRQINPT writes the data blocks to the output file in the order preferred for PHREEQE.

If one accidentally entered a wrong keyword, that keyword data block can be aborted by entering 'exit' during the first question of that keyword block.

During modification of an existing reference file, the user may choose to keep, delete, or modify keyword data blocks as they appear on the screen. Extra data blocks may be inserted by answering delete when PHRQINPT recalls the 'END' card from the reference file.

If one does so, the program at this point then behaves as if there were no reference file at all and will ask the user for the name of a keyword.

At the conclusion of each simulation, the user has several options: (1) stop, (2) continue with the next simulation on the optional reference file (if it exists), (3) define a new reference file, (4) define the previous output as the new reference, or (5) just continue on entering values without a reference file. All further input to PHRQINPT will be appended to the same output file during a single session.

As examples of the use of PHRQINPT, Attachment B is a record of an interactive terminal session in which a PHREEQE input data set was constructed a priori. Attachment C records a session in which the previously constructed data set of Attachment B is modified. Attachment D contains a listing of the PHRQINPT source code and Attachments E and F list the data files required by PHREEQE.

ADAPTING PHRQINPT TO OTHER SYSTEMS

The program is written in Prime Fortran 77[a]. In transporting the program to another computer, several changes may be required:

Logical file #1, which is assigned to the terminal during input/output, may need to be changed.

Open statements may need to be changed to adapt to the different convention of file naming.

Internal reads, "read (STRING, . . .)", may or may not be supported. Buffer-In statements can be substituted.

Long format statements may need to be broken down into several shorter ones.

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[a] Mention of brand name in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

Because of the unusually large number of dynamic variables in the program, procedures may be needed to ensure that it will run properly. On the Prime computer, this problem can be avoided by compiling PHRQINPT with the -save option, making the variables static. Because many of the variables are used in CALL statements, they should not be placed in COMMON.

REFERENCES

Parkhurst, D. L., Thorstenson, D. C., and Plummer, L. N., 1980, PHREEQE-A computer program for geochemical calculations: U.S. Geological Survey Water-Resources Investigations 80-96, 210 p., National Technical Information Services Report PB 81-167 801, Springfield, VA 22161.

Plummer, L. N., Parkhurst, D. L., and Thorstenson, D. C., 1983, Development of reaction models for ground-water systems: Geochimica et Cosmochimica Acta, v. 47, p. 665-686.

Attachment A. - Description of input variables to PHREEQE

(From Parkhurst, Thorstenson, and Plummer, 1980)

DESCRIPTION OF INPUT

PHREEQE is designed to perform a sequence of simulations in a single computer run. Each simulation consists of two separate problems:

1. Process an initial solution or solutions and

2. Model a reaction (starting from the initial solution(s)).

Many pathways for a simulation are accessable with a card input data deck; that is, no program modification should be necessary. Required input begins with a title card followed by an option card. Depending on the options selected, additional data are supplied using various "Keyword" data blocks. A data block consists of a Keyword card followed by appropriate data. The Keyword informs the program of the type and format of the data to follow. ELEMENTS and SPECIES, if they are used, should be the first two data blocks while the other keyword blocks may follow in any order. The keyword END denotes the end of the input data and is required once for each simulation. After the calculations for one simulation are completed, the program starts the data input process again, beginning with a new title and option card.

The general types of reactions that can be simulated are as follows:

1. Mixing of two solutions.

2. Titrating one solution with a second solution.

3. Adding or subtracting a net stoichiometric reaction (changing total concentrations of elements in proportion to a given stoichiometry).

4. Adding a net stoichiometric reaction until the phase boundary of a specified mineral is reached.

5. Equilibrating with mineral phases (mineral equilibrium can be specified with reaction types 1, 2, 3, 4, or 6 as well). Any condition which can be written in the form

$$\log (K_p) = \sum_i b_{p,i} \cdot \log (a_i),$$

where

a_i is activity of the i^{th} aqueous species,

$b_{p,i}$ is the stoichiometric coefficient of the

i^{th} aqueous species in the p^{th} phase, and

K_p is the equilibrium constant for the p^{th} phase,

is considered a mineral phase. This definition of mineral equilibrium includes the following:

a. Maintaining the aqueous phase in equilibrium with one or more minerals, such as calcite, $Fe(OH)_3$, or gypsum;

b. Equilibration of a mineral-water system with a gas (CO_2, CH_4, H_2S);

c. Apparent ion exchange in the sense that a ratio of two aqueous ion activities is kept constant.

Any combination of the above can be included in the MINERALS keyword input provided the Gibbs Phase Rule is not violated.

6. Changing temperature.

These six types of reaction (processes) may be used in various combinations. For example, one could add a net stoichiometric reaction to a starting solution while maintaining mineral equilibrium and increasing temperature.

In each type of reaction, an initial solution must be specified. There are three ways to provide a starting solution for a reaction. (1) The total concentrations of elements (and other necessary information such as pH, and temperature) may be input using the SOLUTION n keyword. n is either 1 or 2 and indicates the number of the array where the solution data will be stored. Any stoichiometric reaction or simple mineral equilibration is performed on solution number 1 alone. Solution number 2 is required only for mixing and titrating. (2) The second method of providing a starting solution for a reaction is to save the final solution from the reaction step of the previous simulation (provided more than one simulation is made in a run). IOPT(7) is used to specify the solution number into which the final solution will be saved. In the subsequent simulation no new solution should be read into that solution number. (3) Finally, if no reaction solution is saved and no new solutions are input, the solutions from the previous simulation remain in memory. Thus, a solution can be input once but can be used as the starting solution for several simulations.

One of the principle applications of PHREEQE is intended to be simulation of reactions based on observed water analyses, which will generally show an apparent electrical imbalance as a result of analytical errors. Because we use the electrical neutrality criterion in solving for pH, it is important to consider this apparent charge imbalance. Various options are available to achieve charge balance or to maintain a charge imbalance in the computations. Care should be taken in choosing the appropriate option and interpreting the results. Only perfect chemical analyses would produce electrical neutrality in an initial solution. Lacking these, the solution may be left electrically unbalanced by setting IOPT(2) = 0. When a reaction is modeled the final calculated solution will have the same electrical imbalance as the initial solution. If IOPT(2) = 1, the pH of the initial solution will be adjusted to produce electrical neutrality in that solution. It may be that the pH of the initial solution is well known and it is more reasonable to add relatively inert ions like K^+ or Cl^- to balance the solution electrically. In this case set IOPT(2) = 2, and use the keyword NEUTRAL and associated input to specify K and Cl. The amount of Cl or K added will be listed in the output. One final alternative is to attribute the charge error to the most suspect analysis, e.g. carbon or sodium, or to a constituent known to be present for which one has no analytical data. Again, set IOPT(2) = 2 and use the NEUTRAL input. Lack of charge balance is a meaningful clue to the errors in analyses and a large error probably makes a solution unsuitable for reaction simulation. By using the various options of the program, one can investigate the significance of analytical errors and their effects on reaction simulations. (Detailed test problems and examples for using PHREEQE are given in the section Test Problems.)

In the following description of the card input, the Fortran format for each card is given. Any Fortran manual will provide a complete explanation of the symbols used in format statements. Briefly, A indicates an alphanumeric character field, I an integer field, F floating point, E single precision exponential, D double precision exponential, and X indicates spaces. The first number following A, I, D, E, or F defines the length of the field, or the number of columns on the card reserved for the field. All integers must be right justified in their fields. All exponential fields, when including an exponent, must be right justified. For floating point and exponential fields, it is suggested that the decimal point always be included. A number preceding a letter is the repeat counter and indicates the number of times the field occurs consecutively on the card. Similarly a number directly preceding a parenthesis indicates the number of times the formats contained within the parentheses are repeated as a group. Any blanks in I, F, E, or D fields are considered to be zeros.

A. Title and option cards.

1. TITLE CARD TITLE
   FORMAT (20A4)
   Eighty characters of titles or comments.

2. OPTION CARD (IOPT(I), I = 1,9), NSTEPS, NCOMPS, VO
   FORMAT (9I1, 1X, 2I2, 6X, F10.5)

   IOPT(1) = 0, No print of thermodynamic data or coefficients of aqueous species.

   = 1, Print the aqueous model data (which are stored on disk) once during the entire computer run.

   IOPT(2) = 0, Initial solutions are not to be charge balanced. Reaction solutions maintain the initial charge imbalance.

   = 1, pH is adjusted in initial solution(s) to obtain charge balance.

   = 2, The total concentration of one of the elements (except H or O) is adjusted to obtain electrical balance. NEUTRAL input is required.

   IOPT(3) = 0, No reactions are modeled. Only the initial solutions are solved.

   = 1, Solution 1 is mixed (a hypothetical constant volume process) with solution 2 in specified reaction steps. STEPS input and a value for NSTEPS are required. MINERALS input may be included.

   = 2, Solution 1 is titrated with solution 2 in specified reaction steps. STEPS input, a value for NSTEPS, and a value for VO are required. MINERALS input may be included.

   = 3, A stoichiometric reaction is added in specified reaction steps. REACTION input, STEPS input, a value for NSTEPS, and a value for NCOMPS are required. MINERALS input may be included.

   = 4, A net stoichiometric reaction is added in NSTEPS equal increments. REACTION input, STEPS input,

a value for NSTEPS, and a value for NCOMPS are required. MINERALS input may be included. Only one value for the total reaction is read in STEPS.

= 5, Solution number 1 is equilibrated with mineral phases only. No other reaction is performed. MINERALS input is required.

= 6, A reaction is added to solution 1 until equilibrium is attained with the first phase in MINERALS input (equilibrium with other MINERALS phases is maintained throughout the reaction). REACTION input, a value for NCOMPS, and MINERALS input are required. No STEPS input is required. Note: there should be a common element in the reaction and the first phase in MINERALS input.

IOPT(4) = 0, The temperature of the reaction solution is (a) the same as the initial solution if adding a reaction, or (b) calculated linearly from the end members if mixing or titrating. No TEMP input required.

= 1, The temperature is constant during the reaction steps and differs from that of the initial solution(s). One value is read in the TEMP input.

= 2, The temperature is varied from T_o to T_f in NSTEPS equal increments during the reaction steps. A value for NSTEPS and two values of temperature, T_o and T_f, (in order) are required in the TEMP input, where T_o is the initial temperature and T_f is the final temperature.

= 3, The temperature of each reaction step is specified in TEMP input, in order. NSTEPS values are read.

IOPT(5) = 0, The pe from the initial solution is held constant during all the reaction steps for the simulation.

= 1, The pe of the reaction solution is determined by the reaction.

IOPT(6) = 0, Activity coefficients are calculated as follows:

a. the WATEQ Debye-Hückel formula is used for all species with GFLAG = 1 (see SPECIES input below),

b. the Davies formula is used for all species with no ion size parameter (DHA = 0, see SPECIES input),

c. the extended Debye-Hückel formula is used for all species with an ion size parameter (DHA 0).

= 1, Activity coefficients are calculated as follows:

a. the WATEQ Debye-Hückel formula is used for all species with GFLAG = 1.

b. the Davies formula is used for all other species.

IOPT(7) = 0, Do not save the aqueous phase composition at the end of a reaction for additional simulations.

= 1, Save the final reaction solution in solution number 1.

= 2, Save the final reaction solution in solution number 2.

IOPT(8) = 0, The debugging print routine is not called.

= 1, A long printout is output at each iteration in each problem. This print is to be used only if there are convergence problems with the program. (See Subroutine PBUG.)

IOPT(9) = 0, No printout of each array to be solved.

= 1, A long printout occurs of the entire array to be solved at each iteration. This print is used only if there are convergence problems. (See Subroutine SLNQ.)

NSTEPS The number of reaction steps. A value is required if IOPT(3) = 1, 2, 3, or 4, or if IOPT(4) = 2 or 3. (Right justified.)

NCOMPS — The number of constituents in a net stoichiometric reaction. A constituent may be any element with an index number between 4 and 30 inclusive. No aqueous species with index numbers greater than 30 may be included as reaction constituents except H_2 and O_2. Any constituent with an index number greater than 30 is assumed to be either H_2 or O_2 and has the effect of raising or lowering the redox state of the solution depending on the assigned valence (THMEAN). A value for NCOMPS is required if IOPT(3) = 3, 4, or 6. (Right justified.)

V0 — The initial volume of solution number 1 when modeling a titration. The unit of V0 must be the same as that of XSTEP (see STEPS input below) if IOPT(3) = 2. Otherwise, V0 is not required.

B. Keyword data blocks. Blocks are preceded by a keyword card. The keywords are numbered and underlined in the following text. Each keyword must begin in the first column of the card. The appropriate cards, which are lettered in the text, must follow in order directly after the keyword.

1. ELEMENTS FORMAT (A8)
This input defines the names and indices of all elements in the aqueous model data base. One card 1.a is read for each element. The index numbers of the elements do not need to be consecutive or sequential. This input block must be terminated with one blank card. Generally these data will be part of the aqueous model stored on disk and read by the program at the beginning of each run. Only changes to the data base need to be in the input card deck.

1.a. TNAME, NELT, TGFW
FORMAT (A8,2X,I2,3X,F10.0)

TNAME — Alphanumeric name of element.

NELT — Index number assigned to the element. Number must be between 4 and 30, inclusive. (Right justified.)

TGFW Gram formula weight of the species used to report the analytical data. If solution data is to include alkalinity, TGFW for the element carbon must be the equivalent weight of the reported alkalinity species. TGFW is not used if the concentrations are entered as molality (IUNITS = 0 in SOLUTION input card 3.b).

1.b. Blank card.

2. SPECIES FORMAT (A8)
This input defines the names, index numbers and composition of all aqueous species in the aqueous model data base. Cards 2.a, 2.b, 2.c, and 2.d are read for each species. The index numbers for the species do not need to be sequential or consecutive. This input block must be terminated with one blank card. To eliminate a species (already in the PHREEQE data array) from the aqueous model only card 2.a followed by a blank card 2.b must be entered. More species changes could then follow or a second blank card would terminate this input block. All species must have association reactions which contain only master species (species numbers less than or equal to 30; see discussion in section, Equilibrium Equations). Reactions containing non-master species must be converted to master species reactions and the appropriate association constants must be calculated before they can be entered into the program. These data are generally stored in the disk file which is read by the program at the beginning of each run and retained for the entire run. Only changes and additions would appear in the input card deck.

2.a. I
FORMAT (I3)

I The index number assigned to the aqueous species. Numbers 4 through 30 are reserved for master species. 250 is the maximum index number for an aqueous species. (Right justified.)

2.b. SNAME, NSP, KFLAG,GFLAG, ZSP, THSP, DHA, ADHSP(1), ADHSP(2), ALKSP
FORMAT (A8,2X,I3,2I1,6F10.3)
Three different formulations are available for the activity coefficient expression.

Three different formulations are available for the activity coefficient expression.

i) Extended Debye-Hückel,

$$\text{Log } \gamma_i = \frac{-A\ z_i^2\ \sqrt{I}}{1 + B\ a_i^o \sqrt{I}}$$

ii) WATEQ Debye-Hückel

$$\text{Log } \gamma_i = \frac{-A\ z_i^2\ \sqrt{I}}{1 + B\ a_i \sqrt{I}} + b_i I$$

iii) Davies

$$\text{Log } \gamma_i = -A\ z_i^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right),$$

where A and B in all three equations are constants depending on the dielectric constant of the solvent and the temperature (Robinson and Stokes, 1970).

SNAME Alphanumeric species name.

NSP The total number of master species in the association reaction that forms this species; do not count the species itself unless the species is a master species. (Right justified.)

KFLAG = 0, The Van't Hoff expression is used to calculate temperature dependence of the association constant for this species.

= 1, An analytical expression is used to calculate temperature dependence of the association constant. Values for ASP are required on card 2.c.

GFLAG = 0, The extended Debye-Hückel or Davies expression (according to IOPT(6)) is used to calculate the activity coefficient for this species if DHA >0 (see below). If DHA = 0 and GFLAG = 0, the Davies equation is always used regardless of IOPT(6).

= 1, The WATEQ Debye-Hückel expression is used to calculate the activity coefficient of this species regardless of the value of IOPT(6).

ZSP The charge on this aqueous species.

THSP The sum of the OPV's of the redox species in this species. (e.g. $FeSO_4^o$ has a THSP = 2 + 6 = 8.)

DHA The extended Debye-Hückel a_i^o term. If this parameter is zero and GFLAG = 0 then the Davies equation is used to calculate the activity coefficient for this species.

ADHSP(1) The a_i term for the WATEQ Debye-Hückel expression.

ADHSP(2) The b_i term for the WATEQ Debye-Hückel expression.

ALKSP The alkalinity assigned to this aqueous species. (See discussion in Numerical Methods section.)

2.c. LKTOSP,DHSP,(ASP(I),I = 1,5)
FORMAT (2F10.3,5E12.5)
Constants used to evaluate the association constant as a function of temperature. The analytical expression has the form:

$$\text{Log}(K) = A_1 + A_2\,T + A_3/T + A_4\,T^2 + A_5/T^2$$

where T is expressed in ^oK.

LKTOSP Log_{10} of the mass action association constant at 25°C (used in Van't Hoff equation).

DHSP Standard enthalpy of the association reaction at 25°C (ΔH_r^o, in kcal/mole); used in the Van't Hoff calculation of the temperature dependence of the association reaction. Required if KFLAG = 0. (A zero or blank will result in no temperature variation in the association constant.)

ASP(1) Constant term in the analytical expression for the association constant, (A_1). The array ASP is used if KFLAG = 1.

ASP(2) Coefficient of $T^{o}K$ in analytic expression, (A_2).

ASP(3) Coefficient of $1/T$ in analytic expression, (A_3).

ASP(4) Coefficient of T^2 in analytic expression, (A_4).

ASP(5) Coefficient of $1/T^2$ in analytic expression, (A_5).

2.d. (LSP(I), CSP(I), I = 1, NSP)
FORMAT 6(I3,F7.3)
List of master species numbers and their coefficients in the mass action association reaction. NSP pairs of values, LSP and CSP, are read. One and only one of these cards is required for each species.

LSP(I) Index number of master species. (Right justified.)

CSP(I) Stoichiometric coefficient of master species in this aqueous species.

For example, using the data base in Attachment A for master species, the reactions below define variables as shown:

$$Ca^{2+} + H^{+} + CO_3^{2-} = CaHCO_3^{+} \quad \text{(species 77)}$$

NSP = 3
LSP(1) = 4, CSP(1) = 1.0; LSP(2) = 1, CSP(2) = 1.0;
LSP(3) = 15, CSP(3) = 1.0.

$$SO_4^{2-} + 8H^{+} + 8e^{-} = S^{2-} + 4H_2O \quad \text{(species 41)}$$

or,

$$SO_4^{2-} + 8H^{+} + 8e^{-} - 4H_2O = S^{2-}$$

NSP = 4
LSP(1) = 16, CSP(1) = 1.0; LSP(2) = 1, CSP(2) = 8.0;
LSP(3) = 2, CSP(3) = 8.0; LSP(4) = 3, CSP(4) = -4.0.

2.e. Blank card.

3. SOLUTION n FORMAT (A8,1X,I1)
This input is used to define a starting solution. n can be either 1 or 2 and indicates the solution number of the data following. Cards 3.a and 3.b are required. Card 3.c is not included if NTOTS = 0. There must be as many card 3.c's as necessary to read NTOTS total concentrations.

3.a. HEAD
FORMAT (20A4)
Title or comments about the solution.

HEAD Alphanumeric heading.

3.b. NTOTS, IALK, IUNITS, PH, PE, TEMP, SDENS
FORMAT (I2,I3,I2,3X,4F10.3)

NTOTS The number of total concentrations to be read from card 3.c input. For example, if the starting solution is a $MgCl_2$ - $NaHCO_3$ solution, NTOTS = 4 (for Mg, Cl, Na, and C). (Right justified.)

IALK Flag which indicates whether total carbon or total alkalinity is to be input. (Right justified.)

= 0 indicates the total concentration of carbon (not alkalinity) is input in the units specified by IUNITS (see below).

= n $4 \leq n \leq 30$, where n is the index number for the element carbon, (in our data base n=15) indicates total alkalinity is being entered. If alkalinity is used (n>0), then IOPT(2) can not be equal to 1. It is theoretically impossible to use pH to achieve electrical neutrality if the alkalinity is fixed. ELEMENTS input may be required. The units of alkalinity are specified by IUNITS (below) and if IUNITS>0, the gram formula weight (GFW) of the element carbon is critically important. The GFW in the case of alkalinity must be the gram equivalent weight (grams/equivalent) of the chemical species in which the alkalinity is reported. The following is a list of species commonly used for reporting alkalinity and their corresponding equivalent weights:

$CaCO_3$	50.0446 g/eq
HCO_3^-	61.0171 g/eq
CO_3^{2-}	30.0046 g/eq.

In our data base 44.010 is the GFW of carbon which is suitable for entering carbon as total CO_2. This GFW must be changed via ELEMENTS input if alkalinity is to be entered as mg/l or ppm (IUNITS = 2 or 3). If IUNITS = 0 alkalinity must be input as eq/kg H_2O and in this case the GFW need not be changed because no conversion of units is necessary. For a discussion of the contribution of the different aqueous species to the total alkalinity see the Numerical Methods section.

IUNITS Flag describing units of input concentrations (right justified). The program makes all of its calculations in terms of molality and any other allowed concentration units (mmoles/l, mg/l, or ppm) must be converted to molality before the calculations may begin. To make the conversions it is necessary to know the gram formula weight (GFW), in g/mole, of the chemical formula in which elemental analyses are reported. The GFW is an input parameter under ELEMENTS input and must be in agreement with the analytical units for each solution data set. (If the units are molality, no conversion is necessary and the GFW's are not used.) Consider silicon as an example: Si is commonly reported as ppm of SiO_2 but may also be given as ppm H_4SiO_4. To convert ppm SiO_2 to moles Si/kg H_2O the GFW for silicon in the ELEMENTS data must be 60.0843. For ppm H_4SiO_4 the GFW must be 96.1147. If the units of the water analysis do not correspond to the GFW for any element, the GFW must be changed using ELEMENTS input or the data must be converted by hand before input into the program. Values of GFW used in the preliminary PHREEQE data base are given in Table 1. Note: All elements must have the same units. It is not possible to enter mg/l of one element and molality of another.

= 0 Concentration of elements entered as molality of each element, or for alkalinity, equivalents/kg H_2O.

= 1 Concentration of elements entered as mmoles/l of each element, or for alkalinity, meq/l.

= 2 Concentration of elements entered as mg/l of the species which has a gram formula weight given in ELEMENTS input. (ELEMENTS input may be required.) For alkalinity see discussion under IALK above.

= 3 Concentration of elements entered as ppm of the species which has a gram formula weight given in ELEMENTS input. (ELEMENTS input may be required.) For alkalinity see discussion under IALK above.

PH The pH of the solution (the approximate pH if IOPT(2) = 1). Required for all solutions.

PE The pe of the solution. Required for all solutions.

TEMP The temperature of the solution in °Celsius.

SDENS The density of the solution. Required if concentrations are input as mmoles/l, mg/l, or ppm. If SDENS is omitted, 1.0 is assumed.

3.c. (LT(I), DTOT(I), I = 1, NTOTS)
FORMAT 5(I4,D11.3)
Total concentrations of elements. Five values of LT and DTOT are read on each card. The card may be repeated in order to enter all the elements desired. All data must appear consecutively in the fields, no blanks or zeros are allowed as values for LT. Omit this card if NTOTS is zero, the case of pure water.

LT Index number of the element. (Right justified.)

DTOT Total concentration of the element in molality, mmoles/l, mg/l, or ppm according to IUNITS.

4. MINERALS FORMAT (A8)
This input defines the phases which will be maintained at equilibrium with each of the reaction solutions. Cards 4.a and 4.b are required for each mineral. Card 4.c is optional for each mineral depending on the value of MFLAG. Unlike SPECIES, MINERALS may be defined in terms of any aqueous species, not just the master species. The input expression for the equilibrium constant must correspond with the input mass action coefficients. Mineral reactions are written as dissociation reactions. MINERALS input must be terminated with a blank card.

4.a. MNAME, NMINO, THMIN, LKTOM, DHMIN, MFLAG,SIMIN
FORMAT (A8,2X,I2,3X,3F10.2,5X,I1,9X,F10.3)
Constant parameters for this mineral.

MNAME Alphanumeric name of mineral.

NMINO Number of different species in the mineral dissociation reaction (including H^+, e^-, and H_2O). NMINO must be less than or equal to 10. (Right justified.)

THMIN The sum of the OPV's of the species in the mineral dissociation reaction.

For example,

$$FeS_2 = Fe^{2+} + 2S^{2-} - 2e^-$$

$$THMIN_{Pyrite} = 1(+2) + 2(-2) - 2(-1) = 0$$

$$Fe(OH)_3 = Fe^{3+} + 3OH^-$$

$$THMIN_{Fe(OH)_3} = 1(+3) + 3(0) = +3$$

$$CaCO_3 = Ca^{2+} + CO_3^{2-}$$

$$THMIN_{CaCO_3} = 1(0) + 1(+4) = +4$$

LKTOM Log of the equilibrium constant at 25°C for the reaction.

DHMIN ΔH_r^o (kcal/mole) for the Van't Hoff expression.

MFLAG = 0, The Van't Hoff expression is used to calculate the temperature dependence of the equilibrium constant.

= 1, The analytical expression is used to calculate the temperature dependence of the equilibrium constant. Card 4.c is required.

SIMIN Saturation index (log(Ion Activity Product/K_{sp})) desired in the final solution. SIMIN = 0.0 would produce equilibrium with the mineral while 1.0 would produce a solution 10 times supersaturated (SI = 1.0). This variable is useful in specifying the partial pressure of a gas. The Henry's law constant for the gas would be entered using the Van't Hoff constant (LKTOM) or analytical expression (AMIN) and the log of the partial pressure would be entered for for SIMIN.

4.b. (LMIN(I), CMIN(I), I=1, NMINO)
FORMAT 5(I4,F11.3)
List of species index numbers and stoichiometric coefficients in the dissociation reaction for this mineral. NMINO pairs of numbers, LMIN and CMIN, are read. The maximum value of NMINO is 10. If NMINO is greater than 5, a second card 4.b is required.

LMIN(I) Index number of species (not necessarily master species) in the dissociation reaction for this mineral. (Right justified.)

CMIN(I) Stoichiometric coefficient of species in dissociation reaction.

For example, using the data for aqueous species index numbers in Attachment A,

i. $CaCO_3 = Ca^{2+} + CO_3^{2-}$

NMINO = 2
LMIN(1) = 4, CMIN(1) = 1.0;
LMIN(2) = 15, CMIN(2) = 1.0.

ii. $FeS_2 + 2e^- = Fe^{2+} + 2S^{2-}$

or,

$FeS_2 = Fe^{2+} + 2S^{2-} - 2e^-$

NMIN0 = 3
LMIN(1) = 8, CMIN(1) = 1.0;
LMIN(2) = 41, CMIN(2) = 2.0;
LMIN(3) = 2, CMIN(3) = -2.0.

iii. $CaSO_4 \cdot 2H_2O = Ca^{2+} + SO_4^{2-} + 2H_2O$

NMIN0 = 3
LMIN(1) = 4, CMIN(1) = 1.0;
LMIN(2) = 16, CMIN(2) = 1.0;
LMIN(3) = 3, CMIN(3) = 2.0.

iv. Ca^{2+} - Na^+ ion exchange. (Assumes composition of exchanger does not change.)

$Na_2(ex) + Ca^{2+} = Ca(ex) + 2Na^+$

or

$Na_2(ex) - Ca(ex) = 2Na^+ - Ca^{2+}$

NMIN0 = 2
LMIN(1) = 6, CMIN(1) = 2.0;
LMIN(2) = 4, CMIN(2) = -1.0.

LKTOM = $\frac{a_{Na^+}^2}{a_{Ca^{2+}}}$ at exchange equilibrium.

v. Fix CO_2 partial pressure.

$CO_{2(gas)} + H_2O = H_2CO_{3(aq)}$

or

$CO_{2(gas)} = H_2CO_{3(aq)} - H_2O$

NMIN0 = 2
LMIN(1) = 35, CMIN(1) = 1.0;
LMIN(2) = 3, CMIN(2) = -1.0,
LKTOM = Henry's law constant for CO_2,
SIMIN = Log P_{CO_2} desired.

4.c. AMIN(I), I = 1,5
FORMAT (5E12.5)
Equilibrium constant expression of the form:

$$\text{Log}(K) = A_1 + A_2\ T + A_3/T + A_4\ T^2 + A_5/T^2,$$

for the mineral dissociation reaction where T is ^{o}K.
This card is used only if MFLAG = 1.

AMIN(1) Constant coefficient of analytical expression, (A_1 above).
AMIN(2) Coefficient of $T^{o}K$ in analytical expression, (A_2).
AMIN(3) Coefficient of 1/T in analytical expression, (A_3).
AMIN(4) Coefficient of T^2 in analytical expression, (A_4).
AMIN(5) Coefficient of $1/T^2$ in analytical expression, (A_5).

4.d. Blank card.

5. LOOK MIN FORMAT (A8)
The purpose of this input is simply to provide information on the saturation state of the aqueous phase with respect to desired minerals. The minerals in this block of input do not affect the calculations of the initial solution or any of the reaction solutions. This input is never mandatory. The Ion Activity Product (IAP) and saturation index (SI = log (IAP/K)) of each of these minerals is printed in the output following each solution description. Only the minerals which contain elements present in the solution are printed. The input following this card is identical to the input for MINERALS (see above). This input must be terminated with a blank card.

The list of "look minerals" is maintained for the duration of the run and any new "look mineral" is simply added to the list. If a "look mineral" is added that has the identical 8 letter name as another mineral in the list, the new mineral replaces the old mineral. The word DELETE as a mineral name will eliminate all of the minerals in the list and new minerals may be added. Only thirty nine "look minerals" are allowed. LOOK MIN

input is generally placed in the disk file which is read at the beginning of each run. The input card deck need only contain additions and changes to that permanent list.

6. TEMP — FORMAT (A8)
This input varies the temperature during the reaction steps. It is required input if IOPT(4) is greater than 0. Only one card 6.a is necessary unless IOPT(4) = 3. In that case as many cards as necessary to input NSTEPS values are required.

6.a. XTEMP
FORMAT (8F10.1)

XTEMP Temperature in degrees Celsius.
If IOPT(4) = 1, one value of XTEMP is coded.
If IOPT(4) = 2, two values of XTEMP are coded, T_o and T_f (in order).
If IOPT(4) = 3, NSTEPS values of XTEMP are coded (no blank fields permitted).

7. STEPS — FORMAT (A8)
This input defines the steps of the reaction process. The input has a different meaning depending on the value of IOPT(3) (option card).

IOPT(3) = 1, XSTEP is the fraction of solution 1 to be mixed with solution 2. NSTEPS values are read.

IOPT(3) = 2, XSTEP is the volume of solution 2 to be titrated into solution 1. XSTEP must have the same units as V0 (option card). NSTEPS values are read.

IOPT(3) = 3, XSTEP is the moles of reaction to be added to solution 1. NSTEP values are read.

IOPT(3) = 4, Only one value of XSTEP is read. XSTEP is the total number of moles of reaction to be added in NSTEPS steps. NSTEPS reaction solutions

will be calculated. The I^{th} solution will have I*XSTEP/NSTEPS moles of reaction added to solution 1.

7.a. XSTEP
FORMAT (8F10.3)

XSTEP — Reaction increments as defined above.

8. REACTION FORMAT (A8)
This input describes the stoichiometry and valence of the elements to be added as a reaction. STEPS input (see above) defines the total number of moles of this reaction to be added. The REACTION process changes the total aqueous concentration of an element by the stoichiometric coefficient (CREAC) times the total moles of reaction (XSTEP). (However, the final total concentration in the reaction solution may also be altered by mass transfer to achieve equilibrium with minerals specified in MINERALS input.) It is necessary to consider the charge balance of the reaction which is added. A charge imbalance by an input error or by intent is equivalent to adding acid or base. If the reaction is a simulation from a known solution to another known solution it is possible to add an inert electrical charge equal to the difference in the charge imbalance between the two solutions. Set LREAC(I) = 0, CREAC(I) = charge imbalance (equivalents/kgH_2O) and THMEAN(I)=0.0. This will eliminate implicit addition of acid or base. Card 8.a is repeated as often as necessary to read NCOMPS (option card) reaction constituents.

8.a. (LREAC(I), CREAC(I), THMEAN(I), I = 1,NCOMPS)
FORMAT 4(I4,2F8.3)
This input defines a net stoichiometric reaction. Four triples of numbers are read on each card. Enough cards must be included to read NCOMPS triples of numbers.

LREAC(I) — Index number of element for the reaction. LREAC must be between 4 and 30 inclusive. If LREAC is greater than 30 the program considers this constituent to be H_2 or O_2 and only uses CREAC and THMEAN (below) to change the oxidation state of the reaction solution. (Right justified.)

CREAC(I) Stoichiometric coefficient of the element in the reaction.

THMEAN(I) The OPV of the element in the reaction (e.g. carbon as carbonate: THMEAN = +4; carbon as methane: THMEAN = -4; ferrous iron: +2; and ferric iron: +3). An element may be included more than once in a reaction to accomodate different valence states of the element.

The variables which affect a reaction simulation are IOPT(3), NSTEPS, and NCOMPS from the option card, REACTION input and STEPS input. The following examples use the species index numbers from Attachment A.

i. Gypsum is added to the initial solution in 5 equal increments of 0.005 moles, to a total of .025 moles. Calcite equilibrium is maintained in each of the five steps.

IOPT(3) = 4 (net reaction added linearly).
NSTEPS = 5 (5 reaction steps).
NCOMPS = 2 (2 constituents, Ca and S).
LREAC(1) = 4, CREAC(1) = 1.0, THMEAN(1) = 0.0 (Ca),
LREAC(2) = 16, CREAC(2) = 1.0, THMEAN(2) = 6.0 (S).
MINERALS input, calcite.
XSTEP(1) = .025 (total moles of reaction to be added).

The total calcium at the completion of the first reaction step is given by:

$$Ca_{tot} = Ca_{tot(initial)} + .005 + MIN_{calcite}.$$

ii. Suppose mass balance between two solutions shows calcite, gypsum, and dolomite dissolving (+) and precipitating (-) in proportions of -1:1.5:1. The net reaction is written:

-	1 Ca			- 1 C			Calcite
+	1.5 Ca				+ 1.5 S		Gypsum
+	1 Ca	+	1 Mg	+ 2 C			Dolomite
	1.5 Ca	+	1 Mg	+ 1 C	+ 1.5 S		NET

Three points along this possible path are modeled by (arbitrarily) adding 10^{-4}, 10^{-3}, and 10^{-2} moles of the net reaction.

IOPT(3) = 3 (add net reaction in specified steps).
NSTEPS = 3 (number of steps).
NCOMPS = 4 (number of constituents in the reaction).
LREAC(1) = 4, CREAC(1) = 1.5, THMEAN(1) = 0.0 (Ca);
LREAC(2) = 5, CREAC(2) = 1.0, THMEAN(2) = 0.0 (Mg);
LREAC(3) = 15, CREAC(3) = 1.0, THMEAN(3) = 4.0 (C);
LREAC(4) = 16, CREAC(4) = 1.5, THMEAN(4) = 6.0 (S).
XSTEP(1) = 10^{-4}, XSTEP(2) = 10^{-3}, XSTEP(3) = 10^{-2}.
(Reaction increments in moles, reaction is not cumulative.)

9. NEUTRAL FORMAT (A8)
This input defines the elements to be used to adjust the initial solution(s) to electrical neutrality. One element with a master species cation and one element with a master species anion are input. H^+ and e^- are not valid entries. A master cation and anion are required in order to add one or the other element according to the charge imbalance. Species are not subtracted, eliminating the possibility of negative total concentrations. This input is required only if IOPT(2) = 2. (Note that this is not equivalent to adding or subtracting charge as discussed in REACTION; remember that IOPT(2) = 0 will maintain an original charge imbalance during a simulation.)

9.a. LPOS, LNEG
FORMAT (2I5)

LPOS	Index number of an element with a cation master species. (Right justified.)
LNEG	Index number of an element with a anion master species. (Right justified.)

10. SUMS FORMAT (A8)
This input sums molalities of aqueous species which are then printed in the output of the run. These sums do not affect the calculations in any way and are never mandatory. These sums could, for example, be used to define an alternate sum of species for the alkalinity. The "sums" are defined by lists of species numbers, so that each time a sequence number for a species is listed, the sum is incremented by the molality of that species. If the species has, for example, two carbonate ions and the total carbonate is the sum which is desired then the species should be listed twice in that sum. Up to 10 dif-

ferent sums may be defined. Each sum may have up to 50 species. Cards 10.a and 10.b are required for each sum. This input, after all sums have been defined, must be terminated with one blank card.

As in LOOK MIN input the sums are kept for the duration of the run but it is possible to add or replace sums or delete the entire set in any single simulation. Any sum input in this data block will be added to the list of sums if the name (SUNAME) is different from all other sum names. A sum with the identical name will replace the sum already in the list. The word DELETE as a sum name will eliminate all the sums known to the computer.

10.a. SUNAME, NSUM
FORMAT (A8,2X,I2)

SUNAME — Alphanumeric name to be printed to identify the sum.

NSUM — The number of index numbers to be read on card(s) 10.b; NSUM 50. (Right justified.)

10.b. (LSUM(I,J), J = 1, NSUM)
FORMAT (20I4)
List of species numbers to define the sum. Twenty index numbers are read on this card. The card may be repeated as many times as necessary to input NSUM index numbers.

LSUM — Index numbers of species in sum. (Right justified.)

Note: repeat cards 10.a and 10.b for each sum.

10.c. Blank card. One blank card at the end of all sums is required to terminate this input.

11. END — FORMAT (A8)
This card terminates input operations for a single simulation. Initial solution(s) and reaction solution(s) are computed as directed by the preceeding input. Any computer run has at least one END card.

Attachment B. - Example using PHRQINPT to construct input data set *a priori*.

```
ENTER OUTPUT FILE NAME
EXAMPLE.1

ENTER REFERENCE FILE NAME:  (HIT <CR> TO OMIT)


INPUT THE TITLE
ADD OXYGEN AT PYRITE-CALCITE-GOETHITE EQUILIBRIUM

ADD OXYGEN AT PYRITE-CALCITE-GOETHITE EQUILIBRIUM
O.K.?
Y

INPUT IOPT(1)
0

INPUT IOPT(2)
1

INPUT IOPT(3)
3

INPUT IOPT(4)
0

INPUT IOPT(5)
1

INPUT IOPT(6)
1

INPUT IOPT(7)
0

INPUT IOPT(8)
0

INPUT IOPT(9)
0

INPUT NSTEPS
5

INPUT NCOMPS
1

013011000  5 1       0.0
O.K.?
Y
```

```
******************
KEYWORD DATA BLOCKS
******************


ENTER KEYWORD.
SOLUTION


--------
SOLUTION
--------


INPUT SOLUTION NUMBER
1

SOLUTION 1
O.K.?
Y

INPUT HEAD
PURE WATER

PURE WATER
O.K.?
Y

INPUT NTOTS
0

INPUT PH
7

 SOLUTION
              PH            THE PH OF THE SOLUTION (THE APPROXIMATE PH
                            IF IOPT(2) = 1)
 FORMAT (F10.3)


INPUT PH
7.

INPUT PE
4.
```

```
INPUT TEMP
25.

 0  0 0   7.        4.        25.        1.0
O.K.?
Y

********************
KEYWORD DATA BLOCKS
********************


ENTER KEYWORD.
MINERALS


--------
MINERALS
--------


PRE-CONSTRUCTED MINERAL DATA ARE AVAILABLE.
DO YOU WISH TO HAVE ANY OF THEM?
Y

   1 CALCITE     2 ARAGONIT    3 DOLOMITE    4 SIDERITE    5 RHODOCHR
   6 STRONTIT    7 GYPSUM      8 ANHYDRIT    9 CELESTIT   10 BARITE
  11 HYDROXAP   12 VIVIANIT   13 FLUORITE   14 FEOH3A     15 HEMATITE
  16 PYRITE     17 GOETHITE   18 GIBBSITE   19 CHALCEDY   20 QUARTZ
  21 KAOLINIT   22 SEPIOLIT   23 FES PPT    24 BIRNESIT   25 MANGANIT
  26 SIL GEL    27 SIL GLAS   28 SEP PPT    29 MACKINIT   30 MUSCOVIT
  31 MICROCLN   32 CO2 GAS    33 O2 GAS     34 H2 GAS     35 N2 GAS
  36 H2S GAS    37 CH4 GAS    38 NH3 GAS

ENTER THE INDEX NUMBER OF MINERAL. (TYPE <STOP> TO EXIT)
16

PYRITE     4      0.0    -18.48     11.3          0
   1  -2.0         2  -2.0         8  1.0         42  2.0
O.K.?
Y

ENTER THE INDEX NUMBER OF MINERAL. (TYPE <STOP> TO EXIT)
17

GOETHITE   3   3.0        0.486    -14.48         0
 115 1.0          3 2.0          1 -3.0
O.K.?
```

```
Y

ENTER THE INDEX NUMBER OF MINERAL. (TYPE <STOP> TO EXIT)
1

CALCITE    2   4.0        -8.480    -2.297          1
  15 1.0           4 1.0
-171.9065   -.077993    2839.319      71.595
O.K.?
Y

ENTER THE INDEX NUMBER OF MINERAL. (TYPE <STOP> TO EXIT)
STOP

MORE MINERALS TO BE TYPED IN FROM THE TERMINAL?
N

********************
KEYWORD DATA BLOCKS
********************



ENTER KEYWORD.
STEPS


--------
STEPS
--------



INPUT XSTEP(1)
0.0

INPUT XSTEP(2)
0.001

INPUT XSTEP(3)
0.005

INPUT XSTEP(4)
0.01

INPUT XSTEP(5)
0.05

0.0        0.001      0.005      0.01       0.05
O.K.?
```

```
Y

******************
KEYWORD DATA BLOCKS
******************


ENTER KEYWORD.
REACTION


--------
REACTION
--------


INPUT LREAC(1)
?

 REACTION
             LREAC          INDEX NUMBER OF ELEMENT FOR THE REACTION.
                            LREAC MUST BE BETWEEN 4 AND 30 INCLUSIVE.
                            IF LREAC IS GREATER THAN 30 THE PROGRAM
                            CONSIDERS THIS CONSTITUENT TO BE H2 OR
                            O2 AND ONLY USES CREAC AND THMEAN
                            TO CHANGE THE OXIDATION STATE OF THE
                            REACTION SOLUTION.
 FORMAT (I4)
 NOTE:  FOR A LISTING OF MASTER SPECIES AND ELEMENTS,
        ENTER <LIST>.


INPUT LREAC(1)
32

INPUT CREAC(1)
1.

INPUT THMEAN(1)
4.

  321.      4.
O.K.?
Y

******************
KEYWORD DATA BLOCKS
```

```
**********

ENTER KEYWORD.
END

--------
END
--------

MORE SIMULATIONS?
N
**** STOP
```

Listing of constructed file: EXAMPLE.1

```
ADD OXYGEN AT PYRITE-CALCITE-GOETHITE EQUILIBRIUM
013011000  5 1       0.0
SOLUTION 1
PURE WATER
 0  0 0   7.        4.        25.        1.0
MINERALS
PYRITE     4      0.0    -18.48     11.3          0
   1  -2.0        2  -2.0        8  1.0        42  2.0
GOETHITE   3   3.0        0.486    -14.48         0
 115 1.0           3 2.0          1 -3.0
CALCITE    2   4.0       -8.480    -2.297         1
  15 1.0           4 1.0
-171.9065   -.077993    2839.319      71.595

STEPS
0.0       0.001     0.005     0.01      0.05
REACTION
  321.      4.
END
```

Attachment C. - Example using PHRQINPT to modify an existing reference file.

EXAMPLE 2

```
ENTER OUTPUT FILE NAME
EXAMPLE.2

ENTER REFERENCE FILE NAME:  (HIT <CR> TO OMIT)
EXAMPLE.1

TITLE CARD:
ADD OXYGEN AT PYRITE-CALCITE-GOETHITE EQUILIBRIUM
ENTER OPTION.  (1=KEEP, 2=REPLACE)
1

OPTION CARD:
013011000  5 1       0.0
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=REPLACE)
2

OLD IOPT(1)=0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(2)=1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(3)=3
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(4)=0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(5)=1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(6)=1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(7)=0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(8)=0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD IOPT(9)=0
```

```
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD NSTEPS= 5
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
7

OLD NCOMPS= 1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


013011000  7 1       0.0
O.K.?
Y

******************
KEYWORD DATA BLOCKS
******************



KEYWORD:
SOLUTION 1
ENTER OPTION.  (1=KEEP, 2=ELIMINATE)
1


--------
SOLUTION
--------



SOLUTION CARD:
PURE WATER
 0  0 0   7.        4.        25.        1.0
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=REPLACE)
2

OLD SOLUTION NUMBER=1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


SOLUTION 1
O.K.?
Y

OLD HEAD=
PURE WATER
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
```

```
PURE WATER
O.K.?
Y

OLD NTOTS= 0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD PH=7.
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD PE=4.
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
0.0

OLD TEMP=25.
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


 0  0 0   7.        0.0       25.        1.0
O.K.?
Y

********************
KEYWORD DATA BLOCKS
********************



KEYWORD:
MINERALS
ENTER OPTION.  (1=KEEP, 2=ELIMINATE)
1


--------
MINERALS
--------



MINERALS CARD:
PYRITE     4      0.0    -18.48     11.3          0
   1  -2.0        2  -2.0        8  1.0        42  2.0
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=ELIMINATE)
1
```

```
MINERALS CARD:
GOETHITE   3   3.0        0.486    -14.48         0
 115 1.0          3 2.0          1 -3.0
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=ELIMINATE)
1

MINERALS CARD:
CALCITE    2   4.0       -8.480    -2.297         1
  15 1.0           4 1.0
-171.9065   -.077993    2839.319      71.595
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=ELIMINATE)
2

OLD MNAME=CALCITE
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD NMINO= 2
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD THMIN=4.0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD LKTOM=-8.480
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD DHMIN=-2.297
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD MFLAG=1
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD SIMIN=
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
0.2

CALCITE    2   4.0       -8.480    -2.297         1         0.2
O.K.?
Y

OLD LMIN(1)=  15
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD CMIN(1)= 1.0
```

```
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD LMIN(2)=   4
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD CMIN(2)= 1.0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


  15 1.0          4 1.0
O.K.?
Y

OLD AMIN(1)=-171.9065
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD AMIN(2)=-.077993
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD AMIN(3)=2839.319
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD AMIN(4)=  71.595
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD AMIN(5)=
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


-171.9065   -.077993    2839.319      71.595
O.K.?
Y

******************
KEYWORD DATA BLOCKS
******************



KEYWORD:
STEPS
ENTER OPTION.  (1=KEEP, 2=ELIMINATE)
1
```

```
--------
STEPS
--------


STEPS    CARD:
0.0       0.001     0.005     0.01      0.05
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=REPLACE)
2

OLD XSTEP(1)=0.0
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD XSTEP(2)=0.001
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD XSTEP(3)=0.005
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD XSTEP(4)=0.01
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD XSTEP(5)=0.05
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)


OLD XSTEP(6)=
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
0.1

OLD XSTEP(7)=
KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NOT, REENTER THE DATA)
0.2

0.0       0.001     0.005     0.01      0.05      0.1       0.2
O.K.?
Y

******************
KEYWORD DATA BLOCKS
******************
```

```
KEYWORD:
REACTION
ENTER OPTION.  (1=KEEP, 2=ELIMINATE)
1


--------
REACTION
--------



REACTION CARD:
  321.      4.
ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=REPLACE)
1

**********
KEYWORD DATA BLOCKS
**********



KEYWORD:
END
ENTER OPTION.  (1=KEEP, 2=ELIMINATE)
1


--------
END
--------


MORE SIMULATIONS?
N
**** STOP
```

Listing of constructed file: EXAMPLE.2

```
ADD OXYGEN AT PYRITE-CALCITE-GOETHITE EQUILIBRIUM
013011000  7 1       0.0
SOLUTION 1
PURE WATER
 0  0 0   7.        0.0       25.        1.0
MINERALS
PYRITE     4      0.0    -18.48     11.3          0
   1  -2.0         2  -2.0         8  1.0        42  2.0
GOETHITE   3   3.0         0.486    -14.48         0
 115 1.0           3 2.0           1 -3.0
CALCITE    2   4.0        -8.480    -2.297         1          0.2
  15 1.0           4 1.0
-171.9065   -.077993    2839.319      71.595

STEPS
0.0       0.001     0.005     0.01      0.05      0.1       0.2
REACTION
  321.      4.
END
```

Attachment D. - Source code listing of PHRQINPT.

```
      PROGRAM PHRQINPT                                                  A   1
C                                                                       A   2
C                                                                       A   3
C             **PROGRAM TO FORMAT INPUT-DATA FOR PHREEQE**              A   4
C                                                                       A   5
C     THIS INTERACTIVE PROGRAM WILL SET UP THE INPUT FILE OF PHREEQE    A   6
C     BY ASKING THE USER VALUES OF THE VARIABLES.  ALL QUESTIONS        A   7
C     SHOULD BE SELF-EXPLANATORY.  IF YOU DON'T UNDERSTAND THE          A   8
C     USE OF A CERTAIN VARIABLE, A SHORT EXPLANATION OF THAT            A   9
C     VARIABLE IS AVAILABLE BY ENTERING A "?".  IN SOME CASES,          A  10
C     HELP IS ALSO OBTAINABLE BY ENTERING SOMETHING THAT IS             A  11
C     INCOMPATIBLE WITH THE VARIABLE OR JUST A <CR>.  TO BE             A  12
C     ON THE SAFE SIDE, HOWEVER, A "?" IS RECOMMENDED.                  A  13
C                                                                       A  14
C     AFTER EACH RECORD OF CARD IS COMPLETED, IT WILL BE PRINTED        A  15
C     ON THE SCREEN AND YOU WILL BE ASKED WHETHER THIS CARD             A  16
C     IS ALL RIGHT.  IF YOU ANSWER 'NO', THE PROGRAM WILL TAKE          A  17
C     THE VARIABLES ON THE CARD, PRINT THEM INDIVIDUALLY, AND YOU       A  18
C     WILL BE GIVEN THE CHANCE OF CORRECTING ANY OF THEM.  IF YOU       A  19
C     ANSWER 'YES', THE PROGRAM WILL GO ON TO THE NEXT CARD AND YOU     A  20
C     WILL NOT HAVE ANY MORE CHANCE OF CORRECTING ANY VARIABLES ON      A  21
C     THAT CARD.                                                        A  22
C                                                                       A  23
C                                                                       A  24
C         -WRITTEN BY GEORGE W. FLEMING  AND  L. NIEL PLUMMER-          A  25
C                              SUMMER, 1980.                            A  26
C                        LAST UPDATE--AUGUST, 1983.                     A  27
C                                                                       A  28
C     ************************************************************      A  29
C     ****** NOTE:  MUST COMPILE WITH -SAVE OPTION ON PRIME ******      A  30
C     ************************************************************      A  31
C                                                                       A  32
C                                                                       A  33
      DIMENSION IOPT(9),LT(2,30),DTOT(2,30),ADHSP(250,2),ASP(250,5)     A  34
     1,LSP(250,6),CSP(250,6),AMIN(2,100,5),XTEMP(50),XSTEP(50)          A  35
     2,LREAC(30),CREAC(30),THMEAN(30),JSUB(11)                          A  36
     3,NELT(30),TGFW(30),NI(250),NSP(250),KFLAG(250),ZSP(250),ISDEL(250)A  37
     4,THSP(250),ALKSP(250),NMINO(2,100),THMIN(2,100),MFLAG(2,100)      A  38
     5,LMIN(2,100,10),CMIN(2,100,10),IMINERAL(2),NSUM(10),LSUM(10,50)   A  39
     6,IMORE(11),TEMP(2),PE(2),PH(2),SDENS(2),IUNITS(2),HEAD(2)         A  40
     7,NTOTS(2),IREQUIRED(11),ICHECK(2,4:30),MUSED(100)                 A  41
     8,IORDER(11),NSOLUTION(2),IALK(2),SIMIN(2,100),IMAX(9)             A  42
      COMMON /REFF/ JOPTION,IOPEN,JLINE                                 A  43
      COMMON /REFF1/ I                                                  A  44
      COMMON /PN/ NFLAG                                                 A  45
      COMMON /EE/ EXIT,LIST,LINE,JFLAG                                  A  46
      COMMON /PT/ MNAME0,NMINO0(100),THMIN0,LKTOM0,DHMIN0,MFLAG0(100)   A  47
     1,SIMIN0,LMIN0(100,10),CMIN0,AMIN0,IMIN0,SUB,ICOL1,ICOL2(0:30)     A  48
     2,ICOL3,ICOL4,SPEC,OPV(30)                                         A  49
      REAL ICOL3(0:30)                                                  A  50
```

```
      LOGICAL YN,EXIT,LIST,STOP,OK                                        A  51
      INTEGER GFLAG(250),OUT                                              A  52
      CHARACTER *80 TITLE,LINE,HEAD,JLINE(3)                              A  53
      CHARACTER *72 TFILE                                                 A  54
      CHARACTER *8 SUB(11),KEYWORD(20),TNAME(30),SNAME(250),MNAME(2,100)  A  55
     1,SUNAME(10),DELETE,ICOL1(0:30),ICOL4(0:30),CSP,MNAME0(100)          A  56
     2,SPEC(30),CREAC,THMEAN,EQUIVWT,SUB0(11)                            A  57
      CHARACTER *12 OPTION,VO,PH,PE,TEMP,SDENS,TGFW,ZSP,THSP,DHA(250)     A  58
     1,ADHSP,ALKSP,LKTOSP(250),THMIN,LKTOM(2,100),DHMIN(2,100),SIMIN      A  59
     2,XTEMP,XSTEP,DTOT,CMIN,DHSP(250),AMIN,ASP,BLANK,CMIN0(100,10)       A  60
     3,THMIN0(100),LKTOM0(100),DHMIN0(100),SIMIN0(100),AMIN0(100,5)       A  61
      DATA SUB/'SOLUTION','ELEMENTS','SPECIES ','MINERALS','LOOK MIN',    A  62
     1'TEMP    ','STEPS   ','REACTION','NEUTRAL ','SUMS    ','END     '/  A  63
     2SUB0/'solution','elements','species ','minerals','look min',        A  64
     3'temp    ','steps   ','reaction','neutral ','sums    ','end     '/  A  65
      DATA OPTION/'OPTION CARD'/BLANK/'    0.0     '/                     A  66
      DATA IMAX/ 1,2,6,3,1,1,2,1,1/IORDER/2,3,1,4,5,6,7,8,9,10,11/        A  67
     1IMORE/1,1,1,1,1,0,0,0,0,1,0/DELETE/'DELETE  '/                      A  68
C                                                                         A  69
C         READ NECESSARY DATA AND INITIALIZE VARIABLES.                   A  70
C                                                                         A  71
      CALL READFILE                                                       A  72
      CLOSE (UNIT=11)                                                     A  73
      CLOSE (UNIT=12)                                                     A  74
      WRITE (1,1)                                                         A  75
    1 FORMAT ('ENTER OUTPUT FILE NAME')                                   A  76
      READ (1,20) TFILE                                                   A  77
   20 FORMAT (A72)                                                        A  78
      OPEN (UNIT=10,FILE=TFILE,STATUS='UNKNOWN')                          A  79
C                                                                         A  80
      ITIME=0                                                             A  81
    2 CALL OPEN (ITIME)                                                   A  82
    3 JOPEN=IOPEN                                                         A  83
C                                                                         A  84
      DO 101 K=1,11                                                       A  85
      IREQUIRED(K)=0                                                      A  86
  101 JSUB(K)=0                                                           A  87
      DO 103 K=1,100                                                      A  88
  103 MUSED(K)=0                                                          A  89
      DO 104 K=1,250                                                      A  90
  104 ISDEL(K)=0                                                          A  91
      DO 105 K=4,30                                                       A  92
      DO 105 K2=1,2                                                       A  93
  105 ICHECK(K2,K)=0                                                      A  94
      DO 106 K=1,50                                                       A  95
      XSTEP(K)=BLANK                                                      A  96
  106 XTEMP(K)=BLANK                                                      A  97
      DO 102 K=1,30                                                       A  98
      LREAC(K)=0                                                          A  99
      CREAC(K)=BLANK                                                      A 100
```

```
  102 THMEAN(K)=BLANK                                                    A 101
      ISUB=0                                                             A 102
      IELEMENT=0                                                         A 103
      IMINERAL(1)=0                                                      A 104
      IDELETE=0                                                          A 105
      JDELETE=0                                                          A 106
      IMINERAL(2)=0                                                      A 107
      ISPECIE=0                                                          A 108
      ISUM=0                                                             A 109
      NSTART=1                                                           A 110
      OUT=10                                                             A 111
      I=0                                                                A 112
      ISOL=0                                                             A 113
      IERROR=0                                                           A 114
      JOPTION=0                                                          A 115
C                                                                        A 116
      IF (IOPEN.EQ.0)GO TO 10                                            A 117
C                                                                        A 118
C         EXPLANATION OF SOME FLAGS:                                     A 119
C                                                                        A 120
C         ICHECK      -->MAKE SURE THAT FOR EVERY MASTER SPECIES        A 121
C                         ENTERED, THERE IS A CORRESPONDING ELEMENT.     A 122
C         IERROR      -->FLAG TO SEE IF IT IS OK TO END THE             A 123
C                         SIMULATION.                                    A 124
C         JSUB        -->KEEPS TRACK OF WHICH DATA BLOCK IS USED,       A 125
C                         AND WHICH ISN'T.                               A 126
C         MUSED       -->KEEPS TRACK OF WHICH MINERAL DATA HAS BEEN     A 127
C                         CALLED.                                        A 128
C         ISDEL       -->SPECIES TO BE DELETED.                         A 129
C         IELEMENT    -->NUMBER OF ELEMENTS.                            A 130
C         IMINERAL(1)-->NUMBER OF MINERALS.                             A 131
C         IMINERAL(2)-->NUMBER OF LOOK MINS.                            A 132
C         IMIN0       -->NUMBER OF PRE-CONSTRUCTED MINERAL DATA.        A 133
C         ISPECIE     -->NUMBER OF SPECIES.                             A 134
C         ISUM        -->NUMBER OF SUMS.                                A 135
C         IDELETE     -->SET TO 1 IF ALL MINERALS ARE TO BE DELETED.    A 136
C         JDELETE     -->SET TO 1 IF ALL OLD SUMS ARE TO BE DELETED.    A 137
C         I           -->WHICH DATA BLOCK IS THE USER USING.            A 138
C         NFLAG       -->SET TO 1 IF THE VARIABLE IS SEEN BY THE USER   A 139
C                         THE SECOND TIME.                               A 140
C         JFLAG       -->USER'S RESPONSE FLAG                           A 141
C         IREQUIRED   -->WHICH DATA BLOCKS ARE REQUIRED.                A 142
C         IMASTER     -->IS THE SPECIES OR ELEMENT ENTERED 'MASTER'?    A 143
C         IOPEN       -->IF IT IS > 0, A REFERENCE FILE IS USED.        A 144
C         JOPTION     -->IF IOPEN > 0, WHAT DOES THE USER WANT TO DO    A 145
C                         WITH EACH CARD.                                A 146
C         ITIME       -->NUMBER OF TIMES SUBROUTINE OPEN IS CALLED.     A 147
C         ILINE       -->NUMBER OF LINES TO BE READ FROM THE REFERENCE  A 148
C                         FILE.                                          A 149
C         IMAX        -->MAXIMUM VALUES PERMITTED FOR EACH OPTION.      A 150
```

```
C         IORDER     -->THE ORDER THAT THE DATA BLOCKS ARE TO BE          A 151
C                       PRINTED.                                          A 152
C         IMORE      -->IS IT OK TO CALL A CERTAIN DATA BLOCK MORE        A 153
C                       THAN ONCE.                                        A 154
C                                                                         A 155
C                                                                         A 156
C       *** THE TITLE ***                                                 A 157
C                                                                         A 158
      WRITE (1,94)                                                        A 159
   94 FORMAT (/'TITLE CARD:')                                             A 160
      CALL REF (1,1,4)                                                    A 161
      IF (IOPEN.EQ.0.OR.JOPTION.NE.1)GO TO 10                             A 162
      TITLE=JLINE(1)                                                      A 163
      GO TO 90                                                            A 164
   10 NFLAG=0                                                             A 165
      CALL QUESTA ($1000,0,'THE TITLE',9,TITLE,'A80 ',0,0)                A 166
      WRITE (1,9110)                                                      A 167
      WRITE (1,1731) TITLE                                                A 168
      IF (.NOT.OK()) GO TO 10                                             A 169
C                                                                         A 170
C       *** OPTIONS ***                                                   A 171
C                                                                         A 172
   90 IF (IOPEN.EQ.0)GO TO 91                                             A 173
      WRITE (1,95) OPTION                                                 A 174
   95 FORMAT (/,A11,':')                                                  A 175
      CALL REF (1,1,1)                                                    A 176
      IF (JOPTION.EQ.3.OR.IOPEN.EQ.0)GO TO 91                             A 177
      READ (JLINE(1),9991)(IOPT(N),N=1,9),NSTEPS,NCOMPS,VO                A 178
      IF (JOPTION.EQ.1)GO TO 92                                           A 179
      GO TO 91                                                            A 180
   91 DO 200 N=NSTART,9                                                   A 181
      CALL QUESTB ($290,N,'IOPT',4,IOPT(N),'I1  ',0,IMAX(N),0)            A 182
  200 CONTINUE                                                            A 183
      IF ((IOPT(3).LE.4.AND.IOPT(3).GE.1).OR.IOPT(4).GE.2) GO TO 250      A 184
      NSTEPS=0                                                            A 185
      GO TO 300                                                           A 186
C                                                                         A 187
C       *** NSTEPS ***                                                    A 188
C                                                                         A 189
  250 CALL QUESTB ($2200,0,'NSTEPS',6,NSTEPS,'I2  ',1,50,0)               A 190
  300 IF (IOPT(3).EQ.3.OR.IOPT(3).EQ.4.OR.IOPT(3).EQ.6)GO TO 301          A 191
      NCOMPS=0                                                            A 192
      GO TO 400                                                           A 193
C                                                                         A 194
C       *** NCOMPS ***                                                    A 195
C                                                                         A 196
  301 CALL QUESTB ($2300,0,'NCOMPS',6,NCOMPS,'I2  ',1,100,0)              A 197
  400 IF (IOPT(3).EQ.2) GO TO 430                                         A 198
      VO=' 0.0'                                                           A 199
      GO TO 500                                                           A 200
```

```
C                                                                       A 201
C       *** VO ***                                                      A 202
C                                                                       A 203
  430 CALL QUESTA ($2400,0,'VO',2,VO,'A10 ',1,0)                        A 204
  500 WRITE (1,9110)                                                    A 205
      WRITE (1,9991) (IOPT(I),I=1,9),NSTEPS,NCOMPS,VO                   A 206
      IF (OK()) GO TO 92                                                A 207
      NSTART=1                                                          A 208
      GO TO 91                                                          A 209
C                                                                       A 210
C         SET FLAGS FOR THE DATA BLOCKS THAT ARE REQUIRED.              A 211
C                                                                       A 212
   92 IF (IOPT(3).EQ.5.OR.IOPT(3).EQ.6)IREQUIRED(4)=1                   A 213
      IF (IOPT(2).EQ.2)IREQUIRED(9)=1                                   A 214
      IF (IOPT(3).GE.1.AND.IOPT(3).LE.4)IREQUIRED(7)=1                  A 215
      IF (IOPT(3).EQ.3.OR.IOPT(3).EQ.4.OR.IOPT(3).EQ.6)IREQUIRED(8)=1   A 216
      IF (IOPT(4).NE.0)IREQUIRED(6)=1                                   A 217
C                                                                       A 218
C         KEYWORD DATA BLOCKS.                                          A 219
C         THE PROGRAM IS DESIGNED SO THAT THE DATA BLOCKS CAN BE        A 220
C         ENTERED IN ANY ORDER.  CERTAIN DATA BLOCKS, SUCH AS           A 221
C         'ELEMENTS', 'SPECIES', 'MINERALS', ETC., CAN BE CALLED        A 222
C         UPON MORE THAN ONCE.  IN THAT CASE, NEW ELEMENTS, SPECIES,    A 223
C         MINERALS, ETC., WILL JUST BE ATTACHED TO THE END OF THE       A 224
C         DATA BLOCK.  AT THE END OF THE SIMULATION, THE PROGRAM        A 225
C         RE-ARRANGES THE DATA BLOCKS AND PRINTS THEM IN A PREFERRED    A 226
C         ORDER.                                                        A 227
C                                                                       A 228
C         IF YOU ACCIDENTALLY ENTERED A DATA BLOCK THAT YOU DO NOT      A 229
C         WISH TO USE, ENTER 'EXIT' AS THE FIRST COMMAND AFTER YOU'VE   A 230
C         ENTERED THE DATA BLOCK NAME.                                  A 231
C                                                                       A 232
  531 ISUB=1                                                            A 233
  621 WRITE(1,601)                                                      A 234
  601 FORMAT (/,19('*'),/,'KEYWORD DATA BLOCKS',/,19('*'),//)           A 235
      IF (IOPEN.EQ.0)GO TO 604                                          A 236
  612 READ (13,9001,END=608,ERR=650) KEYWORD(ISUB),NSOL                 A 237
      DO 609 I=1,11                                                     A 238
  609 IF (KEYWORD(ISUB).EQ.SUB(I))GO TO 615                             A 239
  650 GO TO 612                                                         A 240
C                                                                       A 241
C         IF THE KEYWORD DATA BLOCKS ARE NOT ALLOWED, DON'T BOTHER      A 242
C         TO ASK THE USER.                                              A 243
C                                                                       A 244
  615 IF (I.EQ.6.AND.IOPT(4).EQ.0)GO TO 612                             A 245
      IF (I.EQ.7.AND.(IOPT(3).EQ.0.OR.IOPT(3).EQ.5.OR.IOPT(3).EQ.6))    A 246
     1GO TO 612                                                         A 247
      IF (I.EQ.8.AND.NCOMPS.EQ.0)GO TO 612                              A 248
      IF (I.EQ.9.AND.IOPT(2).NE.2)GO TO 612                             A 249
      WRITE (1,613)                                                     A 250
```

```
  613 FORMAT (/,'KEYWORD:')                                              A 251
      IF (I.EQ.1)GO TO 660                                               A 252
      WRITE (1,9050)KEYWORD(ISUB)                                        A 253
      GO TO 670                                                          A 254
  660 WRITE (1,9001)KEYWORD(ISUB),NSOL                                   A 255
  670 CALL REF (0,1,2)                                                   A 256
      IF (I.NE.11)GO TO 120                                              A 257
      IOPEN=0                                                            A 258
  120 IF (JOPTION.EQ.1)GO TO 620                                         A 259
      JOPTION=0                                                          A 260
      IF (I.EQ.11) GO TO 604                                             A 261
      GO TO 621                                                          A 262
  608 IOPEN=0                                                            A 263
      GO TO 531                                                          A 264
  604 WRITE (1,603)                                                      A 265
  603 FORMAT (/,'ENTER KEYWORD.')                                        A 266
      READ (1,20) LINE                                                   A 267
      READ (LINE,*,ERR=622) IHELP                                        A 268
      IF (IHELP.GT.11.OR.IHELP.LT.1)GO TO 4200                           A 269
C                                                                        A 270
C         HE ASKED FOR HELP..                                            A 271
C                                                                        A 272
      GO TO (4148,4150,4146,4152,4154,4156,4158,4160,4162,4164,4166),    A 273
     1IHELP                                                              A 274
  622 READ (LINE,9050,ERR=4200) KEYWORD(ISUB)                            A 275
      READ (LINE,810,ERR=820) NSOL                                       A 276
  810 FORMAT (9X,I1)                                                     A 277
      GO TO 830                                                          A 278
  820 NSOL=0                                                             A 279
  830 DO 610 I=1,11                                                      A 280
      IF (KEYWORD(ISUB).EQ.SUB0(I)) GO TO 620                            A 281
      IF (KEYWORD(ISUB).EQ.SUB(I)) GO TO 620                             A 282
  610 CONTINUE                                                           A 283
      GO TO 4200                                                         A 284
C                                                                        A 285
C         AH, A LEGITIMATE KEYWORD...                                    A 286
C                                                                        A 287
  620 IF(JSUB(I).EQ.1.AND.IMORE(I).EQ.0)GO TO 630                        A 288
      JSUB(I)=1                                                          A 289
      GO TO 640                                                          A 290
  630 WRITE (1,635)                                                      A 291
  635 FORMAT (/,'YOU HAVE ALREADY USED IT ONCE'/)                        A 292
      GO TO 621                                                          A 293
  640 WRITE (1,639) KEYWORD(ISUB)                                        A 294
  639 FORMAT (//,8('-'),/,A8,/,8('-'),//)                                A 295
      II=I-3                                                             A 296
      GO TO (1700,1725,1750,3260,3250,3270,3280,3900,6000,7000,950), I   A 297
      STOP                                                               A 298
C                                                                        A 299
C  ----------------                                                      A 300
```

```
C  SOLUTION DATA BLOCK                                                    A 301
C  ---------------------                                                  A 302
C                                                                        A 303
 1700 CONTINUE                                                           A 304
      ISOL=ISOL+1                                                        A 305
      IF (ISOL.LE.2) GO TO 1510                                          A 306
      WRITE (1,1300)                                                     A 307
 1300 FORMAT ('ONLY 2 SOLUTIONS ARE ALLOWED. ')                          A 308
      ISOL=2                                                             A 309
      GO TO 531                                                          A 310
 1510 IF (IOPEN.EQ.0.AND.NSOL.EQ.0)GO TO 1739                            A 311
      IF (NSOL.EQ.1.OR.NSOL.EQ.2) GO TO 1500                             A 312
      JOPTION=0                                                          A 313
      GO TO 1492                                                         A 314
 1500 NSOLUTION(ISOL)=NSOL                                               A 315
      IF (IOPEN.EQ.0) GO TO 1400                                         A 316
      WRITE (1,1736) SUB(I)                                              A 317
 1736 FORMAT (/,A8,' CARD:')                                             A 318
      CALL REF (2,1,0)                                                   A 319
      READ (JLINE(1),1731) HEAD(ISOL)                                    A 320
 1731 FORMAT (A80)                                                       A 321
      READ (JLINE(2),9003) NTOTS(ISOL),IALK(ISOL),IUNITS(ISOL),PH        A 322
     1 (ISOL),PE(ISOL),TEMP(ISOL),SDENS(ISOL)                            A 323
      IF (NTOTS(ISOL).EQ.0)GO TO 1734                                    A 324
      CALL REF(1,1,0)                                                    A 325
      READ (JLINE(1),9004) (LT(ISOL,M),DTOT(ISOL,M),M=1,5)               A 326
      IF (NTOTS(ISOL).LE.5)GO TO 1734                                    A 327
      LLINE=INT((NTOTS(ISOL)-1)/5)                                       A 328
      DO 1738 KLINE=1,LLINE                                              A 329
      CALL REF (1,1,0)                                                   A 330
 1738 READ (JLINE(1),9004) (LT(ISOL,M),DTOT(ISOL,M),M=KLINE*5+1,         A 331
     1 (KLINE+1)*5)                                                      A 332
 1734 CALL REF (0,1,1)                                                   A 333
      IF (JOPTION.EQ.1.AND.IALK(ISOL).GT.0)GO TO 1752                    A 334
      IF (JOPTION.EQ.1)GO TO 531                                         A 335
C                                                                        A 336
C       *** SOLUTION NUMBER ***                                          A 337
C                                                                        A 338
 1739 CALL QUESTB ($1492,0,'SOLUTION NUMBER',15,NSOLUTION(ISOL),'I1  '   A 339
     1,1,2,1)                                                            A 340
      IF (.NOT.EXIT)GO TO 1730                                           A 341
      JSUB(1)=0                                                          A 342
 1753 GO TO 531                                                          A 343
 1730 WRITE (1,1001) NSOLUTION(ISOL)                                     A 344
 1001 FORMAT (/,'SOLUTION',1X,I1)                                        A 345
      IF (.NOT.OK()) GO TO 1739                                          A 346
 1400 IREQUIRED(1)=0                                                     A 347
C                                                                        A 348
C       *** HEAD ***                                                     A 349
C                                                                        A 350
```

```
      IF (JOPTION.EQ.2) NFLAG=1                                          A 351
 1488 CALL QUESTA ($4300,0,'HEAD',4,HEAD(ISOL),'A80 ',0,0)               A 352
      WRITE (1,9110)                                                     A 353
      WRITE (1,1731)HEAD(ISOL)                                           A 354
      IF (.NOT.OK()) GO TO 1488                                          A 355
C                                                                        A 356
C       *** NTOTS ***                                                    A 357
C                                                                        A 358
 1713 CALL QUESTB ($4320,0,'NTOTS',5,NTOTS(ISOL),'I2  ',0,100,0)         A 359
 1714 IF (NTOTS(ISOL).NE.0)GO TO 1727                                    A 360
      IALK(ISOL)=0                                                       A 361
      IUNITS(ISOL)=0                                                     A 362
      GO TO 1718                                                         A 363
C                                                                        A 364
C       *** IALK ***                                                     A 365
C                                                                        A 366
 1727 CALL QUESTB ($4340,0,'IALK',4,IALK(ISOL),'I3  ',0,0,0)             A 367
      JUMP=0                                                             A 368
      IF (IALK(ISOL)) 4340,1715,1708                                     A 369
 1708 IF (IALK(ISOL).GT.30.OR.IALK(ISOL).LT.4) GO TO 4340                A 370
C                                                                        A 371
C       *** IUNITS ***                                                   A 372
C                                                                        A 373
 1715 CALL QUESTB ($4360,0,'IUNITS',6,IUNITS(ISOL),'I2  ',0,3,0)         A 374
C                                                                        A 375
C       *** PH ***                                                       A 376
C                                                                        A 377
 1718 CALL QUESTA ($4380,0,'PH',2,PH(ISOL),'A10 ',1,0)                   A 378
C                                                                        A 379
C       *** PE ***                                                       A 380
C                                                                        A 381
 1723 CALL QUESTA ($4400,0,'PE',2,PE(ISOL),'A10 ',1,0)                   A 382
C                                                                        A 383
C       *** TEMP ***                                                     A 384
C                                                                        A 385
 1724 CALL QUESTA ($4420,0,'TEMP',4,TEMP(ISOL),'A10 ',1,0)               A 386
      IF (IUNITS(ISOL).NE.0) GO TO 1482                                  A 387
      SDENS(ISOL)=' 1.0'                                                 A 388
      GO TO 1490                                                         A 389
C                                                                        A 390
C       *** SDENS ***                                                    A 391
C                                                                        A 392
 1482 CALL QUESTA ($4440,0,'SDENS',5,SDENS(ISOL),'A10 ',1,0)             A 393
 1490 WRITE (1,9110)                                                     A 394
      WRITE (1,9003) NTOTS(ISOL),IALK(ISOL),IUNITS(ISOL),PH(ISOL)        A 395
     1,PE(ISOL),TEMP(ISOL),SDENS(ISOL)                                   A 396
      IF (.NOT.OK()) GO TO 1713                                          A 397
      IF (IALK(ISOL).EQ.0)GO TO 1726                                     A 398
 1752 WRITE (1,1006)                                                     A 399
 1006 FORMAT (/,'HAS THE APPROPRIATE CARBON ELEMENT-CARD BEEN',          A 400
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     1' CONSTRUCTED?')                                                  A 401
      JUMP=1                                                            A 402
      IF (.NOT.YN()) GO TO 1728                                         A 403
      GO TO (1726,1753,1726,1726),JOPTION+1                             A 404
C                                                                       A 405
C         ADD AN EXTRA ELEMENT CARD FOR HIM...                          A 406
C                                                                       A 407
 1728 WRITE (1,1709)                                                    A 408
 1709 FORMAT (/,'WHAT IS THE GRAM EQUIVALENT WEIGHT (GRAMS/EQUIVALENT'  A 409
     1,') OF THE',/,'CHEMICAL SPECIES IN WHICH THE ALKALINITY IS',      A 410
     2' REPORTED?')                                                     A 411
      WRITE (1,1710)                                                    A 412
 1710 FORMAT (//,'FOR EXAMPLE:',/,19X,'CACO3      50.0446 G/EQ',/,19X   A 413
     1,'HCO3-     61.0171 G/EQ',/,19X,'CO3--     30.0046 G/EQ.',//)     A 414
      READ (1,1731) LINE                                                A 415
      READ (LINE,*,ERR=1728) EQ                                         A 416
      EQUIVWT=LINE(1:8)                                                 A 417
      JSUB(2)=2                                                         A 418
      WRITE (1,1712)                                                    A 419
 1712 FORMAT (//,'ELEMENTS DATA BLOCK WILL BE CONSTRUCTED AUTOMATICALLY' A 420
     1,//)                                                              A 421
      IF (IELEMENT.LT.27)GO TO 1004                                     A 422
      WRITE (1,1002)                                                    A 423
 1002 FORMAT (1X,52('*'),/,1X,'WARNING:  NUMBER OF ELEMENTS EXCEEDS ',  A 424
     1'MAXIMUM POSSIBLE.',/,1X,'CARBON CARD IS DELETED.',/,1X,52('*')/) A 425
      GO TO (1726,1753),JOPTION+1                                       A 426
 1004 IELEMENT=IELEMENT+1                                               A 427
      TNAME(IELEMENT)='C'                                               A 428
      NELT(IELEMENT)=IALK(ISOL)                                         A 429
      TGFW(IELEMENT)=EQUIVWT                                            A 430
      GO TO 1600                                                        A 431
 1601 IF (JOPTION.EQ.1)GO TO 1753                                       A 432
 1726 IF (IUNITS(ISOL).GE.2.AND.IUNITS(ISOL).LE.3.AND.IELEMENT.EQ.0)    A 433
     1 IREQUIRED(2)=1                                                   A 434
      IF (NTOTS(ISOL).EQ.0)GO TO 531                                    A 435
 1320 M=1                                                               A 436
 1310 N2=1                                                              A 437
C                                                                       A 438
C       *** LT ***                                                      A 439
C                                                                       A 440
 1326 CALL QUESTB ($4100,M,'LT',2,LT(ISOL,M),'I4  ',1,10000,2)          A 441
      IF (.NOT.LIST)GO TO 1057                                          A 442
 1361 CALL LISTM                                                        A 443
      GO TO (1326,1356),N2                                              A 444
 1057 N2=2                                                              A 445
C                                                                       A 446
C       *** DTOT ***                                                    A 447
C                                                                       A 448
 1356 CALL QUESTA ($4100,M,'DTOT',4,DTOT(ISOL,M),'All ',1,2)            A 449
      IF (LIST)GO TO 1361                                               A 450
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      M=M+1                                                                  A 451
      IF (M.LE.NTOTS(ISOL)) GO TO 1310                                       A 452
      WRITE (1,9110)                                                         A 453
      WRITE (1,9004) (LT(ISOL,M),DTOT(ISOL,M),M=1,NTOTS(ISOL))               A 454
      IF (.NOT.OK())GO TO 1320                                               A 455
      GO TO 531                                                              A 456
 1725 CONTINUE                                                               A 457
C                                                                           A 458
C   --------------------                                                    A 459
C    ELEMENTS DATA BLOCK                                                    A 460
C   --------------------                                                    A 461
C                                                                           A 462
      IELEMENT=IELEMENT+1                                                    A 463
      IF (IOPEN.EQ.0)GO TO 1729                                              A 464
 1536 CALL REF (1,0,0)                                                       A 465
      IF (JOPTION.EQ.0)GO TO 1530                                            A 466
      WRITE (1,1736) SUB(I)                                                  A 467
      WRITE (1,1731)JLINE(1)                                                 A 468
      CALL REF (0,0,3)                                                       A 469
      GO TO (1530,1531,1531,1536), JOPTION+1                                 A 470
 1531 READ (JLINE(1),9102) TNAME(IELEMENT),NELT(IELEMENT),TGFW(IELEMENT)     A 471
      IREQUIRED(2)=0                                                         A 472
      IF (JOPTION.EQ.1) GO TO 1600                                           A 473
C                                                                           A 474
C       *** TNAME ***                                                       A 475
C                                                                           A 476
 1729 CALL QUESTA ($4102,0,'TNAME',5,TNAME(IELEMENT),'A8  ',0,3)            A 477
      IF (.NOT.LIST)GO TO 1549                                               A 478
      CALL LISTM                                                             A 479
      GO TO 1729                                                             A 480
 1549 IF (.NOT.EXIT)GO TO 1550                                               A 481
 1530 IELEMENT=IELEMENT-1                                                    A 482
      IF (IELEMENT.EQ.0)JSUB(2)=0                                            A 483
      GO TO 531                                                              A 484
 1550 IREQUIRED(2)=0                                                         A 485
C                                                                           A 486
C       *** NELT ***                                                        A 487
C                                                                           A 488
      CALL QUESTB ($4104,0,'NELT',4,NELT(IELEMENT),'I2  ',4,30,2)            A 489
      IF (.NOT.LIST) GO TO 1558                                              A 490
      CALL LISTM                                                             A 491
      GO TO 1550                                                             A 492
 1558 DO 1547 M=1,IELEMENT-1                                                 A 493
 1547 IF (NELT(IELEMENT).EQ.NELT(M))GO TO 1548                               A 494
      GO TO 1570                                                             A 495
 1548 WRITE (1,1551) NELT(M)                                                 A 496
 1551 FORMAT (/,'WARNING:  ELEMENT #',I2,' IS ALREADY ENTERED.'/)            A 497
C                                                                           A 498
C       *** TGFW ***                                                        A 499
C                                                                           A 500
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 1570 CALL QUESTA ($4106,0,'TGFW',4,TGFW(IELEMENT),'A10 ',1,2)          A 501
      IF (.NOT.LIST) GO TO 1580                                        A 502
      CALL LISTM                                                       A 503
      GO TO 1570                                                       A 504
 1580 WRITE (1,9110)                                                   A 505
      WRITE (1,9102) TNAME(IELEMENT),NELT(IELEMENT),TGFW(IELEMENT)     A 506
      IF (.NOT.OK()) GO TO 1729                                        A 507
C                                                                      A 508
C         KEEP TRACK OF ELEMENTS AND SPECIES                           A 509
C                                                                      A 510
 1600 IF(ICHECK(2,NELT(IELEMENT)).EQ.1)GO TO 1557                      A 511
      ICHECK(1,NELT(IELEMENT))=1                                       A 512
      GO TO 1575                                                       A 513
 1557 ICHECK(2,NELT(IELEMENT))=0                                       A 514
 1575 IF (I.EQ.1)GO TO 1601                                            A 515
      IF (IELEMENT.EQ.27) GO TO 531                                    A 516
      IF (IOPEN.NE.0)GO TO 1725                                        A 517
      WRITE (1,1573)                                                   A 518
 1573 FORMAT (/,'MORE ELEMENTS?')                                      A 519
      IF (YN()) GO TO 1725                                             A 520
      GO TO 531                                                        A 521
 1750 CONTINUE                                                         A 522
C                                                                      A 523
C  ------------------                                                  A 524
C  SPECIES DATA BLOCK                                                  A 525
C  ------------------                                                  A 526
C                                                                      A 527
      ISPECIE=ISPECIE+1                                                A 528
      IF (IOPEN.EQ.0)GO TO 1590                                        A 529
 1523 CALL REF (1,0,0)                                                 A 530
      IF (JOPTION.EQ.0)GO TO 1529                                      A 531
      WRITE (1,1736)SUB(I)                                             A 532
      WRITE (1,1731)JLINE(1)                                           A 533
      READ (JLINE(1),9202) NI(ISPECIE)                                 A 534
      CALL REF (3,1,3)                                                 A 535
      GO TO (1521,1521,1523),JOPTION                                   A 536
      CALL REF (0,0,2)                                                 A 537
      IF (JOPTION.EQ.2) GO TO 1523                                     A 538
      ISDEL(ISPECIE)=1                                                 A 539
      GO TO 1750                                                       A 540
 1521 READ (JLINE(1),9203) SNAME(ISPECIE),NSP(ISPECIE),KFLAG           A 541
     1(ISPECIE),GFLAG(ISPECIE),ZSP(ISPECIE),THSP(ISPECIE),DHA(ISPECIE) A 542
     2,ADHSP(ISPECIE,1),ADHSP(ISPECIE,2),ALKSP(ISPECIE)                A 543
      READ (JLINE(2),9204) LKTOSP(ISPECIE),DHSP(ISPECIE),              A 544
     1(ASP(ISPECIE,MMM),MMM=1,5)                                       A 545
      READ (JLINE(3),9205) (LSP(ISPECIE,MMM),CSP(ISPECIE,MMM),         A 546
     1MMM=1,NSP(ISPECIE))                                              A 547
      IF (JOPTION.EQ.1) GO TO 1670                                     A 548
C                                                                      A 549
C       *** I ***                                                      A 550
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C                                                                       A 551
 1590 CALL QUESTB ($4110,0,'I',1,NI(ISPECIE),'I3  ',4,250,1)            A 552
      IF (.NOT.EXIT) GO TO 1654                                         A 553
 1529 ISPECIE=ISPECIE-1                                                 A 554
      IF (ISPECIE.EQ.0)JSUB(3)=0                                        A 555
      IF (IOPEN.NE.0)GO TO 531                                          A 556
      GO TO 1933                                                        A 557
 1654 WRITE (1,9110)                                                    A 558
      WRITE (1,9202) NI (ISPECIE)                                       A 559
      IF (.NOT.OK()) GO TO 1590                                         A 560
      IF(ISDEL(ISPECIE).NE.1) GO TO 1660                                A 561
      IF (JOPTION.EQ.2)GO TO 1750                                       A 562
      GO TO 1934                                                        A 563
C                                                                       A 564
C       *** SNAME ***                                                   A 565
C                                                                       A 566
 1660 CALL QUESTA ($4112,0,'SNAME',5,SNAME(ISPECIE),'A8  ',0,0)         A 567
C                                                                       A 568
C         IS IT A MASTER SPECIE....                                     A 569
C                                                                       A 570
 1670 IMASTER=0                                                         A 571
      IF (NI(ISPECIE).LE.30.AND.NI(ISPECIE).GT.3.AND.ISDEL(ISPECIE)     A 572
     1.NE.1)IMASTER=1                                                   A 573
      IF (JOPTION.EQ.1.AND.IMASTER.EQ.0)GO TO 1750                      A 574
      IF (IMASTER.EQ.0.OR.(NFLAG.EQ.1.AND.JOPTION.NE.2))GO TO 1676      A 575
C                                                                       A 576
C         KEEP TRACK OF ELEMENTS AND SPECIES...                         A 577
C                                                                       A 578
      IF (ICHECK(1,NI(ISPECIE)).EQ.1)GO TO 1679                         A 579
      ICHECK(2,NI(ISPECIE))=1                                           A 580
      GO TO 1595                                                        A 581
 1679 ICHECK(1,NI(ISPECIE))=0                                           A 582
 1595 IF (JOPTION.EQ.1)GO TO 1750                                       A 583
C                                                                       A 584
C         IF IT IS A MASTER SPECIES, A LOT OF VARIABLES CAN BE          A 585
C         DETERMINED WITHOUT ASKING THE USER...                         A 586
C                                                                       A 587
      NSP(ISPECIE)=1                                                    A 588
      KFLAG(ISPECIE)=0                                                  A 589
      CSP(ISPECIE,1)=' 1.0'                                             A 590
      LSP(ISPECIE,1)=NI(ISPECIE)                                        A 591
      LKTOSP(ISPECIE)=' 0.0'                                            A 592
      DHSP(ISPECIE)=' 0.0'                                              A 593
      DO 1678 NII=1,5                                                   A 594
 1678 ASP(ISPECIE,NII)=' 0.0'                                           A 595
      GO TO 1690                                                        A 596
C                                                                       A 597
C       *** NSP ***                                                     A 598
C                                                                       A 599
 1676 CALL QUESTB ($4114,0,'NSP',3,NSP(ISPECIE),'I3  ',0,6,0)           A 600
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C                                                                       A 601
C       *** KFLAG ***                                                   A 602
C                                                                       A 603
 1680 CALL QUESTB ($4116,0,'KFLAG',5,KFLAG(ISPECIE),'I2  ',0,1,0)       A 604
C                                                                       A 605
C       *** GFLAG ***                                                   A 606
C                                                                       A 607
 1690 CALL QUESTB ($4118,0,'GFLAG',5,GFLAG(ISPECIE),'I2  ',0,1,0)       A 608
C                                                                       A 609
C       *** ZSP ***                                                     A 610
C                                                                       A 611
 1780 CALL QUESTA ($4120,0,'ZSP',3,ZSP(ISPECIE),'A10 ',1,0)             A 612
C                                                                       A 613
C       *** THSP ***                                                    A 614
C                                                                       A 615
 1790 CALL QUESTA ($4122,0,'THSP',4,THSP(ISPECIE),'A10 ',1,0)           A 616
C                                                                       A 617
C       *** DHA ***                                                     A 618
C                                                                       A 619
 1880 CALL QUESTA ($4124,0,'DHA',3,DHA(ISPECIE),'A10 ',1,0)             A 620
      IF (GFLAG(ISPECIE).EQ.1)GO TO 1891                                A 621
      ADHSP(ISPECIE,1)=' 0.0'                                           A 622
      ADHSP(ISPECIE,2)=' 0.0'                                           A 623
      GO TO 1740                                                        A 624
C                                                                       A 625
C       *** ADHSP ***                                                   A 626
C                                                                       A 627
 1891 M=1                                                               A 628
 1892 CALL QUESTA ($1897,M,'ADHSP',5,ADHSP(ISPECIE,M),'A10 ',1,0)       A 629
      M=M+1                                                             A 630
      IF (M.EQ.3)GO TO 1740                                             A 631
      GO TO 1892                                                        A 632
 1897 GO TO (4126,4128), M                                              A 633
C                                                                       A 634
C       *** ALKSP ***                                                   A 635
C                                                                       A 636
 1740 CALL QUESTA ($4130,0,'ALKSP',5,ALKSP(ISPECIE),'A10 ',1,0)         A 637
      WRITE (1,9110)                                                    A 638
      WRITE (1,9203)SNAME(ISPECIE),NSP(ISPECIE),KFLAG(ISPECIE),         A 639
     1GFLAG(ISPECIE),ZSP(ISPECIE),THSP(ISPECIE),DHA(ISPECIE),           A 640
     2ADHSP(ISPECIE,1),ADHSP(ISPECIE,2),ALKSP(ISPECIE)                  A 641
      IF (.NOT.OK()) GO TO 1660                                         A 642
 1960 IF(IMASTER.EQ.0)GO TO 1967                                        A 643
      GO TO 1930                                                        A 644
C                                                                       A 645
C       *** LKTOSP ***                                                  A 646
C                                                                       A 647
 1967 CALL QUESTA ($4132,0,'LKTOSP',6,LKTOSP(ISPECIE),'A10 ',1,0)       A 648
C                                                                       A 649
C        *** DHSP ***                                                   A 650
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C                                                                       A 651
 1970 CALL QUESTA ($4136,0,'DHSP',4,DHSP(ISPECIE),'A10 ',1,0)           A 652
      IF (KFLAG(ISPECIE).EQ.1)GO TO 1986                                A 653
C                                                                       A 654
C       *** ASP ***                                                     A 655
C                                                                       A 656
      DO 1988 K=1,5                                                     A 657
 1988 ASP(ISPECIE,K)=' 0.0'                                             A 658
      GO TO 1990                                                        A 659
 1986 K=1                                                               A 660
 1987 CALL QUESTA ($4138,K,'ASP',3,ASP(ISPECIE,K),'A12 ',1,0)           A 661
      K=K+1                                                             A 662
      IF (K.LT.6)GO TO 1987                                             A 663
 1990 WRITE (1,9110)                                                    A 664
      WRITE (1,9204) LKTOSP(ISPECIE),DHSP(ISPECIE),(ASP(ISPECIE,I8),    A 665
     1I8=1,5)                                                           A 666
      IF (.NOT.OK()) GO TO 1960                                         A 667
 1910 K=1                                                               A 668
      IF (NSP(ISPECIE).EQ.0)GO TO 1930                                  A 669
 1912 K2=1                                                              A 670
C                                                                       A 671
C       *** LSP, CSP ***                                                A 672
C                                                                       A 673
 1915 IF (K2.EQ.1) CALL QUESTB ($4142,K,'LSP',3,LSP(ISPECIE,K),'I3  ',1 A 674
     1,30,2)                                                            A 675
      IF (K2.EQ.2) CALL QUESTA ($4144,K,'CSP',3,CSP(ISPECIE,K),'A7  ',1 A 676
     1,2)                                                               A 677
      IF (.NOT.LIST)GO TO 1922                                          A 678
      CALL LISTM                                                        A 679
      GO TO 1915                                                        A 680
 1922 IF (K2.EQ.2) GO TO 1923                                           A 681
      K2=2                                                              A 682
      GO TO 1915                                                        A 683
 1923 K=K+1                                                             A 684
      IF (K.GT.NSP(ISPECIE)) GO TO 1940                                 A 685
      GO TO 1912                                                        A 686
 1940 WRITE (1,9110)                                                    A 687
      WRITE (1,9205)(LSP(ISPECIE,MM),CSP(ISPECIE,MM),MM=1,NSP(ISPECIE)) A 688
      IF (.NOT.OK())GO TO 1910                                          A 689
 1930 IF (IOPEN.NE.0)GO TO 1750                                         A 690
      WRITE (1,1931)                                                    A 691
 1931 FORMAT (/,'MORE SPECIES?')                                        A 692
      IF (YN())GO TO 1750                                               A 693
 1933 WRITE (1,1932)                                                    A 694
 1932 FORMAT (/,'ANY SPECIES TO DELETE?')                               A 695
 1936 IF (.NOT.YN())GO TO 531                                           A 696
      ISDEL(ISPECIE+1)=1                                                A 697
      JSUB(3)=1                                                         A 698
      GO TO 1750                                                        A 699
 1934 WRITE (1,1935)                                                    A 700
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 1935 FORMAT (/,'MORE SPECIES TO DELETE?')                              A 701
      GO TO 1936                                                       A 702
C                                                                      A 703
C     ------------------                                               A 704
C     MINERALS DATA BLOCK                                              A 705
C     ------------------                                               A 706
C                                                                      A 707
 3260 CONTINUE                                                         A 708
      IF (IMIN0.EQ.0.OR.IOPEN.NE.0)GO TO 3100                          A 709
C                                                                      A 710
C         MINERAL DATA AVAILABLE...                                    A 711
C                                                                      A 712
      WRITE (1,3002)                                                   A 713
 3002 FORMAT (/,'PRE-CONSTRUCTED MINERAL DATA ARE AVAILABLE.'/,        A 714
     1'DO YOU WISH TO HAVE ANY OF THEM?')                             A 715
      IF (.NOT.YN())GO TO 3100                                         A 716
C                                                                      A 717
C         PRINT THE LIST OF MINERALS.....                              A 718
C                                                                      A 719
 3004 WRITE(1,3003)(K,MNAME0(K),K=1,IMIN0)                             A 720
 3003 FORMAT (/20(1X,5(I3,1X,A8,2X,:)/))                               A 721
 3021 WRITE (1,3005)                                                   A 722
 3005 FORMAT (/,'ENTER THE INDEX NUMBER OF MINERAL. (TYPE <STOP> TO'   A 723
     1,' EXIT)')                                                      A 724
      READ (1,1731) LINE                                               A 725
      IF (LINE(1:4).EQ.'STOP'.OR.LINE(1:4).EQ.'stop') GO TO 3010       A 726
      READ (LINE,*,ERR=3004) INDEX                                     A 727
      IF (INDEX.GT.IMIN0.OR.INDEX.LT.1)GO TO 3004                      A 728
      IF (MUSED(INDEX).EQ.1)GO TO 3012                                 A 729
      MUSED(INDEX)=1                                                   A 730
      GO TO 3013                                                       A 731
 3012 WRITE (1,3014) INDEX                                             A 732
 3014 FORMAT (//,'MINERAL # ',I3,' HAS ALREADY BEEN ENTERED.'//)       A 733
      GO TO 3021                                                       A 734
 3013 IMINERAL(1)=IMINERAL(1)+1                                        A 735
      IM=IMINERAL(1)                                                   A 736
      IREQUIRED(4)=0                                                   A 737
      MNAME(1,IM)=MNAME0(INDEX)                                        A 738
      NMINO(1,IM)=NMINO0(INDEX)                                        A 739
      THMIN(1,IM)=THMIN0(INDEX)                                        A 740
      LKTOM(1,IM)=LKTOM0(INDEX)                                        A 741
      DHMIN(1,IM)=DHMIN0(INDEX)                                        A 742
      MFLAG(1,IM)=MFLAG0(INDEX)                                        A 743
      SIMIN(1,IM)=SIMIN0(INDEX)                                        A 744
      DO 3006 K2=1,NMINO(1,IM)                                         A 745
      LMIN(1,IM,K2)=LMIN0(INDEX,K2)                                    A 746
 3006 CMIN(1,IM,K2)=CMIN0(INDEX,K2)                                    A 747
 3015 LFLAG=1                                                          A 748
      GO TO 3032                                                       A 749
 3020 DO 3008 K2=1,5                                                   A 750
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3008 AMIN(1,IM,K2)=AMIN0(INDEX,K2)                                          A 751
     GO TO 3210                                                             A 752
3024 IF (MFLAG(II,IM).EQ.1) GO TO 3020                                      A 753
3000 IF (OK()) GO TO 3016                                                   A 754
     WRITE (1,3017)                                                         A 755
3017 FORMAT ('DO YOU WISH TO CHANGE SIMIN?')                                A 756
     IF (.NOT.YN())GO TO 3019                                               A 757
     LFLAG=3                                                                A 758
     GO TO 3167                                                             A 759
3009 WRITE (1,3022)                                                         A 760
3022 FORMAT ('DO YOU WISH TO CHANGE ANYTHING ELSE?')                        A 761
     IF (.NOT.YN())GO TO 3015                                               A 762
3019 LFLAG=2                                                                A 763
     GO TO 3102                                                             A 764
3016 LFLAG=0                                                                A 765
     GO TO 3021                                                             A 766
3010 WRITE (1,3011)                                                         A 767
3011 FORMAT (/,'MORE MINERALS TO BE TYPED IN FROM THE TERMINAL?')           A 768
     IF (.NOT.YN()) GO TO 3061                                              A 769
3100 IF (IOPEN.EQ.0)GO TO 3221                                              A 770
     IMINERAL(II)=IMINERAL(II)+1                                            A 771
     IM=IMINERAL(II)                                                        A 772
3062 CALL REF (1,0,0)                                                       A 773
     IF (JOPTION.NE.0)GO TO 3056                                            A 774
3059 IMINERAL(II)=IMINERAL(II)-1                                            A 775
3061 IF (IMINERAL(II).EQ.0)JSUB(I)=0                                        A 776
     GO TO 531                                                              A 777
3056 WRITE (1,1736) SUB(I)                                                  A 778
     WRITE (1,1731)JLINE(1)                                                 A 779
      READ (JLINE(1),9302)MNAME(II,IM),NMINO(II,IM),THMIN(II,IM)            A 780
    1,LKTOM(II,IM),DHMIN(II,IM),MFLAG(II,IM),SIMIN(II,IM)                   A 781
     IF (MNAME(II,IM).NE.DELETE)GO TO 3051                                  A 782
     CALL REF (0,0,2)                                                       A 783
     GO TO (3063,3062),JOPTION                                              A 784
3063 IDELETE=1                                                              A 785
     GO TO 3062                                                             A 786
3051 NLINE=2                                                                A 787
     IF (NMINO(II,IM).GT.5)NLINE=3                                          A 788
     IF (MFLAG(II,IM).NE.1)NLINE=NLINE-1                                    A 789
     CALL REF (NLINE,1,3)                                                   A 790
     READ (JLINE(1),9303)(LMIN(II,IM,MMM),CMIN(II,IM,MMM),MMM=1,5)          A 791
     IF (NMINO(II,IM).LE.5)GO TO 3054                                       A 792
     READ (JLINE(2),9303)(LMIN(II,IM,MMM),CMIN(II,IM,MMM),MMM=6             A 793
    1,NMINO(II,IM))                                                         A 794
3054 IF (MFLAG(II,IM).NE.1)GO TO 3057                                       A 795
     READ (JLINE(NLINE),9304) (AMIN(II,IM,MMM),MMM=1,5)                     A 796
3057 GO TO (3102,3062), JOPTION-1                                           A 797
     IREQUIRED(I)=0                                                         A 798
     GO TO 3100                                                             A 799
C                                                                           A 800
```

```
C       *** MNAME ***                                                          A 801
C                                                                              A 802
 3221 IMINERAL(II)=IMINERAL(II)+1                                              A 803
      IM=IMINERAL(II)                                                          A 804
      LFLAG=0                                                                  A 805
 3102 CALL QUESTA ($8000,0,'MNAME',5,MNAME(II,IM),'A8  ',0,1)                  A 806
      IF (EXIT) GO TO 3059                                                     A 807
 3106 IREQUIRED(I)=0                                                           A 808
C                                                                              A 809
C       *** NMINO ***                                                          A 810
C                                                                              A 811
 3110 CALL QUESTB ($8002,0,'NMINO',5,NMINO(II,IM),'I2  ',1,10,0)               A 812
C                                                                              A 813
C       *** THMIN ***                                                          A 814
C                                                                              A 815
 3120 CALL QUESTA ($8004,0,'THMIN',5,THMIN(II,IM),'A10 ',1,0)                  A 816
C                                                                              A 817
C       *** LKTOM ***                                                          A 818
C                                                                              A 819
 3130 CALL QUESTA ($8006,0,'LKTOM',5,LKTOM(II,IM),'A10 ',1,0)                  A 820
C                                                                              A 821
C       *** DHMIN ***                                                          A 822
C                                                                              A 823
 3140 CALL QUESTA ($8008,0,'DHMIN',5,DHMIN(II,IM),'A10 ',1,0)                  A 824
C                                                                              A 825
C       *** MFLAG ***                                                          A 826
C                                                                              A 827
 3150 CALL QUESTB ($8010,0,'MFLAG',5,MFLAG(II,IM),'I1  ',0,1,0)                A 828
      IF (LFLAG.EQ.2) GO TO 3032                                               A 829
C                                                                              A 830
C       *** SIMIN ***                                                          A 831
C                                                                              A 832
 3167 CALL QUESTA ($8012,0,'SIMIN',5,SIMIN(II,IM),'A10 ',1,0)                  A 833
      IF (LFLAG.EQ.3)GO TO 3009                                                A 834
 3032 WRITE (1,9110)                                                           A 835
      WRITE (1,9302) MNAME(II,IM),NMINO(II,IM),THMIN(II,IM),LKTOM(II,IM)       A 836
     1,DHMIN(II,IM),MFLAG(II,IM),SIMIN(II,IM)                                  A 837
      IF (LFLAG.EQ.1)GO TO 3187                                                A 838
      IF (LFLAG.EQ.2) LFLAG=4                                                  A 839
      IF (.NOT.OK()) GO TO 3102                                                A 840
      IF (LFLAG.EQ.4) NFLAG=1                                                  A 841
C                                                                              A 842
C       *** LMIN, CMIN ***                                                     A 843
C                                                                              A 844
 3190 K=1                                                                      A 845
 3192 K2=1                                                                     A 846
 3195 IF (K2.EQ.1) CALL QUESTB ($8014,K,'LMIN',4,LMIN(II,IM,K),'I4  ',0        A 847
     1,0,2)                                                                   A 848
      IF (K2.EQ.2) CALL QUESTA ($8016,K,'CMIN',4,CMIN(II,IM,K),'A11 ',1        A 849
     1,2)                                                                     A 850
```

```
      IF (.NOT.LIST)GO TO 3191                                          A 851
      CALL LISTM                                                        A 852
      GO TO 3195                                                        A 853
 3191 IF (K2.EQ.2) GO TO 3186                                           A 854
      K2=2                                                              A 855
      GO TO 3195                                                        A 856
 3186 K=K+1                                                             A 857
      IF (K.LE.NMINO(II,IM)) GO TO 3192                                 A 858
      WRITE (1,9110)                                                    A 859
 3187 WRITE (1,9303) (LMIN(II,IM,K),CMIN(II,IM,K),K=1,NMINO(II,IM))     A 860
      IF (LFLAG.EQ.1) GO TO 3024                                        A 861
      IF (.NOT.OK()) GO TO 3190                                         A 862
      IF(MFLAG(II,IM).EQ.1)GO TO 3201                                   A 863
      IF (LFLAG.EQ.4) GO TO 3016                                        A 864
      IF (IOPEN.NE.0)GO TO 3100                                         A 865
      GO TO 3010                                                        A 866
C                                                                       A 867
C       *** AMIN ***                                                    A 868
C                                                                       A 869
 3201 IF (LFLAG.EQ.4) NFLAG=1                                           A 870
 3200 K=1                                                               A 871
 3207 CALL QUESTA ($8018,K,'AMIN',4,AMIN(II,IM,K),'A12 ',1,0)           A 872
      K=K+1                                                             A 873
      IF (K.LT.6)GO TO 3207                                             A 874
      WRITE (1,9110)                                                    A 875
 3210 WRITE (1,9304)(AMIN(II,IM,K),K=1,5)                               A 876
      IF (LFLAG.EQ.1) GO TO 3000                                        A 877
      IF (.NOT.OK()) GO TO 3200                                         A 878
      IF (LFLAG.EQ.4) GO TO 3016                                        A 879
      IF (IOPEN.NE.0)GO TO 3100                                         A 880
      GO TO 3010                                                        A 881
 3250 CONTINUE                                                          A 882
C                                                                       A 883
C     ------------------                                                A 884
C     LOOK MIN DATA BLOCK                                               A 885
C     ------------------                                                A 886
C                                                                       A 887
      IF(IMINERAL(2).NE.0.OR.IOPEN.NE.0)GO TO 3100                      A 888
      WRITE (1,3251)                                                    A 889
 3251 FORMAT (/,'DO YOU WANT TO DELETE ALL OLD MINERALS?')              A 890
      IF (YN())IDELETE=1                                                A 891
      IF (IDELETE.EQ.1) JSUB(I)=1                                       A 892
C                                                                       A 893
C         SINCE LOOK MIN IS ALMOST IDENTICAL TO MINERAL,                A 894
C         WHY NOT USE MINERAL SECTION AND SAVE SOME SPACE?              A 895
C                                                                       A 896
      GO TO 3100                                                        A 897
 3270 CONTINUE                                                          A 898
C                                                                       A 899
C     ---------------                                                   A 900
```

```
C     TEMP DATA BLOCK                                                    A 901
C     ---------------                                                    A 902
C                                                                        A 903
      IF(IOPT(4).EQ.0)GO TO 3320                                         A 904
      NTEMP=IOPT(4)                                                      A 905
      IF (IOPT(4).EQ.3)NTEMP=NSTEPS                                      A 906
      IF (IOPEN.EQ.0)GO TO 3308                                          A 907
      READ (13,9501)(XTEMP(K3),K3=1,NTEMP)                               A 908
      WRITE (1,1736) SUB(I)                                              A 909
      WRITE (1,9501)(XTEMP(K3),K3=1,NTEMP)                               A 910
      CALL REF (0,0,1)                                                   A 911
      IF (JOPTION.NE.1) GO TO 3308                                       A 912
      IREQUIRED(6)=0                                                     A 913
      GO TO 531                                                          A 914
C                                                                        A 915
C       *** XTEMP ***                                                    A 916
C                                                                        A 917
 3308 K=1                                                                A 918
 3307 CALL QUESTA ($8020,K,'XTEMP',5,XTEMP(K),'A10 ',1,1)                A 919
      IF (.NOT.EXIT)GO TO 3312                                           A 920
      JSUB(6)=0                                                          A 921
      GO TO 531                                                          A 922
 3312 K=K+1                                                              A 923
      IF (K.LE.NTEMP)GO TO 3307                                          A 924
      IREQUIRED(6)=0                                                     A 925
      WRITE (1,9110)                                                     A 926
      WRITE (1,9501)(XTEMP(K),K=1,NTEMP)                                 A 927
      IF (OK())GO TO 531                                                 A 928
      GO TO 3308                                                         A 929
 3320 WRITE (1,3321)                                                     A 930
 3321 FORMAT (/,'ERROR:  TEMP DATA BLOCK NOT REQUIRED WHEN IOPT(4) ='    A 931
     1,' 0',//)                                                          A 932
      JSUB(6)=0                                                          A 933
      GO TO 531                                                          A 934
 3280 CONTINUE                                                           A 935
C                                                                        A 936
C     ----------------                                                   A 937
C     STEPS DATA BLOCK                                                   A 938
C     ----------------                                                   A 939
C                                                                        A 940
      IF(IOPT(3).EQ.0.OR.IOPT(3).EQ.5.OR.IOPT(3).EQ.6)GO TO 3630         A 941
      NSTEP=NSTEPS                                                       A 942
      IF (IOPT(3).EQ.4)NSTEP=1                                           A 943
      IF (IOPEN.EQ.0)GO TO 3608                                          A 944
      READ (13,9501)(XSTEP(K3),K3=1,NSTEP)                               A 945
      WRITE (1,1736) SUB(I)                                              A 946
      WRITE (1,9501)(XSTEP(K3),K3=1,NSTEP)                               A 947
      CALL REF (0,0,1)                                                   A 948
      GO TO (3801,3801,3608), JOPTION                                    A 949
 3801 IREQUIRED(7)=0                                                     A 950
```

```
      IF (JOPTION.NE.2) GO TO 531                                        A 951
C                                                                        A 952
C       *** XSTEP ***                                                    A 953
C                                                                        A 954
 3608 K=1                                                                A 955
 3607 CALL QUESTA ($3620,K,'XSTEP',5,XSTEP(K),'A10 ',1,1)                A 956
      IF (.NOT.EXIT)GO TO 3606                                           A 957
      JSUB(7)=0                                                          A 958
      GO TO 531                                                          A 959
 3606 K=K+1                                                              A 960
      IF (K.LE.NSTEP)GO TO 3607                                          A 961
      IREQUIRED(7)=0                                                     A 962
      WRITE (1,9110)                                                     A 963
      WRITE (1,9501)(XSTEP(K),K=1,NSTEP)                                 A 964
      IF (OK())GO TO 531                                                 A 965
      GO TO 3608                                                         A 966
 3620 GO TO (8022,8024,8026,8028),IOPT(3)                                A 967
 3630 WRITE (1,3631) IOPT(3)                                             A 968
 3631 FORMAT (/,'ERROR:  STEPS DATA BLOCK NOT ALLOWED WHEN IOPT(3) ='    A 969
     1,1X,I1,//)                                                         A 970
      JSUB(7)=0                                                          A 971
      GO TO 531                                                          A 972
 3900 CONTINUE                                                           A 973
C                                                                        A 974
C     ------------------                                                 A 975
C     REACTION DATA BLOCK                                                A 976
C     ------------------                                                 A 977
C                                                                        A 978
      IF (NCOMPS.NE.0)GO TO 3902                                         A 979
      WRITE (1,3901)                                                     A 980
 3901 FORMAT (//,'ERROR:   REACTION DATA BLOCK NOT ALLOWED WHEN',        A 981
     1' NCOMPS = 0',//)                                                  A 982
      JSUB(8)=0                                                          A 983
      GO TO 531                                                          A 984
 3902 IF (IOPEN.EQ.0)GO TO 5010                                          A 985
      READ (13,9701)(LREAC(K3),CREAC(K3),THMEAN(K3),K3=1,NCOMPS)         A 986
      WRITE (1,1736) SUB(I)                                              A 987
      WRITE (1,9701)(LREAC(K3),CREAC(K3),THMEAN(K3),K3=1,NCOMPS)         A 988
      CALL REF (0,0,1)                                                   A 989
      IF (JOPTION.EQ.2) GO TO 5010                                       A 990
      IREQUIRED(8)=0                                                     A 991
      IF (JOPTION.EQ.1) GO TO 531                                        A 992
C                                                                        A 993
C       *** THMEAN, LREAC, CREAC ***                                     A 994
C                                                                        A 995
 5010 K=1                                                                A 996
 5012 K2=1                                                               A 997
 5015 IF (K2.EQ.1) CALL QUESTB ($8032,K,'LREAC',5,LREAC(K),'I4  ',0,0,3) A 998
      IF (K2.EQ.2) CALL QUESTA ($8034,K,'CREAC',5,CREAC(K),'A8  ',1,3)   A 999
      IF (K2.EQ.3) CALL QUESTA ($8036,K,'THMEAN',6,THMEAN(K),'A8  ',1,3) A1000
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      IF (.NOT.EXIT)GO TO 5023                                          A1001
 5300 JSUB(8)=0                                                         A1002
      GO TO 531                                                         A1003
 5023 IF (.NOT.LIST) GO TO 5025                                         A1004
      CALL LISTM                                                        A1005
      GO TO 5015                                                        A1006
 5025 IF (K2.EQ.3) GO TO 5026                                           A1007
      K2=K2+1                                                           A1008
      IREQUIRED(8)=0                                                    A1009
      GO TO 5015                                                        A1010
 5026 K=K+1                                                             A1011
      IF (K.GT.NCOMPS) GO TO 5027                                       A1012
      GO TO 5012                                                        A1013
 5027 WRITE (1,9110)                                                    A1014
      WRITE (1,9701) (LREAC(K),CREAC(K),THMEAN(K),K=1,NCOMPS)           A1015
      IF (OK()) GO TO 531                                               A1016
      GO TO 5010                                                        A1017
 6000 CONTINUE                                                          A1018
C                                                                       A1019
C     ------------------                                                A1020
C     NEUTRAL DATA BLOCK                                                A1021
C     ------------------                                                A1022
C                                                                       A1023
      IF(IOPT(2).NE.2)GO TO 6040                                        A1024
      IF (IOPEN.EQ.0)GO TO 6010                                         A1025
      CALL REF (1,1,1)                                                  A1026
      GO TO (6100,6110,6110,6010),JOPTION+1                             A1027
 6100 JSUB(9)=0                                                         A1028
      GO TO 531                                                         A1029
 6110 READ(JLINE(1),9801)LPOS,LNEG                                      A1030
      IREQUIRED(9)=0                                                    A1031
      IF (JOPTION.EQ.1)GO TO 531                                        A1032
C                                                                       A1033
C       *** LPOS ***                                                    A1034
C                                                                       A1035
 6010 CALL QUESTB ($8038,0,'LPOS',4,LPOS,'I5  ',0,0,3)                  A1036
      IF (.NOT.EXIT)GO TO 6016                                          A1037
      JSUB(9)=0                                                         A1038
      GO TO 531                                                         A1039
 6016 IF (.NOT.LIST)GO TO 6017                                          A1040
      CALL LISTM                                                        A1041
      GO TO 6010                                                        A1042
 6017 IREQUIRED(9)=0                                                    A1043
C                                                                       A1044
C       *** LNEG ***                                                    A1045
C                                                                       A1046
 6020 CALL QUESTB ($8040,0,'LNEG',4,LNEG,'I5  ',0,0,2)                  A1047
      IF (.NOT.LIST)GO TO 6030                                          A1048
      CALL LISTM                                                        A1049
      GO TO 6020                                                        A1050
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 6030 WRITE (1,9110)                                                    A1051
      WRITE (1,9801)LPOS,LNEG                                           A1052
      IF (OK()) GO TO 531                                               A1053
      GO TO 6000                                                        A1054
 6040 WRITE (1,6041)                                                    A1055
 6041 FORMAT (/,'ERROR:  NEUTRAL DATA BLOCK IS REQUIRED ONLY IF IOPT'   A1056
     1,'(2) = 2',//)                                                    A1057
      JSUB(9)=0                                                         A1058
      GO TO 531                                                         A1059
 7000 CONTINUE                                                          A1060
C                                                                       A1061
C     ---------------                                                   A1062
C     SUMS DATA BLOCK                                                   A1063
C     ---------------                                                   A1064
C                                                                       A1065
      IF(ISUM.NE.0.OR.IOPEN.NE.0)GO TO 7001                             A1066
C                                                                       A1067
C         DELETE ALL OLD SUMS....                                       A1068
C                                                                       A1069
      WRITE (1,7003)                                                    A1070
 7003 FORMAT (/,'DO YOU WANT TO DELETE ALL OLD SUMS?')                  A1071
      IF (YN())JDELETE=1                                                A1072
 7001 ISUM=ISUM+1                                                       A1073
      IF (IOPEN.EQ.0)GO TO 7010                                         A1074
 7116 CALL REF (1,0,0)                                                  A1075
      IF (JOPTION.EQ.0)GO TO 7111                                       A1076
      WRITE (1,1736) SUB(I)                                             A1077
      WRITE (1,1731)JLINE(1)                                            A1078
      READ (JLINE(1),9901) SUNAME(ISUM),NSUM(ISUM)                      A1079
      IF (SUNAME(ISUM).NE.DELETE)GO TO 7120                             A1080
      CALL REF (0,0,2)                                                  A1081
      GO TO (7111,7117,7116),JOPTION+1                                  A1082
 7117 JDELETE=1                                                         A1083
      GO TO 7116                                                        A1084
 7120 READ (13,9902)(LSUM(ISUM,M3),M3=1,NSUM(ISUM))                     A1085
      WRITE (1,9902) (LSUM(ISUM,M3),M3=1,NSUM(ISUM))                    A1086
      CALL REF (0,0,3)                                                  A1087
      GO TO (7111,7001,7010,7116),JOPTION+1                             A1088
C                                                                       A1089
C       *** SUNAME ***                                                  A1090
C                                                                       A1091
 7010 CALL QUESTA ($8042,0,'SUNAME',6,SUNAME(ISUM),'A8  ',0,1)          A1092
      IF (.NOT.EXIT)GO TO 7020                                          A1093
 7111 ISUM=ISUM-1                                                       A1094
      IF (ISUM.EQ.0)JSUB(10)=0                                          A1095
      GO TO 531                                                         A1096
C                                                                       A1097
C       *** NSUM ***                                                    A1098
C                                                                       A1099
 7020 CALL QUESTB ($8044,0,'NSUM',4,NSUM(ISUM),'I2  ',0,50,0)           A1100
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      WRITE (1,9110)                                                    A1101
      WRITE (1,9901) SUNAME(ISUM),NSUM(ISUM)                            A1102
      IF (.NOT.OK())GO TO 7010                                          A1103
C                                                                       A1104
C       *** LSUM ***                                                    A1105
C                                                                       A1106
 7030 K=1                                                               A1107
 7037 CALL QUESTB ($8046,K,'LSUM',4,LSUM(ISUM,K),'I4  ',0,10000,0)      A1108
      K=K+1                                                             A1109
      IF (K.LE.NSUM(ISUM))GO TO 7037                                    A1110
      WRITE (1,9110)                                                    A1111
      WRITE (1,9902) (LSUM(ISUM,K),K=1,NSUM(ISUM))                      A1112
      IF (.NOT.OK())GO TO 7030                                          A1113
      IF (JOPTION.EQ.2)GO TO 7001                                       A1114
      WRITE (1,7051)                                                    A1115
 7051 FORMAT (/,'MORE SUMS?')                                           A1116
      IF (YN())GO TO 7000                                               A1117
      GO TO 531                                                         A1118
C                                                                       A1119
C  ---------------                                                      A1120
C  END DATA BLOCK                                                       A1121
C  ---------------                                                      A1122
C                                                                       A1123
  950 CONTINUE                                                          A1124
      JOPTION=0                                                         A1125
      KKK=1                                                             A1126
  954 IF (IREQUIRED(KKK).EQ.1)GO TO 952                                 A1127
  953 KKK=KKK+1                                                         A1128
      IF (KKK.EQ.11)GO TO 958                                           A1129
      GO TO 954                                                         A1130
C                                                                       A1131
C         OOPS!!   HE LEFT OUT A DATA BLOCK.                            A1132
C                                                                       A1133
  952 WRITE (1,955)SUB(KKK)                                             A1134
  955 FORMAT (/,'ERROR:  ',A8,' DATA BLOCK IS REQUIRED'/)               A1135
      IERROR=1                                                          A1136
      GO TO 953                                                         A1137
  958 IF (IERROR.EQ.0)GO TO 957                                         A1138
      JSUB(11)=0                                                        A1139
      IERROR=0                                                          A1140
      GO TO 531                                                         A1141
C                                                                       A1142
C         EXCLUDE ELEMENTS OR SPECIES THAT ARE ALREADY IN PHREEQE'S     A1143
C         THERMODYNAMIC DATA.                                           A1144
C                                                                       A1145
  957 DO 951 JL=4,30                                                    A1146
      IF (ICOL2(JL).EQ.0)GO TO 951                                      A1147
      ICHECK(1,ICOL2(JL))=0                                             A1148
      ICHECK(2,ICOL2(JL))=0                                             A1149
  951 CONTINUE                                                          A1150
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      JJ=1                                                              A1151
  943 JJJ=4                                                             A1152
  942 IF (ICHECK(JJ,JJJ).EQ.1)GO TO (944,945),JJ                        A1153
  949 JJJ=JJJ+1                                                         A1154
      IF (JJJ.EQ.31)GO TO 946                                           A1155
      GO TO 942                                                         A1156
  946 JJ=JJ+1                                                           A1157
      IF (JJ.EQ.3)GO TO 947                                             A1158
      GO TO 943                                                         A1159
  944 WRITE (1,948)JJJ                                                  A1160
  948 FORMAT ('ERROR:  SPECIES #',I2,' WAS NOT ENTERED.')               A1161
  938 IERROR=1                                                          A1162
      GO TO 949                                                         A1163
  945 WRITE (1,937)JJJ                                                  A1164
  937 FORMAT ('ERROR:  ELEMENT #',I2,' WAS NOT ENTERED.')               A1165
      GO TO 938                                                         A1166
  947 IF (IERROR.EQ.0)GO TO 959                                         A1167
C                                                                       A1168
C         HE ISN'T ALLOWED TO END.                                      A1169
C                                                                       A1170
      IERROR=0                                                          A1171
      JSUB(11)=0                                                        A1172
      GO TO 531                                                         A1173
C                                                                       A1174
C         EVERYTHING NEEDED IS PRESENT.                                 A1175
C                                                                       A1176
  959 GO TO 9010                                                        A1177
 5001 WRITE (1,5000)                                                    A1178
 5000 FORMAT ('MORE SIMULATIONS?')                                      A1179
      IF (.NOT.YN())GO TO 50                                            A1180
      IF (JOPEN.EQ.0)GO TO 5003                                         A1181
 5006 READ (13,1731,END=5003)LINE                                       A1182
      WRITE(1,5005)                                                     A1183
 5005 FORMAT(/,'DO YOU WISH TO USE THE NEXT SIMULATION IN YOUR',        A1184
     1' REFERENCE?')                                                    A1185
      IF (.NOT.YN())GO TO 5008                                          A1186
      BACKSPACE 13                                                      A1187
      IOPEN=1                                                           A1188
      GO TO 3                                                           A1189
 5008 READ (13,5009,END=5003)LINE                                       A1190
 5009 FORMAT (A3)                                                       A1191
      IF (LINE(1:3).EQ.'END')GO TO 5006                                 A1192
      GO TO 5008                                                        A1193
 5003 WRITE (1,5002)                                                    A1194
 5002 FORMAT (/,'DO YOU WISH TO DEFINE THE PREVIOUS OUTPUT AS '         A1195
     1,/,1X,'YOUR NEW REFERENCE?')                                      A1196
      IF (.NOT.YN())GO TO 2                                             A1197
C                                                                       A1198
C         WRITE THE OUTPUT ONTO THE REFERENCE FILE.                     A1199
C                                                                       A1200
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      OUT=13                                                            A1201
      CLOSE (UNIT=13)                                                   A1202
      OPEN (UNIT=13,FILE='REF',STATUS='UNKNOWN')                        A1203
      REWIND 13                                                         A1204
      GO TO 9010                                                        A1205
  999 ENDFILE (UNIT=13)                                                 A1206
      REWIND 13                                                         A1207
      IOPEN=1                                                           A1208
C                                                                       A1209
C         LET'S TRY AGAIN...                                            A1210
C                                                                       A1211
      GO TO 3                                                           A1212
   50 ENDFILE (UNIT=10)                                                 A1213
      STOP                                                              A1214
C                                                                       A1215
 9010 CONTINUE                                                          A1216
C                                                                       A1217
C         WRITE TO FILE.....                                            A1218
C                                                                       A1219
      ITER=1                                                            A1220
C                                                                       A1221
C          PRINT TITLE CARD.                                            A1222
C                                                                       A1223
      WRITE (OUT,1731)TITLE                                             A1224
C                                                                       A1225
C         PRINT OPTION CARD.                                            A1226
C                                                                       A1227
      WRITE (OUT,9991) (IOPT(I),I=1,9),NSTEPS,NCOMPS,VO                 A1228
 9991 FORMAT (9I1,1X,2I2,6X,A10)                                        A1229
      DO 9999 L=1,11                                                    A1230
      IF (JSUB(IORDER(L)).LT.1) GO TO 9999                              A1231
      IF (IORDER(L).EQ.1)GO TO 9000                                     A1232
      WRITE (OUT,9050)SUB(IORDER(L))                                    A1233
 9050 FORMAT (A8)                                                       A1234
      GO TO (9100,9200,9300,9300,9500,9600,9700,9800,9900,9999),IORDER(L A1235
     1)-1                                                               A1236
C                                                                       A1237
C         PRINT SOLUTION DATA BLOCK.                                    A1238
C                                                                       A1239
 9000 WRITE (OUT,9001) SUB(1),NSOLUTION(ITER)                           A1240
 9001 FORMAT (A8,1X,I1)                                                 A1241
      WRITE (OUT,1731) HEAD(ITER)                                       A1242
      WRITE (OUT,9003) NTOTS(ITER),IALK(ITER),IUNITS(ITER),PH(ITER)     A1243
     1, PE(ITER),TEMP(ITER),SDENS(ITER)                                 A1244
 9003 FORMAT(I2,I3,I2,3X,4A10)                                          A1245
      IF (NTOTS(ITER).EQ.0)GO TO 9005                                   A1246
      WRITE (OUT,9004)(LT(ITER,M),DTOT(ITER,M),M=1,NTOTS(ITER))         A1247
 9004 FORMAT (6(5(I4,A11),:,/))                                         A1248
 9005 IF (ISOL.EQ.ITER) GO TO 9999                                      A1249
      ITER=2                                                            A1250
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      GO TO 9000                                                        A1251
C                                                                       A1252
C         PRINT ELEMENTS DATA BLOCK.                                    A1253
C                                                                       A1254
 9100 DO 9103 MM=1,IELEMENT                                             A1255
 9103 WRITE (OUT,9102) TNAME(MM),NELT(MM),TGFW(MM)                      A1256
 9102 FORMAT(A8,2X,I2,3X,A10)                                           A1257
      WRITE (OUT,9110)                                                  A1258
 9110 FORMAT (1X)                                                       A1259
      GO TO 9999                                                        A1260
C                                                                       A1261
C         PRINT SPECIES DATA BLOCK.                                     A1262
C                                                                       A1263
 9200 DO 9206 MM=1,ISPECIE                                              A1264
      WRITE (OUT,9202) NI(MM)                                           A1265
 9202 FORMAT (I3)                                                       A1266
      IF(ISDEL(MM).EQ.0)GO TO 9207                                      A1267
      WRITE (OUT,9110)                                                  A1268
      GO TO 9206                                                        A1269
 9207 WRITE (OUT,9203) SNAME(MM),NSP(MM),KFLAG(MM),GFLAG(MM),ZSP(MM)    A1270
     1,THSP(MM),DHA(MM),ADHSP(MM,1),ADHSP(MM,2),ALKSP(MM)               A1271
 9203 FORMAT (A8,2X,I3,2I1,6A10)                                        A1272
      WRITE (OUT,9204) LKTOSP(MM),DHSP(MM),(ASP(MM,M),M=1,5)            A1273
 9204 FORMAT (2A10,5A12)                                                A1274
      WRITE (OUT,9205)(LSP(MM,M),CSP(MM,M),M=1,NSP(MM))                 A1275
 9205 FORMAT (6(I3,A7))                                                 A1276
 9206 CONTINUE                                                          A1277
      WRITE (OUT,9110)                                                  A1278
      GO TO 9999                                                        A1279
C                                                                       A1280
C         PRINT MINERALS OR LOOK MIN DATA BLOCK.                        A1281
C                                                                       A1282
 9300 NM=IORDER(L)-3                                                    A1283
      IF (NM.NE.2.OR.IDELETE.NE.1)GO TO 9301                            A1284
      WRITE (OUT,9050) DELETE                                           A1285
 9301 IM=IMINERAL(NM)                                                   A1286
      DO 9305 MM=1,IM                                                   A1287
      WRITE (OUT,9302) MNAME(NM,MM),NMINO(NM,MM),THMIN(NM,MM),LKTOM(NM  A1288
     1,MM),DHMIN(NM,MM),MFLAG(NM,MM),SIMIN(NM,MM)                       A1289
 9302 FORMAT (A8,2X,I2,3X,3A10,5X,I1,9X,A10)                            A1290
      WRITE (OUT,9303) (LMIN(NM,MM,M),CMIN(NM,MM,M),M=1,NMINO(NM,MM))   A1291
 9303 FORMAT (2(5(I4,A11,:),/))                                         A1292
      IF(MFLAG(NM,MM).NE.1)GO TO 9305                                   A1293
      WRITE (OUT,9304) (AMIN(NM,MM,M),M=1,5)                            A1294
 9305 CONTINUE                                                          A1295
      WRITE (OUT,9110)                                                  A1296
 9304 FORMAT (5A12)                                                     A1297
      GO TO 9999                                                        A1298
C                                                                       A1299
C         PRINT TEMP DATA BLOCK.                                        A1300
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C                                                                       A1301
 9500 WRITE (OUT,9501) (XTEMP(IF),IF=1,NTEMP)                           A1302
 9501 FORMAT (7(8(A10,:),/))                                            A1303
      GO TO 9999                                                        A1304
C                                                                       A1305
C         PRINT STEP DATA BLOCK.                                        A1306
C                                                                       A1307
 9600 WRITE (OUT,9501) (XSTEP(IF),IF=1,NSTEP)                           A1308
      GO TO 9999                                                        A1309
C                                                                       A1310
C         PRINT REACTION DATA BLOCK.                                    A1311
C                                                                       A1312
 9700 WRITE (OUT,9701)(LREAC(M),CREAC(M),THMEAN(M),M=1,NCOMPS)          A1313
 9701 FORMAT (8(4(I4,2A8,:),/))                                         A1314
      GO TO 9999                                                        A1315
C                                                                       A1316
C         PRINT NEUTRAL DATA BLOCK.                                     A1317
C                                                                       A1318
 9800 WRITE (OUT,9801)LPOS,LNEG                                         A1319
 9801 FORMAT (2I5)                                                      A1320
      GO TO 9999                                                        A1321
C                                                                       A1322
C         PRINT SUMS DATA BLOCK.                                        A1323
C                                                                       A1324
 9900 IF (JDELETE.NE.1)GO TO 9904                                       A1325
      WRITE (OUT,9302) DELETE                                           A1326
 9904 DO 9903 MM=1,ISUM                                                 A1327
      WRITE (OUT,9901)SUNAME(MM),NSUM(MM)                               A1328
 9901 FORMAT (A8,2X,I2)                                                 A1329
 9903 WRITE (OUT,9902) (LSUM(MM,M),M=1,NSUM(MM))                        A1330
 9902 FORMAT(20I4)                                                      A1331
      WRITE (OUT,9110)                                                  A1332
 9999 CONTINUE                                                          A1333
C                                                                       A1334
      IF (OUT.EQ.10) GO TO 5001                                         A1335
      GO TO 999                                                         A1336
C                                                                       A1337
C        HELP MESSAGES....                                              A1338
C                                                                       A1339
  290 NSTART=N                                                          A1340
      GO TO (2000,2020,2040,2060,2080,2100,2120,2140,2160),N            A1341
 1000 WRITE (1,1010)                                                    A1342
 1010 FORMAT (/1X,'TITLE CARD',2X,'TITLE',/,1X,'FORMAT (A80)',          A1343
     1/,1X,'EIGHTY CHARACTERS OF TITLES OR COMMENTS.'//)                A1344
      GO TO 10                                                          A1345
 2000 WRITE (1,2010) OPTION                                             A1346
 2010 FORMAT (/1X,A11,/,13X,'IOPT(1) = 0, NO PRINT OF',                 A1347
     1' THERMODYNAMIC DATA OR COEFFICIENTS',/,26X,'OF AQUEOUS',         A1348
     2' SPECIES.',//,21X,'= 1, PRINT THE AQUEOUS MODEL DATA',           A1349
     3' (WHICH ARE STORED',/26X,'ON DISK) ONCE DURING THE ENTIRE',      A1350
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    4' COMPUTER RUN.',/,1X,'FORMAT (I1)',//)                              A1351
     GO TO 91                                                             A1352
2020 WRITE (1,2030) OPTION                                                A1353
2030 FORMAT(/1X,A11,/,13X,'IOPT(2) = 0, INITIAL SOLUTIONS',               A1354
    1' ARE NOT TO BE CHARGE BALANCED.',/,26X,'REACTION SOLUTIONS',        A1355
    2' MAINTAIN THE INITIAL CHARGE',/,26X,'IMBALANCE.',//,21X,'= 1,',     A1356
    3' PH IS ADJUSTED IN INITIAL SOLUTION(S) TO',/,26X,'OBTAIN CHARGE',   A1357
    4' BALANCE.',//,21X,'= 2, THE TOTAL CONCENTRATION OF ONE OF THE',     A1358
    5' ELEMENTS',/,26X,'(EXCEPT H OR O) IS ADJUSTED TO OBTAIN',           A1359
    6' ELECTRICAL',/,26X,'BALANCE.  NEUTRAL INPUT IS REQUIRED.',/,1X,'F   A1360
    7ORMAT (I1)',//)                                                      A1361
     GO TO 91                                                             A1362
2040 WRITE (1,2050) OPTION                                                A1363
2050 FORMAT (/1X,A11,/,13X,'IOPT(3) = 0, NO REACTIONS ARE',               A1364
    1' MODELED.  ONLY THE INITIAL',/,26X,'SOLUTIONS ARE SOLVED.'//,       A1365
    221X,'= 1, SOLUTION 1 IS MIXED (A HYPOTHETICAL CONSTANT',/,26X,       A1366
    3'VOLUME PROCESS) WITH SOLUTION 2 IN SPECIFIED',/,26X,'REACTION',     A1367
    4' STEPS.  STEPS INPUT AND A VALUE FOR',/,26X,'NSTEPS ARE REQUIRED'   A1368
    5,'.  MINERALS INPUT MAY BE',/,26X,'INCLUDED.',//,21X,'= 2,',         A1369
    6' SOLUTION 1 IS TITRATED WITH SOLUTION 2 IN SPECI-',/,26X,           A1370
    7'FIED REACTION STEPS.  STEPS INPUT, A VALUE FOR',/,26X,'NSTEPS,',    A1371
    8' AND A VALUE FOR V0 ARE REQUIRED.',/,26X,'MINERALS INPUT MAY',      A1372
    9' BE INCLUDED.',//,21X,'= 3, A',                                     A1373
    !' STOICHIOMETRIC REACTION IS ADDED IN SPECIFIED',/,26X,'REACTION',    A1374
    @' STEPS.  REACTION  INPUT, STEPS INPUT,',/,26X,'A VALUE FOR',        A1375
    #' NSTEPS, AND A VALUE FOR NCOMPS ARE',/,26X,'REQUIRED.  MINERALS',   A1376
    $' INPUT MAY BE INCLUDED.'///' HIT <RETURN> FOR MORE INFORMATION.')   A1377
     READ (1,20) LINE                                                     A1378
     WRITE(1,2055)                                                        A1379
2055 FORMAT(21X,'= 4, A NET STOICHIOMETRIC',                              A1380
    ^' REACTION IS ADDED IN NSTEPS',/,26X,'EQUAL INCREMENTS.  REACTION'   A1381
    &,' INPUT, STEPS INPUT,',/,26X,'A VALUE FOR NSTEPS, AND A VALUE FOR   A1382
    * NCOMPS ARE',/,26X,'REQUIRED.  MINERALS INPUT MAY BE INCLUDED.',     A1383
    ('  ONLY',/,26X,'ONE VALUE FOR THE TOTAL REACTION IS READ IN STEPS.   A1384
    )',//,21X,'= 5, SOLUTION NUMBER 1 IS EQUILIBRATED WITH MINERAL',      A1385
    -/,26X,'PHASES ONLY.  NO OTHER REACTION IS PERFORMED.',/,26X,         A1386
    ='MINERALS INPUT IS REQUIRED.',//,21X,'= 6, A REACTION IS ADDED',     A1387
    +' TO SOLUTION 1 UNTIL EQUI-',/,26X,'LIBRIUM IS ATTAINED WITH THE',   A1388
    |' FIRST PHASE IN',/,26X,'MINERAL INPUT (EQUILIBRIUM WITH OTHER',     A1389
    :' MINERALS',/,26X,'PHASES IS MAINTAINED THROUGHOUT THE REACTION)',   A1390
    /'.',/,26X,'REACTION INPUT, A VALUE FOR NCOMPS, AND MINERALS',/,      A1391
    ]26X,'INPUT ARE REQUIRED.  NO STEPS INPUT IS REQUIRED.',/,26X,        A1392
    ['NOTE:  THERE SHOULD BE A COMMON ELEMENT IN THE',/,26X,'REACTION',   A1393
    ~' AND THE FIRST PHASE IN MINERALS INPUT.',/,1X,'FORMAT (I1)',//)     A1394
     GO TO 91                                                             A1395
2060 WRITE (1,2070) OPTION                                                A1396
2070 FORMAT (/1X,A11,/,13X,'IOPT(4) = 0, THE TEMPERATURE OF',             A1397
    1' THE REACTION SOLUTION IS',/,26X,'A) THE SAME AS THE INITIAL',      A1398
    2' SOLUTION IF ADDING',/,26X,'A REACTION, OR B) CALCULATED LINEARLY   A1399
    3 FROM THE',/,26X,'END MEMBERS IF MIXING OR TITRATING.  NO TEMP',     A1400
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     4/,26X,'INPUT IS REQUIRED.',//,21X,'= 1, THE TEMPERATURE IS',          A1401
     5' CONSTANT DURING THE REACTION',/,26X,'STEPS AND DIFFERS FROM THAT    A1402
     6 OF THE INITIAL SOL-',/,26X,'UTION(S).  ONE VALUE IS READ IN THE',    A1403
     7' TEMP INPUT.'//,21X,'= 2, THE TEMPERATURE IS VARIED FROM T(O) TO'    A1404
     8,' T(F) IN',/,26X,'NSTEPS EQUAL INCREMENTS, DURING THE REACTION',/    A1405
     9,26X,'STEPS.',//,21X,'= 3, THE TEMPERATURE',                          A1406
     $' OF EACH REACTION STEP IS SPEC-',/,26X,'IFIED IN TEMP INPUT, IN'     A1407
     %,' ORDER.  NSTEPS VALUES',/,26X,'ARE READ.',/,1X,'FORMAT (I1)',//)    A1408
      GO TO 91                                                              A1409
2080 WRITE (1,2090) OPTION                                                  A1410
2090 FORMAT (/1X,A11,/,13X,'IOPT(5) = 0, THE PE FROM THE',                  A1411
     1' INITIAL SOLUTION IS HELD CON-',/,26X,'STANT DURING ALL THE',        A1412
     2' REACTION STEPS FOR THE',/,26X,'SIMULATION.'//,21X,'= 1, THE PE',    A1413
     3' OF THE REACTION SOLUTION IS DETERMINED',/,26X,'BY THE REACTION.'    A1414
     4,/,1X,'FORMAT (I1)',//)                                               A1415
      GO TO 91                                                              A1416
2100 WRITE (1,2110) OPTION                                                  A1417
2110 FORMAT (/1X,A11,/,13X,'IOPT(6) = 0, DEBYE-HUCKEL',                     A1418
     1' ACTIVITY COEFFICIENTS ARE USED FOR',/,26X,'THE CALCULATIONS.  ('    A1419
     2,'SEE SPECIES INPUT).',//,21X,'= 1, DAVIES ACTIVITY COEFFICIENTS',    A1420
     3' ARE USED.  (SEE',/,26X,'SPECIES INPUT)',/,1X,'FORMAT (I1)',//)      A1421
      GO TO 91                                                              A1422
2120 WRITE (1,2130) OPTION                                                  A1423
2130 FORMAT (/1X,A11,/,13X,'IOPT(7) = 0, DO NOT SAVE THE',                  A1424
     1' AQUEOUS PHASE COMPOSITION AT',/,26X,'THE END OF A REACTION FOR',    A1425
     2' ADDITIONAL SIMU-',/,26X,'LATIONS.',//,21X,'= 1, SAVE THE FINAL',    A1426
     3' REACTION SOLUTION IN SOLUTION',/,26X,'NUMBER 1.',//,21X,'= 2,',     A1427
     4' SAVE THE FINAL REACTION SOLUTION IN SOLUTION',/,26X,'NUMBER 2.'     A1428
     5,/,1X,'FORMAT (I1)',//)                                               A1429
      GO TO 91                                                              A1430
2140 WRITE (1,2150) OPTION                                                  A1431
2150 FORMAT (/1X,A11,/,13X,'IOPT(8) = 0, THE DEBUGGING PRINT'               A1432
     1,' ROUTINE IS NOT CALLED.',//,21X,'= 1, A LONG PRINTOUT IS OUTPUT'    A1433
     2,' AT EACH ITERATION IN',/,26X,'EACH PROBLEM.  THIS PRINT IS TO BE    A1434
     3 USED ONLY',/,26X,'IF THERE ARE CONVERGENCE PROBLEM WITH THE',        A1435
     4/,26X,'PROGRAM.  (SEE SUBROUTINE PBUG)',/,1X,'FORMAT (I1)',//)        A1436
      GO TO 91                                                              A1437
2160 WRITE (1,2170) OPTION                                                  A1438
2170 FORMAT (/1X,A11,/,13X,'IOPT(9) = 0, NO PRINTOUT OF EACH',              A1439
     1' ARRAY INVERTED.',//,21X,'= 1, A LONG PRINTOUT OCCURS OF THE',       A1440
     2' ENTIRE ARRAY TO',/,26X,'BE INVERTED AT EACH ITERATION.  THIS',      A1441
     3' PRINT IS',/,26X,'USED ONLY IF THERE ARE CONVERGENCE PROBLEMS.',     A1442
     4/,26X,'(SEE SUBROUTINE SLNQ)',/,1X,'FORMAT (I1)',//)                  A1443
      GO TO 91                                                              A1444
2200 WRITE (1,2210) OPTION                                                  A1445
2210 FORMAT (/1X,A11,/,13X,'NSTEPS',7X,'THE NUMBER OF'                      A1446
     1,' STEPS.  A VALUE IS',/,26X,'REQUIRED IF IOPT(3) = 1, 2, 3,',        A1447
     2'OR 4, OR IF',/,26X,'IOPT(4) = 2 OR 3.',/,1X,'FORMAT (I2)',//)        A1448
      GO TO 250                                                             A1449
2300 WRITE (1,2310) OPTION                                                  A1450
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2310 FORMAT (/1X,A11,/,13X,'NCOMPS',7X,'THE NUMBER OF CONSTIT',          A1451
    1'UENTS IN A NET STOICHIO-',/26X,'METRIC REACTION.  A CONSTITUENT M  A1452
    2AY BE ANY',/,26X,'ELEMENT WITH AN INDEX NUMBER BETWEEN 4 AND',      A1453
    3/,26X,'30 INCLUSIVE.  NO AQUEOUS SPECIES WITH INDEX',/,26X,'NUMBER  A1454
    4S GREATER THAN 30 MAY BE INCLUDED AS',/,26X,'REACTION CONSTITUENTS  A1455
    5 EXCEPT H2 AND O2.  ANY',/,26X,'CONSTITUENT WITH AN INDEX NUMBER G  A1456
    6REATER THAN',/,26X,'30 IS ASSUMED TO BE EITHER H2 OR O2 AND HAS',/  A1457
    7,26X,'THE EFFECT OF RAISING OR LOWERING THE REDOX',/,26X,'STATE OF  A1458
    8 THE SOLUTION DEPENDING ON THE AS-',/,26X,'SIGNED VALENCE (THMEAN)  A1459
    9.  A VALUE FOR NCOMPS',/,26X,'IS REQUIRED IF IOPT(3) = 3, 4, OR 6.  A1460
    !',/,1X,'FORMAT (I2)',//)                                            A1461
     GO TO 301                                                           A1462
2400 WRITE (1,2410) OPTION                                               A1463
2410 FORMAT (/1X,A11,/,13X,'VO',11X,'THE INITIAL VOLUME OF SO',          A1464
    1'LUTION NUMBER 1 WHEN',/26X,'MODELING A TITRATION.  THIS UNIT OF V  A1465
    2O MUST',/,26X,'BE THE SAME AS THAT OF XSTEP (SEE STEPS INPUT)',/,2  A1466
    36X,'IF IOPT(3) = 2.  OTHERWISE, VO IS NOT REQUIRED',/,1X,'FORMAT (  A1467
    4F10.5)',//)                                                         A1468
     GO TO 430                                                           A1469
4146 WRITE (1,4147) SUB(1)                                               A1470
4147 FORMAT (/1X,A8,10X,'THIS INPUT IS USED TO DEFINE A STARTING'        A1471
    1,' SOLU-',/,19X,'TION.',//)                                         A1472
     GO TO 621                                                           A1473
4148 WRITE (1,4149) SUB(2)                                               A1474
4149 FORMAT (/1X,A8,10X,'THIS INPUT DEFINES THE NAMES AND INDICES',      A1475
    1' OF ALL',/,19X,'ELEMENTS IN THE AQUEOUS MODEL DATA BASE.',//)      A1476
     GO TO 621                                                           A1477
4150 WRITE (1,4151) SUB(3)                                               A1478
4151 FORMAT (/1X,A8,10X,'THIS INPUT DEFINES THE NAMES, INDEX NUMB'       A1479
    1'ERS AND',/,19X,'COMPOSITION OF ALL AQUEOUS SPECIES IN THE',        A1480
    2' AQUEOUS',/,19X,'MODEL DATA BASE.',//)                             A1481
     GO TO 621                                                           A1482
4152 WRITE (1,4153) SUB(4)                                               A1483
4153 FORMAT (/1X,A8,10X,'THIS INPUT DEFINES THE PHASES WHICH WILL'       A1484
    1,' BE MAIN-',/,19X,'TAINED AT EQUILIBRIUM WITH EACH OF THE'         A1485
    2,' REACTION',/,19X,'SOLUTIONS',//)                                  A1486
     GO TO 621                                                           A1487
4154 WRITE (1,4155) SUB(5)                                               A1488
4155 FORMAT (/1X,A8,10X,'THE PURPOSE OF THIS INPUT IS SIMPLY TO '        A1489
    1,'PROVIDE',/,19X,'INFORMATION ON THE SATURATION STATE OF THE'       A1490
    2,' AQUEOUS',/,19X,'PHASE WITH RESPECT TO DESIRED MINERALS.  '       A1491
    3,'THE',/,19X,'MINERALS IN THIS BLOCK OF INPUT DO NOT AFFECT'        A1492
    4,' THE',/,19X,'CALCULATIONS OF THE INITIAL SOLUTION OR ANY '        A1493
    5,'OF THE',/,19X,'REACTION SOLUTIONS.  THIS INPUT IS NEVER'          A1494
    6,' MANDATORY.',//)                                                  A1495
     GO TO 621                                                           A1496
4156 WRITE (1,4157) SUB(6)                                               A1497
4157 FORMAT (/1X,A8,10X,'THIS INPUT VARIES THE TEMPERATURE DURING'       A1498
    1,' THE',/,19X,'REACTION STEPS.',//)                                 A1499
     GO TO 621                                                           A1500
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4158 WRITE (1,4159) SUB(7)                                              A1501
4159 FORMAT (/1X,A8,10X,'THIS INPUT DEFINES THE STEPS OF THE '          A1502
    1,'REACTION PROCESS.',//)                                           A1503
     GO TO 621                                                          A1504
4160 WRITE (1,4161) SUB(8)                                              A1505
4161 FORMAT (/1X,A8,10X,'THIS INPUT DESCRIBES THE STOICHIOMETRY'        A1506
    1,' AND VALENCE',/,19X,'OF THE ELEMENTS TO BE ADDED AS A'           A1507
    2,' REACTION.',//)                                                  A1508
     GO TO 621                                                          A1509
4162 WRITE (1,4163) SUB(9)                                              A1510
4163 FORMAT (/1X,A8,10X,'THIS INPUT DEFINES THE ELEMENTS TO BE '        A1511
    1,'USED TO',/,19X,'ADJUST THE INITIAL SOLUTION(S) TO ELECTRI'       A1512
    2,'CAL',/,19X,'NEUTRALITY.',//)                                     A1513
     GO TO 621                                                          A1514
4164 WRITE (1,4165) SUB(10)                                             A1515
4165 FORMAT (/1X,A8,10X,'THIS INPUT SUMS MOLALITIES OF AQUEOUS'         A1516
    1,' SPECIES WHICH',/,19X,'ARE THEN PRINTED IN THE OUTPUT OF THE'    A1517
    2,' RUN.  THESE',/,19X,'SUMS DO NOT AFFECT THE CALCULATIONS IN'     A1518
    3,' ANY WAY AND',/,19X,'ARE NEVER MANDATORY.',//)                   A1519
     GO TO 621                                                          A1520
4166 WRITE (1,4167) SUB(11)                                             A1521
4167 FORMAT (/1X,A8,10X,'THIS CARD TERMINATES INPUT OPERATIONS'         A1522
    1,' FOR A',/,19X,'SINGLE SIMULATION.  ANY COMPUTER RUN HAS '        A1523
    2,'AT LEAST ONE',/,19X,'END CARD.',//)                              A1524
     GO TO 621                                                          A1525
4200 WRITE (1,4210)                                                     A1526
4210 FORMAT (/1X,'POSSIBLE KEYWORDS:',//1X,'(1)ELEMENTS, (2)SPECIES'    A1527
    1,', (3)SOLUTION, (4)MINERALS, (5)LOOK MIN,',/,1X,'(6)TEMP, '       A1528
    2,'(7)STEPS, (8)REACTION, (9)NEUTRAL, (10)SUMS, (11)END',//,1X      A1529
    3,'FORMAT (A8)',//,' FOR MORE INFORMATION ON ANY OF THE DATA'       A1530
    4,' BLOCK, ENTER THE',/,1X,'NUMBER ASSOCIATED WITH IT.',/)          A1531
     GO TO 621                                                          A1532
1492 WRITE (1,1493)SUB(1)                                               A1533
1493 FORMAT (/1X,A8,/,13X,'N',12X,'A NUMBER OF EITHER 1 OR 2 INDICAT'   A1534
    1,'ING THE',/,26X,'SOLUTION NUMBER OF THE FOLLOWING DATA.',/,1X     A1535
    2,'FORMAT (I1)'//)                                                  A1536
     GO TO 1739                                                         A1537
4300 WRITE (1,4310) SUB(1)                                              A1538
4310 FORMAT (/1X,A8,/,13X,'HEAD',/,13X,'FORMAT (A80)',/,13X,            A1539
    1'TITLE OR COMMENTS ABOUT THE SOLUTION.',//)                        A1540
     GO TO 1488                                                         A1541
4320 WRITE (1,4330) SUB(1)                                              A1542
4330 FORMAT (/1X,A8,/,13X,'NTOTS',8X,'THE NUMBER OF TOTAL CONCENTRATION A1543
    1S TO BE',/,26X,'READ FROM CARD INPUT.  FOR EXAMPLE, IF THE',/,26X, A1544
    2'STARTING SOLUTION IS MGCL2-NAHCO3 SOLUTION',/,26X,'NTOTS = 4 (FOR A1545
    3 MG, CL, NA, AND C)',/,1X,'FORMAT (I2)',//)                        A1546
     GO TO 1713                                                         A1547
4340 WRITE (1,4350) SUB(1)                                              A1548
4350 FORMAT (/1X,A8,/,13X,'IALK',9X,'FLAG WHICH INDICATES WHETHER TOTAL A1549
    1 CARBON OR',/,26X,'TOTAL ALKALINITY IS TO BE INPUT.',//,21X,'= 0,  A1550
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     2INDICATES THE TOTAL CONCENTRATION OF CARBON',/,26X,'(NOT ALKALINIT  A1551
     3Y) IS INPUT IN THE UNITS',/,26X,'SPECIFIED BY IUNITS.',//,21X,'= N  A1552
     4, 4<=N<=30, WHERE N IS THE INDEX NUMBER FOR',/,26X,'THE ELEMENT CA  A1553
     5RBON, (IN OUR DATA BASE N=15)',/,26X,'INDICATES TOTAL ALKALINITY I  A1554
     6S BEING ENTERED.',/,26X,'ELEMENTS INPUT MAY BE REQUIRED.  THE UNIT  A1555
     7S OF',/,26X,'ALKALINITY ARE SPECIFIED BY IUNITS',/,26X,'AND IF ',  A1556
     9'IUNITS > 0, THE GRAM FORMULA WEIGHT (GFW)',/,26X,'OF THE ELEMENT'  A1557
     !,' CARBON IS CRITICALLY IMPORTANT.',/,26X,'THE GFW IN THE CASE OF'  A1558
     @,' ALKALINITY MUST BE THE',/,26X,'GRAM EQUIVALENT WEIGHT (GRAMS/EQ  A1559
     #UIVALENT) OF',/,26X,'THE CHEMICAL SPECIES IN WHICH THE ALKALINTY',  A1560
     $/,26X,'IS REPORTED.  THE FOLLOWING IS A LIST OF',///,' HIT <RETURN  A1561
     /> FOR MORE EXPLANATION')                                            A1562
      READ (1,1731) LINE                                                  A1563
      WRITE (1,4355)                                                      A1564
4355 FORMAT(//26X,'SPECIES ',                                             A1565
     %'COMMONLY USED FOR REPORTING ALKA-',/,26X,'LINITY AND THEIR CORRES  A1566
     ^PONDING EQUIVALENT',/,26X,'WEIGHTS:',//,31X,'CACO3',4X,'50.0446 G/  A1567
     &EQ',//,31X,'HCO3-',4X,'61.0171 G/EQ',//,31X,'CO3--',4X,'30.0046 G/  A1568
     *EQ',//,26X,'IN OUR DATA BASE 44.010 IS THE GFW OF CARBON',/,26X,'W  A1569
     (HICH IS SUITABLE FOR ENTERING CARBON AS',/,26X,'TOTAL CO2.  THIS G  A1570
     )FW MUST BE CHANGED VIA',/,26X,'ELEMENTS INPUT IF ALKALINITY IS TO'  A1571
     -,' BE ENTERED',/,26X,'AS MG/L OR PPM (IUNITS = 2 OR 3).  IF IUNITS  A1572
     ='',/,26X,'= 0 ALKALINITY MUST BE INPUT AS EQ/KG H2O AND',/,26X,'IN'  A1573
     +,' THIS CASE THE GFW NEED NOT BE CHANGED SINCE',/,26X,'NO CONVERSI  A1574
     :ON IS NECESSARY.',/,1X,'FORMAT (I3)',//)                            A1575
      GO TO (1714,1752),JUMP+1                                            A1576
4360 WRITE (1,4370) SUB(1)                                                A1577
4370 FORMAT (/1X,A8,/,13X,'IUNITS',7X,'FLAG DESCRIBING UNITS OF INPUT C  A1578
     1ONCENTRATIONS.',/,26X,'THE PROGRAM MAKES ALL OF ITS CALCULATIONS'   A1579
     2,/,26X,'IN TERMS OF MOLALITY AND ANY OTHER ALLOWED',/,26X,'CONCEN'  A1580
     3,'TRATION UNITS (MMOLES/L, MG/L,',/26X,'OR PPM) MUST BE CONVERTED'  A1581
     4,' TO MOLALITY',/26X,'BEFORE THE CALCULATION MAY BEGIN.  TO MAKE',  A1582
     5/26X,'THE CONVERSIONS IT IS NECESSARY TO KNOW THE',/26X,'GRAM FORM  A1583
     6ULA WEIGHT (GFW), IN G/MOLE, OF THE',/26X,'CHEMICAL FORMULA IN WHI  A1584
     7CH ELEMENTAL ANALYSES',/,26X,'ARE REPORTED.  THE GFW IS AN INPUT P  A1585
     8ARAMETER',/,26X,'UNDER ELEMENTS INPUT AND MUST BE IN AGREEMENT',    A1586
     9/,26X,'WITH THE ANALYTICAL UNITS FOR EACH SOLUTION',/,26X,'DATA SE  A1587
     !T.  (IF THE UNITS ARE MOLALITY, NO',/,26X,'CONVERSION IS NECESSARY  A1588
     @ AND THE GFWS ARE NOT',/,26X,'USED.)  NOTE:  ALL ELEMENTS MUST HAV  A1589
     #E',/,26X,'THE SAME UNITS.  IT IS NOT POSSIBLE TO ENTER MG/L',/,26X  A1590
     $,'OF ONE ELEMENT AND MOLALITY OF ANOTHER.',///,' HIT <RETURN> FOR'  A1591
     /,' MORE EXPLANATION')                                               A1592
      READ (1,1731) LINE                                                  A1593
      WRITE (1,4375)                                                      A1594
4375 FORMAT (/21X,'= 0, CONCENTRATION ',                                  A1595
     %'OF ELEMENTS ENTERED AS MOLALITY',/,26X,'OF EACH ELEMENT, OR FO','  A1596
     ^R ALKALINITY, EQUIV-',/,26X,'ALENTS/KG H2O.',//,21X,'= 1, CONCENTR  A1597
     &ATION OF ELEMENTS ENTERED AS MMOLES/L',/,26X,'OF EACH ELEMENT, OR'  A1598
     *,' FOR ALKALINITY, MEQ/L.',//,21X,'= 2, CONCENTRATION OF ELEMENTS   A1599
     (ENTERED AS MG/L',/,26X,'OF THE SPECIES WHICH HAS A GRAM FORMULA',   A1600
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    )/,26X,'WEIGHT GIVEN IN ELEMENTS INPUT.  (ELEMENTS',/,26X,'INPUT MA  A1601
    -Y BE REQUIRED.)',//,21X,'= 3, CONCENTRATION OF ELEMENTS ENTERED AS  A1602
    = PPM',/,26X,'OF THE SPECIES WHICH HAS A GRAM FORMULA',/,26X,'WEIGH  A1603
    +T GIVEN IN ELEMENTS INPUT.  (ELEMENTS',/,26X,'INPUT MAY BE REQUIRE  A1604
    :D.)',/,1X,'FORMAT (I1)',//)                                         A1605
     GO TO 1715                                                          A1606
4380 WRITE (1,4390) SUB(1)                                               A1607
4390 FORMAT (/1X,A8,/,13X,'PH',11X,'THE PH OF THE SOLUTION (THE APPROXI  A1608
    1MATE PH',/,26X,'IF IOPT(2) = 1)',/,1X,'FORMAT (F10.3)',//)          A1609
     GO TO 1718                                                          A1610
4400 WRITE (1,4410) SUB(1)                                               A1611
4410 FORMAT (/1X,A8,/,13X,'PE',11X,'THE PE OF THE SOLUTION. REQUIRED FO  A1612
    1R ALL',/,26X,'SOLUTIONS.',/,1X,'FORMAT (F10.3)',//)                 A1613
     GO TO 1723                                                          A1614
4420 WRITE (1,4430) SUB(1)                                               A1615
4430 FORMAT (/1X,A8,/,13X,'TEMP',9X,'THE TEMPERATURE OF THE SOLUTION IN  A1616
    1 DEGREES',/,26X,'CELCIUS.',/,1X,'FORMAT (F10.3)',//)                A1617
     GO TO 1724                                                          A1618
4440 WRITE (1,4450) SUB(1)                                               A1619
4450 FORMAT (/1X,A8,/,13X,'SDENS',8X,'THE DENSITY OF THE SOLUTION.',/,1  A1620
    1X,'FORMAT (F10.3)',//)                                              A1621
     GO TO 1482                                                          A1622
4100 WRITE (1,4101) SUB(1)                                               A1623
4101 FORMAT (/1X,A8,/,13X,'LT,DTOT',6X,'TOTAL CONCENTRATIONS OF ELEMENT  A1624
    1S.',/,26X,'LT',8X,'INDEX NUMBER OF THE ELEMENT.',//,26X,'DTOT',     A1625
    26X,'TOTAL CONCENTRATION OF THE ELEMENT IN',/,36X,'MOLALITY, MMOLES  A1626
    3/L, MG/L, OR',/,36X,'PPM ACCORDING TO IUNITS.',/,1X,'FORMAT (I4'    A1627
    4,',1X,F11.4)')                                                      A1628
     WRITE (1,4000)                                                      A1629
     GO TO (1326,1356),N2                                                A1630
4102 WRITE (1,4103) SUB(2)                                               A1631
4103 FORMAT (/1X,A8,/,13X,'TNAME',8X,'ALPHANUMERIC NAME OF ELEMENT.',    A1632
    1/,1X,'FORMAT (A8)')                                                 A1633
     WRITE (1,4000)                                                      A1634
4000 FORMAT (' NOTE:  FOR A LISTING OF MASTER SPECIES AND ELEMENTS,'     A1635
    1,/,8X,'ENTER <LIST>.',//)                                           A1636
     GO TO 1729                                                          A1637
4104 WRITE (1,4105) SUB(2)                                               A1638
4105 FORMAT (/1X,A8,/,13X,'NELT',9X,'INDEX NUMBER ASSIGNED TO THE ELEME  A1639
    1NT.  NUMBER',/,26X,'MUST BE BETWEEN 4 AND 30, INCLUSIVE.',/,1X,     A1640
    2'FORMAT (I2)')                                                      A1641
     WRITE (1,4000)                                                      A1642
     GO TO 1550                                                          A1643
4106 WRITE (1,4107) SUB(2)                                               A1644
4107 FORMAT (/1X,A8,/,13X,'TGFW',9X,'GRAM FORMULA WEIGHT OF THE SPECIES  A1645
    1 USED TO',/,26X,'REPORT THE ANALYTICAL DATA.  IF SOLUTION DATA'     A1646
    2,/,26X,'IS TO INCLUDE ALKALINITY, TGFW FOR THE ELEMENT',/,26X,'CAR  A1647
    3BON MUST BE THE EQUIVALENT WEIGHT OF THE',/,26X,'REPORTED ALKALINI  A1648
    4TY SPECIES.',/,1X,'FORMAT (F10.4)')                                 A1649
     WRITE (1,4000)                                                      A1650
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      GO TO 1570                                                        A1651
4110  WRITE (1,4111) SUB(3)                                             A1652
4111  FORMAT (/1X,A8,/,13X,'I',12X,'THE INDEX NUMBER ASSIGNED TO THE AQU A1653
     1EOUS',/,26X,'SPECIES.  NUMBER 4 THROUGH 30 ARE RESERVED',/,26X,   A1654
     2'FOR MASTER SPECIES.  250 IS THE MAXIMUM INDEX',/,26X,'NUMBER FOR A1655
     3AN AQUEOUS SPECIES.',/,1X,'FORMAT (I3)',//)                       A1656
      GO TO 1590                                                        A1657
4112  WRITE (1,4113) SUB(3)                                             A1658
4113  FORMAT (/1X,A8,/,13X,'SNAME',8X,'ALPHANUMERIC SPECIES NAME.',/,1X, A1659
     1'FORMAT (A8)',//)                                                 A1660
      GO TO 1660                                                        A1661
4114  WRITE (1,4115) SUB(3)                                             A1662
4115  FORMAT (/1X,A8,/,13X,'NSP',10X,'THE TOTAL NUMBER OF MASTER SPECIES A1663
     1 IN THE',/,26X,'ASSOCIATION REACTION THAT FORMS THIS SPECIES;',/,2 A1664
     26X,'DO NOT COUNT THE SPECIES ITSELF UNLESS THE',/,26X,'SPECIES IS A1665
     3A MASTER SPECIES.',/,1X,'FORMAT (I3)',//)                         A1666
      GO TO 1676                                                        A1667
4116  WRITE (1,4117) SUB(3)                                             A1668
4117  FORMAT (/1X,A8/,13X,'KFLAG',3X,'= 0, THE VAN''T HOFF EXPRESSION IS A1669
     1 USED TO CALCU-',/,26X,'LATE TEMPERATURE DEPENDENCE OF THE ASSOCIA A1670
     2TION',/,26X,'CONSTANT FOR THIS SPECIES.',//,21X,'= 1, AN ANALYTICA A1671
     3L EXPRESSION IS USED TO CALCU-',/,26X,'LATE TEMPERATURE DEPENDENCE A1672
     4 OF THE ASSOCIATION',/,26X,'CONSTANT.',/,1X,'FORMAT (I1)',//)     A1673
      GO TO 1680                                                        A1674
4118  WRITE (1,4119) SUB(3)                                             A1675
4119  FORMAT (/1X,A8,/,13X,'GFLAG',3X,'= 0, THE EXTENDED DEBYE-HUCKEL OR A1676
     1 DAVIS EXPRES-',/,26X,'SION (ACCORDING TO IOPT(6)) IS USED TO CALC A1677
     2ULATE',/,26X,'THE ACTIVITY COEFFICIENT FOR THIS SPECIES.',//,21X, A1678
     3'= 1, THE WATEQ DEBYE-HUCKEL EXPRESSION IS USED',/,26X,'TO CALCULA A1679
     4TE THE ACTIVITY COEFFICIENT OF THIS',/,26X,'SPECIES REGARDLESS OF  A1680
     5THE VALUE OF IOPT(6)',/,1X,'FORMAT (I1)',//)                      A1681
      GO TO 1690                                                        A1682
4120  WRITE (1,4121) SUB(3)                                             A1683
4121  FORMAT (/1X,A8,/,13X,'ZSP',10X,'THE CHARGE ON THIS AQUEOUS SPECIES A1684
     1.',/,1X,'FORMAT (F10.3)',//)                                      A1685
      GO TO 1780                                                        A1686
4122  WRITE (1,4123) SUB(3)                                             A1687
4123  FORMAT (/1X,A8,/,13X,'THSP',9X,'THE SUM OF THE FORMAL VALENCE OF T A1688
     1HE REDOX',/,26X,'SPECIES IN THIS SPECIES.  (E.G. FESO4 HAS',/,26X, A1689
     2'A THSP = 2 + 6 = 8.)',/,1X,'FORMAT (F10.3)',//)                  A1690
      GO TO 1790                                                        A1691
4124  WRITE (1,4125) SUB(3)                                             A1692
4125  FORMAT (/1X,A8,/,13X,'DHA',10X,'THE EXTENDED DEBYE-HUCKEL A 0 TERM A1693
     1.',/,1X,'FORMAT (F10.3)'//)                                       A1694
      GO TO 1880                                                        A1695
4126  WRITE (1,4127) SUB(3)                                             A1696
4127  FORMAT (/1X,A8,/,13X,'ADHSP(1)',5X,'THE A(I) TERM FOR THE WATEQ DE A1697
     1BYE-HUCKEL EXPRESSION.',/,1X,'FORMAT (F10.3)',//)                 A1698
      GO TO 1892                                                        A1699
4128  WRITE (1,4129) SUB(3)                                             A1700
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4129 FORMAT (/1X,A8,/,13X,'ADHSP(2)',5X,'THE B(I) TERM FOR THE WATEQ DE  A1701
    1BYE-HUCKEL EXPRESSION.',/,1X,'FORMAT (F10.3)',//)                   A1702
     GO TO 1892                                                          A1703
4130 WRITE (1,4131) SUB(3)                                               A1704
4131 FORMAT (/1X,A8,/,13X,'ALKSP',8X,'THE ALKALINITY ASSIGNED TO THIS A  A1705
    1QUEOUS SPECIES.',/,1X,'FORMAT (F10.3)',//)                          A1706
     GO TO 1740                                                          A1707
4132 WRITE (1,4133) SUB(3)                                               A1708
4133 FORMAT (/1X,A8,/,13X,'LKTOSP',7X,'LOG (K) AT 25 DEGREES CELCIUS',   A1709
    1', WHERE',/)                                                        A1710
     WRITE (1,4134)                                                      A1711
4134 FORMAT (26X,'LOG (K) = A1 + A2*T + A3/T + A4*T^2 + A5/T^2')         A1712
     WRITE (1,4135)                                                      A1713
4135 FORMAT (/1X,'FORMAT (F10.3)'//)                                     A1714
     GO TO 1960                                                          A1715
4136 WRITE (1,4137) SUB(3)                                               A1716
4137 FORMAT (/1X,A8,/,13X,'DHSP',9X,'STANDARD ENTHALPY OF THE ASSOCIAT'  A1717
    1,'ION REACTION AT',/,26X,'25 DEGREES CELCIUS ( H(R), IN KCAL/'      A1718
    2,'MOLE ).',/,1X,'FORMAT (F10.3)',//)                                A1719
     GO TO 1970                                                          A1720
4138 WRITE (1,4139) SUB(3),K,K                                           A1721
4139 FORMAT (/1X,A8,/,13X,'ASP(',I1,')',7X,'A',I1,' OF THE FOLLOWING',   A1722
    1' EQUATION:',/)                                                     A1723
     WRITE (1,4134)                                                      A1724
     WRITE (1,4140)                                                      A1725
4140 FORMAT (/1X,'FORMAT (F12.5)')                                       A1726
     GO TO 1987                                                          A1727
4142 WRITE (1,4143) SUB(3)                                               A1728
4143 FORMAT (/1X,A8,/,13X,'LSP',10X,'INDEX NUMBER OF MASTER SPECIES.'    A1729
    1,/,1X,'FORMAT (I3)')                                                A1730
     WRITE (1,4000)                                                      A1731
     GO TO 1915                                                          A1732
4144 WRITE (1,4145) SUB(3)                                               A1733
4145 FORMAT (/1X,A8,/,13X,'CSP',10X,'STOICHIOMETRIC COEFFICIENT OF',     A1734
    1' MASTER SPECIES',/,26X,'IN THIS AQUEOUS SPECIES.',/,1X,'FORMAT'    A1735
    2,' (F7.3)')                                                         A1736
     WRITE (1,4000)                                                      A1737
     GO TO 1915                                                          A1738
8000 WRITE (1,8001) SUB(I)                                               A1739
8001 FORMAT (/1X,A8,/,13X,'MNAME',8X,'ALPHANUMERIC NAME OF MINERAL',/,   A1740
    11X,'FORMAT (A8)',//)                                                A1741
     GO TO 3102                                                          A1742
8002 WRITE (1,8003) SUB(I)                                               A1743
8003 FORMAT (/1X,A8,/,13X,'NMINO',8X,'NUMBER OF DIFFERENT SPECIES IN TH  A1744
    1E MINERAL',/,26X,'DISSOCIATION REACTION (INCLUDING H+, E-, AND',/   A1745
    2,26X,'H2O).  NMINO MUST BE LESS THAN OR EQUAL TO 10.',/,1X,         A1746
    3'FORMAT (I2)',//)                                                   A1747
     GO TO 3110                                                          A1748
8004 WRITE (1,8005) SUB(I)                                               A1749
8005 FORMAT (/1X,A8,/,13X,'THMIN',8X,'THE SUM OF THE VALENCES OF THE RE  A1750
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    1DOX SPECIES',/,26X,'IN THE MINERAL DISSOCIATION REACTION.',/,1X,    A1751
    2'FORMAT (F10.3)',//)                                               A1752
     GO TO 3120                                                         A1753
8006 WRITE (1,8007)SUB(I)                                               A1754
8007 FORMAT (/1X,A8,/,13X,'LKTOM',8X,'LOG OF THE EQUILIBRIUM CONSTANT'  A1755
    1,' AT 25 DEGREES',/,26X,'CELCIUS FOR THE REACTION',/,1X,'FORM AT'  A1756
    2,' (F10.3)',//)                                                    A1757
     GO TO 3130                                                         A1758
8008 WRITE (1,8009) SUB(I)                                              A1759
8009 FORMAT (/1X,A8,/,13X,'DHMIN',8X,'DELTA H(R) (KCAL/MOLE) FOR THE '  A1760
    1,'VANT HOFF',/,26X,'EXPRESSION.',/,1X,'FORMAT (F10.3)'//)          A1761
     GO TO 3140                                                         A1762
8010 WRITE (1,8011) SUB(I)                                              A1763
8011 FORMAT (/1X,A8,/,13X,'MFLAG',3X,'= 0, THE VANT HOFF EXPRESSION IS' A1764
    1,' USED TO CALCU-',/,26X,'LATE THE TEMPERATURE DEPENDENCE OF THE', A1765
    2' EQUIL-',/,26X,'IBRIUM CONSTANT',//,21X,'= 1, THE ANALYTICAL EXP' A1766
    3,'RESSION IS USED TO CALCU-'/,26X,'LATE THE TEMPERATURE DEPENDENCE A1767
    4 OF THE EQUIL-',/,26X,'IBRIUM CONSTANT.',/,1X,'FORMAT (I1)'//)     A1768
     GO TO 3150                                                         A1769
8012 WRITE (1,8013) SUB(I)                                              A1770
8013 FORMAT (/1X,A8,/,13X,'SIMIN',8X,'SATURATION INDEX (LOG(ION ACTIVI' A1771
    1,'TY PRODUCT/K(SP)))',/,26X,'DESIRED IN THE FINAL SOLUTION.  SIMIN A1772
    2 = 0.0',/,26X,'WOULD PRODUCE EQUILIBRIUM WITH THE MINERAL',/,26X,  A1773
    3'WHILE 1.0 WOULD PRODUCE A SOLUTION 10 TIMES',/,26X,'SUPERSATURATE A1774
    4D (SI = 1.0).  THIS VARIABLE IS',/,26X,'USEFUL IN SPECIFYING THE ' A1775
    5,'PARTIAL PRESSURE OF',/,26X,'A GAS.  THE HENRY(S) LAW CONSTANT ', A1776
    6'FOR THE GAS',/,26X,'WOULD BE ENTERED USING THE VANT HOFF (LKTOM)  A1777
    7'/,26X,'OR ANALYTICAL EXPRESSION (AMIN) AND THE LOG OF'/,25X,' THE A1778
    8 PARTIAL PRESSURE WOULD BE ENTERED FOR SIMIN.',/,1X,'FORMAT (F10.3 A1779
    9)',//)                                                             A1780
     GO TO 3167                                                         A1781
8014 WRITE (1,8015) SUB(I)                                              A1782
8015 FORMAT (/1X,A8,/,13X,'LMIN',9X,'INDEX NUMBER OF SPECIES (NOT NECE' A1783
    1,'SSARILY MASTER',/,26X,'SPECIES) IN THE DISSOCIATION REACTION ',  A1784
    2'FOR',/,26X,'THIS MINERAL',/,1X,'FORMAT (I4)')                     A1785
     WRITE (1,3800)                                                     A1786
     GO TO 3195                                                         A1787
8016 WRITE (1,8017) SUB(I)                                              A1788
8017 FORMAT (/1X,A8,/,13X,'CMIN',9X,'STOICHIOMETRIC COEFFICIENT OF ',   A1789
    1'SPECIES IN',/,26X,'DISSOCIATION REACTION.',/,1X,'FORMAT (F11.3)')  A1790
     WRITE (1,3800)                                                     A1791
     GO TO 3195                                                         A1792
8018 WRITE (1,8019) SUB(I),K,K                                          A1793
8019 FORMAT (/1X,A8,/,13X,'AMIN(',I1,')',6X,'A',I1,1X,'OF THE FOLLOWING A1794
    1 MINERAL DISSOCIATION',/,26X,'REACTION:',//,26X,'LOG (K) = A1 +'   A1795
    2,' A2*T + A3/T + A4*T^2 + A5/T^2',//,26X,'WHERE T IS IN DEGREES',  A1796
    3' KELVIN',/,1X,'FORMAT (F12.5)',//)                                A1797
     GO TO 3207                                                         A1798
8020 WRITE (1,8021) SUB(6)                                              A1799
8021 FORMAT (/1X,A8,/,13X,'XTEMP',8X,'TEMPERATURE IN DEGREES CELSIUS.'  A1800
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    1,/,1X,'FORMAT (F10.3)',//)                                          A1801
     GO TO 3307                                                          A1802
8022 WRITE (1,8023) SUB(7)                                               A1803
8023 FORMAT (/1X,A8,/,13X,'XSTEP',8X,'THE FRACTION OF SOLUTION 1 TO BE'  A1804
    1,/,26X,'MIXED WITH SOLUTION 2.')                                    A1805
8030 WRITE (1,8029)                                                      A1806
8029 FORMAT (1X,'FORMAT (F10.9)',//)                                     A1807
     GO TO 3607                                                          A1808
8024 WRITE (1,8025) SUB(7)                                               A1809
8025 FORMAT (/1X,A8,/,13X,'XSTEP',8X,'THE VOLUME OF SOLUTION 2 TO',      A1810
    1' BE',/,26X,'TITRATED INTO SOLUTION 1.  XSTEP MUST',/,26X,'HAVE'    A1811
    2,' THE SAME UNITS AS VO.')                                          A1812
     GO TO 8030                                                          A1813
8026 WRITE (1,8027) SUB(7)                                               A1814
8027 FORMAT (/1X,A8,/,13X,'XSTEP',8X,'THE MOLES OF REACTION TO BE ',     A1815
    1'ADDED',/,26X,'TO SOLUTION 1')                                      A1816
     GO TO 8030                                                          A1817
8028 WRITE (1,8031) SUB(7)                                               A1818
8031 FORMAT (/1X,A8,/,13X,'XSTEP',8X,'THE TOTAL NUMBER OF MOLES OF'      A1819
    1,/,26X,'REACTION TO BE ADDED IN NSTEPS',/,26X,'STEPS.  NSTEPS'      A1820
    2,' REACTION SOLUTIONS'/,26X,'WILL BE CALCULATED.  THE I(TH) SOLU-'  A1821
    3,/,26X,'TION WILL HAVE I*XSTEP/NSTEPS MOLES',/,26X,'OF REACTION'    A1822
    4,' ADDED TO SOLUTION 1.')                                           A1823
     GO TO 8030                                                          A1824
8032 WRITE (1,8033) SUB(8)                                               A1825
8033 FORMAT (/1X,A8,/,13X,'LREAC',8X,'INDEX NUMBER OF ELEMENT FOR THE'   A1826
    1,' REACTION.',/,26X,'LREAC MUST BE BETWEEN 4 AND 30 INCLUSIVE.',/,  A1827
    226X,'IF LREAC IS GREATER THAN 30 THE PROGRAM',/,26X,'CONSIDERS',    A1828
    3' THIS CONSTITUENT TO BE H2 OR ',/,26X,'O2 AND ONLY USES CREAC',    A1829
    4' AND THMEAN',/,26X,'TO CHANGE THE OXIDATION STATE OF THE',/,26X    A1830
    5,'REACTION SOLUTION.',/,1X,'FORMAT (I4)')                           A1831
     WRITE (1,3800)                                                      A1832
     GO TO 5015                                                          A1833
8034 WRITE (1,8035) SUB(8)                                               A1834
8035 FORMAT (/1X,A8,/,13X,'CREAC',8X,'STOICHIOMETRIC COEFFICIENT OF'     A1835
    1,' THE ELEMENT',/,26X,'IN THE REACTION',/,1X,'FORMAT (F8.3)')       A1836
     WRITE (1,3800)                                                      A1837
     GO TO 5015                                                          A1838
8036 WRITE (1,8037) SUB(8)                                               A1839
8037 FORMAT (/1X,A8,/,13X,'THMEAN',7X,'THE VALENCE OF THE ELEMENT IN'    A1840
    1,' THE REACTION.',/,26X,'AN ELEMENT MAY BE INCLUDED MORE THAN',     A1841
    2' ONCE IN',/,26X,'A REACTION TO ACCOMODATE DIFFERENT VALENCE',/,    A1842
    326X,'STATES OF THE ELEMENT.',/,1X,'FORMAT (F8.3)')                  A1843
     WRITE (1,3800)                                                      A1844
     GO TO 5015                                                          A1845
8038 WRITE (1,8039) SUB(9)                                               A1846
8039 FORMAT (/1X,A8,/,13X,'LPOS',9X,'INDEX NUMBER OF AN ELEMENT WITH'    A1847
    1,' A CATION',/,26X,'MASTER SPECIES.',/,1X,'FORMAT (I5)')            A1848
     WRITE (1,3800)                                                      A1849
     GO TO 6010                                                          A1850
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 8040 WRITE (1,8041) SUB(9)                                              A1851
 8041 FORMAT (/1X,A8,/,13X,'LNEG',9X,'INDEX NUMBER OF AN ELEMENT WITH'   A1852
     1,' AN ANION',/,26X,'MASTER SPECIES.',/,1X,'FORMAT (I5)')           A1853
      WRITE (1,3800)                                                     A1854
 3800 FORMAT (1X,'NOTE:  FOR A LISTING OF MASTER SPECIES AND ELEMENTS,'  A1855
     1,/,8X,'ENTER <LIST>.',//)                                          A1856
      GO TO 6020                                                         A1857
 8042 WRITE (1,8043) SUB(10)                                             A1858
 8043 FORMAT (/1X,A8,/,13X,'SUNAME',7X,'ALPHANUMERIC NAME TO BE PRINT'   A1859
     1'ED TO IDENTIFY',/,26X,'THE SUM.',/,1X,'FORMAT (A8)'//)            A1860
      GO TO 7010                                                         A1861
 8044 WRITE (1,8045) SUB(10)                                             A1862
 8045 FORMAT (/1X,A8,/,13X,'NSUM',9X,'THE NUMBER OF INDEX NUMBER TO BE'  A1863
     1,' READ.',/,26X,'NSUM<=50.',/,1X,'FORMAT (I2)'//)                  A1864
      GO TO 7020                                                         A1865
 8046 WRITE (1,8047) SUB (10)                                            A1866
 8047 FORMAT (/1X,A8,/,13X,'LSUM',9X,'INDEX NUMBERS OF SPECIES IN '      A1867
     1,'SUM.',/,1X,'FORMAT (I4)'//)                                      A1868
      GO TO 7037                                                         A1869
      END                                                                A1870
      SUBROUTINE READFILE                                                B   1
C                                                                        B   2
C         THIS SUBROUTINE READS FROM LOGICAL FILE #11,                   B   3
C         PRE-CONSTRUCTED MINERAL CARDS; AND FROM LOGICAL FILE #12,      B   4
C         THE THERMODYNAMIC DATA OF PHREEQE, THE NECESSARY INFORMATIONS  B   5
C         TO CONSTRUCT A MASTER SPECIES AND ELEMENTS TABLE.              B   6
C                                                                        B   7
      REAL ICOL3(0:30),NOUSE6                                            B   8
      CHARACTER *80 LINE                                                 B   9
      CHARACTER *12 THMIN(100),LKTOM(100),DHMIN(100),SIMIN(100)          B  10
     1,CMIN(100,10),AMIN(100,5)                                          B  11
      CHARACTER *8 NONE,MNAME(100),SUB(11),ICOL1(0:30),ICOL4(0:30)       B  12
     1,SPEC(30),KEYWORD,NOUSE2                                           B  13
      COMMON /PT/ MNAME,NMINO(100),THMIN,LKTOM,DHMIN,MFLAG(100)          B  14
     1,SIMIN,LMIN(100,10),CMIN,AMIN,IMINERAL,SUB,ICOL1,ICOL2(0:30)       B  15
     2,ICOL3,ICOL4,SPEC,OPV(30)                                          B  16
      DATA NONE/'********'/                                              B  17
C                                                                        B  18
      LREAD=0                                                            B  19
      DO 40 M=1,30                                                       B  20
   40 ICOL2(M)=0                                                         B  21
      NUM=1                                                              B  22
C                                                                        B  23
C         READ MINERAL CARDS.                                            B  24
C         NOTE:  MAXIMUM NUMBER OF MINERALS IS 100.                      B  25
C                                                                        B  26
      OPEN (UNIT=11,FILE='MINERALS.DATA',STATUS='OLD')                   B  27
      DO 26 M=1,100                                                      B  28
      READ (11,27,END=7)MNAME(M),NMINO(M),THMIN(M),LKTOM(M),DHMIN(M)     B  29
     1,MFLAG(M),SIMIN(M)                                                 B  30
```

```
   27 FORMAT (A8,2X,I2,3X,3A10,5X,I1,9X,A10)                          B  31
      NO2=NMINO(M)                                                    B  32
      IF (NO2.LE.5) GO TO 29                                          B  33
      NO2=5                                                           B  34
   29 READ (11,28) (LMIN(M,M0),CMIN(M,M0),M0=NUM,NO2)                 B  35
   28 FORMAT (5(I4,A11))                                              B  36
      IF (NMINO(M).LE.5.OR.NUM.EQ.6) GO TO 30                         B  37
      NUM=6                                                           B  38
      NO2=NMINO(M)                                                    B  39
      GO TO 29                                                        B  40
   30 IF (MFLAG(M).NE.1) GO TO 26                                     B  41
      READ (11,31) (AMIN(M,M0),M0=1,5)                                B  42
   31 FORMAT (5A12)                                                   B  43
   26 CONTINUE                                                        B  44
    7 IMINERAL=M-1                                                    B  45
C                                                                     B  46
C           READ THERMODYNAMIC DATA OF PHREEQE.                       B  47
C        NOTE: THE DATA BLOCKS OF PHREEQE DATA CAN BE ARRNAGED        B  48
C              IN ANY ORDER.                                          B  49
C                                                                     B  50
      OPEN (UNIT=12,FILE='PHREEQE.DATA',STATUS='OLD')                 B  51
   48 READ (12,11) KEYWORD                                            B  52
   11 FORMAT (A8)                                                     B  53
C                                                                     B  54
C        READ IS REPEATED UNTIL A KEYWORD IS FOUND.                   B  55
C                                                                     B  56
   45 IF (KEYWORD.EQ.SUB(2))GO TO 42                                  B  57
      IF (KEYWORD.EQ.SUB(3))GO TO 44                                  B  58
      READ (12,43,END=50)LINE                                         B  59
   43 FORMAT (A80)                                                    B  60
      READ (LINE,11) KEYWORD                                          B  61
      GO TO 45                                                        B  62
   46 LREAD=LREAD+1                                                   B  63
      IF (LREAD.EQ.2)RETURN                                           B  64
      GO TO 48                                                        B  65
C                                                                     B  66
C        READ SPECIES DATA BLOCK.                                     B  67
C                                                                     B  68
   44 DO 80 JL=1,250                                                  B  69
      READ (12,51) NOUSE1                                             B  70
      IF (NOUSE1.EQ.0)GO TO 46                                        B  71
      READ (12,52)NOUSE2,NOUSE3,NOUSE4,NOUSE5,NOUSE6                  B  72
   51 FORMAT (I3)                                                     B  73
   52 FORMAT (A8,2X,I3,2I1,F10.3,//)                                  B  74
      IF (NOUSE3.GT.6)READ (22,53)                                    B  75
   53 FORMAT (1X)                                                     B  76
      IF (NOUSE1.GT.30)GO TO 80                                       B  77
      SPEC(NOUSE1)=NOUSE2                                             B  78
      OPV(NOUSE1)=NOUSE6                                              B  79
   80 CONTINUE                                                        B  80
```

```
      GO TO 46                                                          B  81
C                                                                       B  82
C         READ ELEMENTS DATA BLOCK.                                     B  83
C                                                                       B  84
   42 DO 8 JL=1,50                                                      B  85
      READ (12,9)ICOL1(0),ICOL2(0),ICOL3(0),ICOL4(0)                    B  86
    9 FORMAT (A8,2X,I2,3X,F10.0,5X,A8)                                  B  87
      IF (ICOL2(0).GT.30)GO TO 8                                        B  88
      IF (ICOL2(0).NE.0)GO TO 100                                       B  89
      JCOL=JL-1                                                         B  90
      GO TO 46                                                          B  91
  100 ICOL1(ICOL2(0))=ICOL1(0)                                          B  92
      ICOL2(ICOL2(0))=ICOL2(0)                                          B  93
      ICOL3(ICOL2(0))=ICOL3(0)                                          B  94
      ICOL4(ICOL2(0))=ICOL4(0)                                          B  95
    8 CONTINUE                                                          B  96
   50 STOP                                                              B  97
C     ***********                                                       B  98
      ENTRY LISTM                                                       B  99
C     ***********                                                       B 100
C                                                                       B 101
C         THIS SUBROUTINE FORMATS AND PRINTS A TABLE OF MASTER          B 102
C         SPECIES AND ELEMENTS.                                         B 103
C                                                                       B 104
      DO 200 MO=1,3                                                     B 105
      ICOL1(MO)=NONE                                                    B 106
      ICOL2(MO)=MO                                                      B 107
      ICOL3(MO)=0.0                                                     B 108
      ICOL4(MO)=NONE                                                    B 109
      OPV(MO)=0.0                                                       B 110
  200 CONTINUE                                                          B 111
      ICOL3(3)=18.0152                                                  B 112
      SPEC(1)='H+       '                                               B 113
      SPEC(2)='E-       '                                               B 114
      SPEC(3)='H2O      '                                               B 115
      WRITE (1,201)                                                     B 116
  201 FORMAT (/34X,'INPUT FORMULA',/,34X,'CORRESPONDING',5X,'MASTER',/  B 117
     1,1X,'ELEMENTS',5X,'#',9X,'GFW',10X,'TO GFW',9X,'SPECIES',6X,'OPV' B 118
     2,/,1X,8('-'),4X,3('-'),4X,10('-'),4X,14('-'),4X,8('-'),4X,5('-')  B 119
     3,/)                                                               B 120
      DO 203 MO=1,30                                                    B 121
      IF (ICOL2(MO).EQ.0)GO TO 203                                      B 122
      WRITE(1,202)ICOL1(MO),ICOL2(MO),ICOL3(MO),ICOL4(MO),SPEC(MO)      B 123
     1,OPV(MO)                                                          B 124
  203 CONTINUE                                                          B 125
  202 FORMAT (1X,A8,4X,I2,5X,F10.4,8X,A8,6X,A8,4X,SP,F4.1,SS)           B 126
      RETURN                                                            B 127
      END                                                               B 128
C                                                                       C   1
      SUBROUTINE REF (ILINE,JOPT,JOPEN)                                 C   2
```

```
C                                                                       C   3
C       THIS SUBROUTINE READS CERTAIN NUMBER OF LINES--ACCORDING        C   4
C       TO THE VALUE OF ILINE--FROM THE REFERENCE FILE, PRINTS          C   5
C       IT(THEM) ON THE SCREEN, AND, DEPENDING ON THE VALUE OF          C   6
C       IOPEN, ASKS A QUESTION CONCERNING THE FATE OF THE LINE(S).      C   7
C                                                                       C   8
C       JOPT:  0 = NO PRINT OF LINES                                    C   9
C              1 = PRINT THE LINES                                      C  10
C       JOPEN: 0 = NO QUESTION ASKED                                    C  11
C              > 0 = QUESTION ASKED                                     C  12
C                                                                       C  13
      COMMON /REFF/ JOPTION,IOPEN,JLINE                                 C  14
      COMMON /REFF1/ I                                                  C  15
      CHARACTER *80 JLINE(3),LINE                                       C  16
C                                                                       C  17
      DO 310 II=1,ILINE                                                 C  18
      READ (13,10,END=99) JLINE(II)                                     C  19
   10 FORMAT (A80)                                                      C  20
      IF (JLINE(II)(1:10).NE.'          ')GO TO 311                     C  21
      IF (II.NE.1) GO TO 311                                            C  22
      JOPTION=0                                                         C  23
      RETURN                                                            C  24
  311 IF (JOPT.EQ.0) GO TO 310                                          C  25
      WRITE (1,300) JLINE(II)                                           C  26
  300 FORMAT (A80)                                                      C  27
  310 CONTINUE                                                          C  28
      IF (JOPEN.EQ.0)RETURN                                             C  29
  402 GO TO (303,400,500,600), JOPEN                                    C  30
  303 WRITE (1,301)                                                     C  31
  301 FORMAT ('ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=REPLACE)')           C  32
  305 READ (1,300) LINE                                                 C  33
      READ (LINE,*,ERR=402) JOPTION                                     C  34
      IF (JOPTION.LE.0.OR.JOPTION.GT.3)GO TO 402                        C  35
      IF ((JOPTION.EQ.3).AND.(JOPEN.EQ.2.OR.JOPEN.EQ.4))GO TO 402       C  36
      RETURN                                                            C  37
   99 IOPEN=0                                                           C  38
      RETURN                                                            C  39
  400 WRITE (1,401)                                                     C  40
  401 FORMAT ('ENTER OPTION.  (1=KEEP, 2=ELIMINATE)')                   C  41
      GO TO 305                                                         C  42
  500 WRITE (1,501)                                                     C  43
  501 FORMAT ('ENTER OPTION.  (1=KEEP, 2=MODIFY, 3=ELIMINATE)')         C  44
      GO TO 305                                                         C  45
  600 WRITE (1,601)                                                     C  46
  601 FORMAT ('ENTER OPTION.  (1=KEEP, 2=REPLACE)')                     C  47
      GO TO 305                                                         C  48
      END                                                               C  49
C                                                                       D   1
      SUBROUTINE SPECL(I)                                               D   2
C                                                                       D   3
```

```
C       THIS SUBROUTINE CHECKS FOR SPECIAL CHARACTERS 'EXIT' AND 'LIST'   D   4
C                                                                         D   5
      COMMON /EE/ EXIT,LIST,LINE,JFLAG                                    D   6
      LOGICAL EXIT,LIST                                                   D   7
      CHARACTER *80 LINE                                                  D   8
C                                                                         D   9
      EXIT=.FALSE.                                                        D  10
      LIST=.FALSE.                                                        D  11
      IF (I.EQ.0) RETURN                                                  D  12
      IF ((LINE(1:4).EQ.'LIST'.OR.LINE(1:4).EQ.'list').AND.(I.EQ.2.OR.    D  13
     1I.EQ.3)) LIST=.TRUE.                                                D  14
      IF ((LINE(1:4).EQ.'EXIT'.OR.LINE(1:4).EQ.'exit').AND.(I.EQ.1.OR.    D  15
     1I.EQ.3)) EXIT=.TRUE.                                                D  16
      RETURN                                                              D  17
      END                                                                 D  18
C                                                                         E   1
      LOGICAL FUNCTION OK                                                 E   2
C                                                                         E   3
C         THIS SUBROUTINE ASKS WHETHER IT IS O.K.                         E   4
C                                                                         E   5
      COMMON /PN/ NFLAG                                                   E   6
      LOGICAL ANSWER,YN                                                   E   7
C                                                                         E   8
      WRITE (1,10)                                                        E   9
   10 FORMAT ('O.K.?')                                                    E  10
      NFLAG=0                                                             E  11
      OK=.TRUE.                                                           E  12
      ANSWER=YN()                                                         E  13
      IF (ANSWER) RETURN                                                  E  14
      NFLAG=1                                                             E  15
      OK=.FALSE.                                                          E  16
      RETURN                                                              E  17
      END                                                                 E  18
C                                                                         F   1
C     THIS SUBROUTINE READS VALUES FROM THE TERMINAL AND CHECKS TO MAKE   F   2
C        SURE THAT IT IS PROPER                                           F   3
C                                                                         F   4
      SUBROUTINE QUESTA (*,J1,CHAR1,L1,STRING,F1,K1,M1)                   F   5
      COMMON /REFF/ JOPTION,IOPEN,JLINE                                   F   6
      COMMON /PN/ NFLAG                                                   F   7
      COMMON /EE/ EXIT,LIST,LINE,JFLAG                                    F   8
      CHARACTER *(*) STRING                                               F   9
      CHARACTER *80 LINE,JLINE(3)                                         F  10
      CHARACTER *72 QUESTION                                              F  11
      CHARACTER *40 FMT                                                   F  12
      CHARACTER *16 CHAR,CHAR1                                            F  13
      CHARACTER *4 F,F1                                                   F  14
      CHARACTER *2 F0(16)                                                 F  15
      LOGICAL EXIT,LIST,NONB                                              F  16
      DATA F0/'1 ','2 ','3 ','4 ','5 ','6 ','7 ','8 ','9 ','10','11'     F  17
```

```
     1,'12','13','14','15','16' /                                          F  18
      DATA QUESTION /'KEEP THE OLD VALUE? (HIT <RETURN> IF YOU DO; IF NO    F  19
     1T, REENTER THE DATA)'/                                                F  20
C                                                                           F  21
C        K=0 ==> STRING                                                     F  22
C        K=1 ==> REAL                                                       F  23
C        K=2 ==> INTEGER                                                    F  24
C                                                                           F  25
      IF (F1.EQ.'A80') F1='/A80'                                            F  26
      GO TO 50                                                              F  27
C     ***********************************************                       F  28
      ENTRY QUESTB (*,J,CHAR,L,IVAL,F,IMIN,IMAX,M)                          F  29
C     ***********************************************                       F  30
      K=2                                                                   F  31
      GO TO 100                                                             F  32
C                                                                           F  33
   50 J=J1                                                                  F  34
      CHAR=CHAR1                                                            F  35
      F=F1                                                                  F  36
      K=K1                                                                  F  37
      L=L1                                                                  F  38
      M=M1                                                                  F  39
C                                                                           F  40
  100 IF (J.GT.0.AND.J.LT.10) I=1                                           F  41
      IF (J.GE.10.AND.J.LT.100) I=2                                         F  42
      IF (J.GE.100) I=3                                                     F  43
      IF (NFLAG.GT.0.OR.JOPTION.EQ.2) GO TO 30                              F  44
      IF (J.GT.0) GO TO 10                                                  F  45
      FMT='(/,''INPUT '',A'//F0(L)//')'                                     F  46
      WRITE (1,FMT) CHAR                                                    F  47
      GO TO 300                                                             F  48
   10 FMT='(/,''INPUT '',A'//F0(L)//','''('',I'//F0(I)//','')''')'          F  49
      WRITE (1,FMT) CHAR,J                                                  F  50
      GO TO 300                                                             F  51
   30 IF (J.GT.0) GO TO 40                                                  F  52
      FMT='(/,''OLD '',A'//F0(L)//','''=='','//F//',/,A72)'                 F  53
      IF (K.EQ.2) WRITE (1,FMT) CHAR,IVAL,QUESTION                          F  54
      IF (K.NE.2) WRITE (1,FMT) CHAR,STRING,QUESTION                        F  55
      GO TO 300                                                             F  56
   40 FMT='(/,''OLD '',A'//F0(L)//','''('',I'//F0(I)//','')=='','//F//',    F  57
     1/,A72)'                                                               F  58
      IF (K.EQ.2) WRITE (1,FMT) CHAR,J,IVAL,QUESTION                        F  59
      IF (K.NE.2) WRITE (1,FMT) CHAR,J,STRING,QUESTION                      F  60
C                                                                           F  61
C     READ RESPONSE                                                         F  62
C                                                                           F  63
  300 JFLAG=0                                                               F  64
      READ (1,105) LINE                                                     F  65
  105 FORMAT(A80)                                                           F  66
C                                                                           F  67
```

```
C         JFLAG=0 ---> PROPER ENTRY                                    F  68
C         JFLAG=1 ---> EXPLANATION IS ASKED                            F  69
C         JFLAG=2 ---> A NULL ANSWER                                   F  70
C         JFLAG=3 ---> ANSWER OF WRONG TYPE                            F  71
C         JFLAG=4 ---> SPECIAL CHARACTERS                              F  72
C                                                                      F  73
      IF (LINE(1:1).NE.'') GO TO 110                                   F  74
      JFLAG=2                                                          F  75
  110 IF (LINE(1:1).EQ.'?') JFLAG=1                                    F  76
      CALL SPECL (M)                                                   F  77
      IF (EXIT.OR.LIST) JFLAG=4                                        F  78
      IF (JFLAG.NE.0) GO TO 200                                        F  79
      GO TO (140,150,120), K+1                                         F  80
  140 STRING=LINE                                                      F  81
      GO TO 200                                                        F  82
  120 READ (LINE,*,ERR=130) IVAL                                       F  83
      GO TO 200                                                        F  84
  150 READ (LINE,*,ERR=130) G                                          F  85
C                                                                      F  86
C     MAKE SURE THAT DECIMAL POINT IS PRESENT                          F  87
C                                                                      F  88
      NONB=.FALSE.                                                     F  89
      DO 155 I2=1,80                                                   F  90
      IF (LINE(I2:I2).NE.' ') NONB=.TRUE.                              F  91
      IF (NONB.AND.LINE(I2:I2).EQ.' ') GO TO 130                       F  92
      IF (LINE(I2:I2).EQ.'.') GO TO 156                                F  93
  155 CONTINUE                                                         F  94
      GO TO 130                                                        F  95
  156 STRING=LINE                                                      F  96
      GO TO 200                                                        F  97
C                                                                      F  98
  130 JFLAG=3                                                          F  99
  200 IF (JFLAG.EQ.2.AND.(NFLAG.NE.0.OR.JOPTION.EQ.2)) GO TO 170       F 100
      IF (JFLAG.EQ.4) RETURN                                           F 101
      IF (JFLAG.NE.0) RETURN 1                                         F 102
  170 IF (K.NE.2.OR.IMAX.LE.IMIN) RETURN                               F 103
      IF (IVAL.GT.IMAX.OR.IVAL.LT.IMIN) RETURN 1                       F 104
      RETURN                                                           F 105
      END                                                              F 106
C                                                                      G   1
      LOGICAL FUNCTION YN                                              G   2
C                                                                      G   3
C          THIS FUNCTION CHECKS FOR YES OR NO ANSWER                   G   4
C                                                                      G   5
      CHARACTER *1 YESNO                                               G   6
C                                                                      G   7
    5 READ (1,10) YESNO                                                G   8
   10 FORMAT (A1)                                                      G   9
      YN=.FALSE.                                                       G  10
      IF (YESNO.EQ.'Y'.OR.YESNO.EQ.'y') GO TO 20                       G  11
```

```
      IF (YESNO.EQ.'N'.OR.YESNO.EQ.'n') RETURN                          G  12
      WRITE (1,30)                                                      G  13
   30 FORMAT ('PLEASE ANSWER ''Y'' OR ''N''.')                          G  14
      GO TO 5                                                           G  15
   20 YN=.TRUE.                                                         G  16
      RETURN                                                            G  17
      END                                                               G  18
C                                                                       H   1
      SUBROUTINE OPEN(ITIME)                                            H   2
C                                                                       H   3
C         THIS SUBROUTINE GIVES THE USER A CHOICE OF CHOOSING A         H   4
C         REFERENCE FILE OR NOT TO USE IT AT ALL.  IF THE               H   5
C         REFERENCE FILE IS DESIRED, IT OPENS THE FILE AND              H   6
C         POSITION THE POINTER SO THAT THE PROGRAM CAN USE IT;          H   7
C         IF REFERENCE FILE IS NOT WANTED, IT SETS IOPEN TO ZERO        H   8
C         AND RETURN TO 'MAIN.                                          H   9
C                                                                       H  10
      COMMON /REFF/ JOPTION,IOPEN,JLINE                                 H  11
      CHARACTER *36 TREAD                                               H  12
      CHARACTER *80 LINE,JLINE(3)                                       H  13
      SAVE TREAD,KOPEN                                                  H  14
      LOGICAL YN                                                        H  15
C                                                                       H  16
      ITIME=ITIME+1                                                     H  17
      IF (ITIME.EQ.1.OR.KOPEN.EQ.0)GO TO 100                            H  18
  120 WRITE (1,110)                                                     H  19
  110 FORMAT (/,'DO YOU WISH TO USE THE SAME REFERENCE FILE?')          H  20
      IF (.NOT.YN()) GO TO 100                                          H  21
      CLOSE (UNIT=13)                                                   H  22
      GO TO 25                                                          H  23
  100 WRITE (1,10)                                                      H  24
   10 FORMAT (/,'ENTER REFERENCE FILE NAME:  (HIT <CR> TO OMIT)')       H  25
      READ (1,20) TREAD                                                 H  26
   20 FORMAT (A36)                                                      H  27
      IF (TREAD(1:1).NE.'')GO TO 25                                     H  28
      IOPEN=0                                                           H  29
      GO TO 30                                                          H  30
   25 OPEN (UNIT=13,FILE=TREAD,STATUS='OLD')                            H  31
      IOPEN=1                                                           H  32
   30 KOPEN=IOPEN                                                       H  33
      RETURN                                                            H  34
      END                                                               H  35
```

Attachment E. - Minerals file read by PHRQINPT as logical file unit 11.

```
CALCITE    2   4.0        -8.480     -2.297          1
  15 1.0          4 1.0
-171.9065   -.077993     2839.319       71.595
ARAGONIT   2   4.0        -8.336     -2.589          1
  15 1.0          4 1.0
-171.9773   -.077993     2903.293       71.595
DOLOMITE   3   8.0        -17.09     -9.436          0
   4 1.0          5 1.0          15 2.0
SIDERITE   2   6.0        -10.57     -6.14           0
   8 1.0         15 1.0
RHODOCHR   2   6.0        -10.41     -2.079          0
   9 1.0         15 1.0
STRONTIT   2          4.0     -9.271     -0.40       1
  12         1.0  15          1.0
155.0305                  -7239.594   -56.58638
GYPSUM     3   6.0        -4.602     -0.028          1
   4 1.0         16 1.0           3 2.0
82.090                    -3853.936   -29.8115
ANHYDRITE  2   6.0        -4.384     -4.3            0
   4 1.0         16 1.0
CELESTIT   2   6.0        -6.578     0.228           0
  12 1.0         16 1.0
BARITE     2   6.0        -9.978     6.141           0
  11 1.0         16 1.0
HYDROXAP   4   0.0        -3.421     -36.155         0
   3 1.0         65 3.0           4 5.0           1 -4.0
VIVIANIT   3   6.0        -36.000    0.0             0
   8 3.0         19 2.0           3 8.0
FLUORITE   2   0.0        -10.96     4.71            0
   4 1.0         20 2.0
FEOH3A     3   3.0        4.891      0.0             0
 115 1.0          3 3.0          1 -3.0
HEMATITE   3   6.0        -4.008     -30.845         0
 115 2.0          3 3.0          1 -6.0
PYRITE     4       0.0    -18.48      11.3           0
   1  -2.0         2  -2.0         8  1.0         42  2.0
GOETHITE   3   3.0         0.486     -14.48          0
 115 1.0          3 2.0          1 -3.0
GIBBSITE   3   0.0        8.77       -22.8           0
  10         1.0   3          3.0   1         -3.0
CHALCEDY   2   0.0        -3.523     4.615           0
  13 1.0          3 -2.0
QUARTZ     2   0.0        -4.006     6.22            0
  13 1.0          3 -2.0
KAOLINIT   4   0.0        -36.921    49.150          0
  10         2.0   3          1.0  13          2.0   1         -6.0
SEPIOLIT   4   0.0        -40.079    26.532          0
   5 2.0         13 3.0          31 4.0           3 -4.5
FES PPT    3   0.0        -3.915     0.0             0
   8 1.0         42 1.0           1 -1.0
```

```
BIRNESIT   4   4.0        18.091     0.0            0
 144 1.0          3 2.0           2 -1.0         1 -4.0
MANGANIT   3   3.0        -0.238     0.0            0
 144 1.0          3 2.0           1 -3.0
SIL GEL    2   0.0        -2.70      5.50           0
  13 1.0          3 -2.0
SIL GLAS   2   0.0        -3.017     4.44           0
  13 1.0          3 -1.0
SEP PPT    4   0.0        -37.212    0.0            0
   5 2.0         13 3.0          31 4.0          3 -4.5
MACKINIT   3   0.0        -4.631     0.0            0
   8 1.0         42 1.0           1 -1.0
MUSCOVIT   4          0.0      12.97    -59.377      0
  10        3.0  13         3.0   7         1.0   1       -10.0
MICROCLN   5          0.0      0.875    -12.467      0
  10        1.0  13         3.0   7         1.0   3        -4.0   1        -4.0
CO2 GAS    1       4.0      -1.468     -4.776        1
  35  1.0
108.3865    0.01985076  -6919.53     -40.45154    669365.0
O2 GAS     1       4.0       -2.96       -1.844       0
  32  1.0
H2 GAS     1      -2.0       -3.15       -1.759       0
  33  1.0
N2 GAS     1       0.0       -3.26      -1.358        0
  49  1.0
H2S GAS    1      -2.0       -0.997     -4.57         0
  43 1.0
CH4 GAS    1      -4.0       -2.86      -3.373        0
  36  1.0
NH3 GAS    1      -3.0       1.77       -8.17         0
  50 1.0
```

Attachment F. - PHREEQE data file read by PHRQINPT as logical file unit 12.

```
ELEMENTS
CA          4    40.08          CA+2
MG          5    24.305         MG+2
NA          6    22.9898        NA+
K           7    39.0983        K+
FE          8    55.847         FE+2
MN          9    54.9380        MN+2
AL         10    26.9815        AL+3
BA         11    137.33         BA+2
SR         12    87.62          SR+2
SI         13    60.0843        SIO2
CL         14    35.453         CL-
C          15    44.0098        CO2
S          16    96.06          SO4-2
N          17    62.0049        NO3-
B          18    10.81          B
P          19    94.9714        PO4-3
F          20    18.9984        F-
LI         21     6.941         LI+
BR         22     79.904        BR-

SPECIES
  1
H+           100 1.0       0.0        9.0                              0.0
 0.0        0.0
  1 1.0
  2
E-           100 -1.0      0.0        0.0                              0.0
 0.0        0.0
  2 1.0
  3
H2O          100 0.0       0.0        0.0                              0.0
 0.0        0.0
  3 1.0
  4
CA+2         101 2.0       0.0        6.0        5.0       0.165       0.0
 0.0        0.0
  4 1.0
  5
MG+2         101 2.0       0.0        8.0        5.5       0.20        0.0
0.0        0.0
  5 1.0
  6
NA+          101 1.0       0.0        4.0        4.0       0.075       0.0
0.0        0.0
  6 1.0
  7
K+           101 1.0       0.0        3.0        3.5       0.015       0.0
0.0        0.0
  7 1.0
```

```
  8
FE+2          100 2.0       2.0       6.0                                   0.0
0.0         0.0
  8 1.0
  9
MN+2          100 2.0       2.0       6.0                                   0.0
 0.0         0.0
  9 1.0
 10
AL+3          100 3.0       0.0       9.0                                   0.0
 0.0         0.0
 10 1.0
 11
BA+2          100 2.0       0.0       5.0                                   0.0
 0.0         0.0
 11 1.0
 12
SR+2          101 2.0       0.0       5.0             5.26      0.121 0.0
 0.0         0.0
 12 1.0
 13
H4SIO4        100 0.0       0.0       0.0                                   0.0
 0.0         0.0
 13 1.0
 14
CL-           101 -1.0      0.0       3.0       3.5         0.015       0.0
 0.0         0.0
 14 1.0
 15
CO3-2         101 -2.0      4.0       4.5       5.4         0.0         2.0
 0.0         0.0
 15 1.0
 16
SO4-2         101 -2.0      6.0       4.0       5.0         -0.04       0.0
 0.0         0.0
 16 1.0
 17
NO3-          100 -1.0      5.0       3.0                                   0.0
 0.0         0.0
 17 1.0
 18
H3BO3         100 0.0       0.0       0.0                                   0.0
0.0         0.0
 18 1.0
 19
PO4-3         100 -3.0      0.0       4.0                                   2.0
 0.0         0.0
 19 1.0
 20
F-            100 -1.0      0.0       3.5                                   0.0
```

```
 0.0        0.0
 20 1.0
 21
LI+           100 1.0        0.0        6.0                              0.0
0.0        0.0
 21 1.0
 22
BR-           100 -1.0       0.0        3.0                              0.0
0.0        0.0
 22 1.0
 31
OH-           200 -1.0       0.0        3.5                              1.0
-13.998    13.345
  3 1.0      1 -1.0
 32
O2 AQ         300 0.0        4.0        0.0                              0.0
-86.08     134.79
  3 2.0      1 -4.0     2 -4.0
 33
H2 AQ         200 0.0        -2.0       0.0                              0.0
-3.15      -1.759
  1 2.0      2 2.0
 34
HCO3-         211 -1.0       4.0        4.5        5.4        0.0        1.0
 10.329     -3.561     107.8871     0.03252849  -5151.79     -38.92561    563713.9
 15 1.0      1 1.0
 35
H2CO3         310 0.0        4.0        0.0                              0.0
 16.681     -5.738     464.1965     0.09344813  -26986.16    -165.75951   2248628.9
 15 1.0      1 2.0      3 -1.0
 36
CH4 AQ        400 0.0        -4.0       0.0                              0.0
 41.071     -61.039
 15 1.0      1 10.0     2 8.0      3 -3.0
 40
HSO4-         210 -1.0       6.0        0.0                              0.0
 1.987      4.91       -5.3505      0.0183412   557.2461
 16 1.0      1 1.0
 41
S-2           400 -2.0       -2.0       5.0                              2.0
 20.735     -28.04
 16 1.0      1 8.0      2 8.0      3 -4.0
 42
HS-           400 -1.0       -2.0       3.5                              1.0
 33.652     -40.14
 16 1.0      1 9.0      2 8.0      3 -4.0
 43
H2S           400 0.0        -2.0       0.0                              0.0
 40.644     -65.44
 16 1.0      1 10.0     2 8.0      3 -4.0
```

```
 48
NO2-          400 -1.0       3.0        3.0                          0.0
 28.57       -43.76
 17 1.0       1 2.0       2 2.0      3 -1.0
 49
N2 AQ         400 0.0        0.0        0.0                          0.0
 207.08      -312.13
 17 2.0       1 12.0      2 10.0     3 -6.0
 50
NH3 AQ        400 0.0       -3.0        0.0                          1.0
 109.83      -174.58
 17 1.0       1 9.0       2 8.0      3 -3.0
 51
NH4+          400 1.0       -3.0        2.5                          0.0
 119.077     -187.055
 17 1.0       1 10.0      2 8.0      3 -3.0
 52
NH4SO4-       500 -1.0       3.0        0.0                          0.0
 120.19      -187.055
 17 1.0       1 10.0      2 8.0     16 1.0      3 -3.0
 57
H2BO3-        200 -1.0       0.0        0.0                          1.0
-9.240       3.224
 18 1.0       1 -1.0
 58
BFOH3-        200 -1.0       0.0        0.0                          0.0
-0.40        1.85
 18 1.0      20 1.0
 59
BF2OH2-       400 -1.0       0.0        0.0                          0.0
7.628        1.635
 18 1.0      20 2.0       1 1.0      3 -1.0
 60
BF3OH-        400 -1.0       0.0        0.0                          0.0
13.666      -1.58
 18 1.0       1 2.0      20 3.0      3 -2.0
 61
BF4-          400 -1.0       0.0        0.0                          0.0
20.274      -1.795
 18 1.0       1 3.0      20 4.0      3 -3.0
 65
HPO4-2        200 -2.0       0.0        4.0                          1.0
 12.346      -3.53
 19 1.0       1 1.0
 66
H2PO4-        200 -1.0       0.0        4.5                          0.0
 19.553      -4.52
 19 1.0       1 2.0
 69
HF AQ         200 0.0        0.0        0.0                          0.0
```

```
 3.169     3.46
  1 1.0    20 1.0
 70
HF2-        200 -1.0      0.0       0.0                          0.0
 3.749     4.55
  1 1.0    20 2.0
 75
CAOH+       300 1.0       0.0       0.0                          1.0
-12.598   14.535
  4 1.0     3 1.0     1 -1.0
 76
CACO3       210 0.0       4.0       0.0                          2.0
3.225     3.547     -1228.732   -0.299440   35512.75     485.818
  4 1.0    15 1.0
 77
CAHCO3+     311 1.0       4.0       0.0       5.4       0.0       1.0
11.435    -0.869    1317.0071   0.34546894  -39916.84    -517.70761  563713.9
  4 1.0    15 1.0     1 1.0
 78
CASO4       200 0.0       6.0       0.0                          0.0
2.309     1.470
  4 1.0    16 1.0
 79
CAPO4-      200 -1.0      0.0       0.0                          2.0
6.459     3.100
  4 1.0    19 1.0
 80
CAHPO4      300 0.0       0.0       0.0                          1.0
15.085    -0.230
  4 1.0     1 1.0    19 1.0
 81
CAH2PO4+    300 1.0       0.0       0.0                          0.0
20.961    -1.120
  4 1.0     1 2.0    19 1.0
 82
CAF+        200 1.0       0.0       0.0                          0.0
0.940     3.798
  4 1.0    20 1.0
 85
MGOH+       300 1.0       0.0       0.0                          1.0
-11.794   15.419
  5 1.0     3 1.0     1 -1.0
 86
MGCO3       210 0.0       4.0       0.0                          2.0
2.981     2.535     -32.172     0.0          1093.486    12.72433
  5 1.0    15 1.0
 87
MGHCO3+     310 1.0       4.0       0.0                          1.0
11.397    -2.775    48.6721     0.03252849  -2614.335     -18.00263  563713.9
  5 1.0     1 1.0    15 1.0
```

```
 88
MGSO4          200 0.0        6.0        0.0                    0.0
2.250      1.4
  5 1.0     16 1.0
 89
MGPO4-         200 -1.0       0.0        0.0                    2.0
6.589      3.100
  5 1.0     19 1.0
 90
MGHPO4         300 0.0        0.0        0.0                    1.0
15.216     -0.230
  5 1.0      1 1.0     19 1.0
 91
MGH2PO4+       300 1.0        0.0        0.0                    0.0
21.066     -1.120
  5 1.0      1 2.0     19 1.0
 92
MGF+           200 1.0        0.0        0.0                    0.0
1.820      4.674
  5 1.0     20 1.0
 95
NACO3-         200 -1.0       4.0        0.0                    2.0
1.268      8.911
  6 1.0     15 1.0
 96
NAHCO3         300 0.0        4.0        0.0                    1.0
10.080     -3.604
  6 1.0      1 1.0     15 1.0
 97
NASO4-         200 -1.0       6.0        0.0                    0.0
0.700      1.120
  6 1.0     16 1.0
 98
NAHPO4-        300 -1.0       0.0        0.0                    1.0
12.636     -3.530
  6 1.0      1 1.0     19 1.0
100
KSO4-          200 -1.0       6.0        0.0                    0.0
0.85       2.25
  7 1.0     16 1.0
101
KHPO4-         300 -1.0       0.0        0.0                    1.0
12.636     -3.530
  7 1.0      1 1.0     19 1.0
105
FEOH+          300 1.0        2.0        0.0                    1.0
-9.500     13.2
  8 1.0      3 1.0      1 -1.0
106
FEOH2          300 0.0        2.0        0.0                    2.0
```

```
-20.570   28.565
  8 1.0     3 2.0     1 -2.0
107
FEOH3-      300 -1.0      2.0       0.0                              3.0
-31.000   30.300
  8 1.0     3 3.0     1 -3.0
108
FESO4       200 0.0       8.0       0.0                              0.0
2.25      3.23
  8 1.0    16 1.0
109
FE(HS)2     500 0.0       -2.0      0.0                              2.0
76.250    -120.280
  8 1.0    16 2.0     1 18.0    2 16.0    3 -8.0
110
FE(HS)3-    500 -1.0      -4.0      0.0                              3.0
111.937   -180.420
  8 1.0    16 3.0     1 27.0    2 24.0    3 -12.0
111
FEHPO4      300 0.0       2.0       0.0                              1.0
15.946    -3.530
  8 1.0     1 1.0    19 1.0
112
FEH2PO4+    300 1.0       2.0       0.0                              0.0
22.253    -4.520
  8 1.0     1 2.0    19 1.0
115
FE+3        200 3.0       3.0       9.0                              0.0
-13.032   10.0
  8 1.0     2 -1.0
116
FEOH+2      400 2.0       3.0       0.0                              0.0
-15.22    20.4
  8 1.0     3 1.0     2 -1.0    1 -1.0
117
FEOH2+      400 1.0       3.0       0.0                              0.0
-18.70    10.0
  8 1.0     3 2.0     1 -2.0    2 -1.0
118
FEOH3       400 0.0       3.0       0.0                              1.0
-26.63    10.0
  8 1.0     3 3.0     1 -3.0    2 -1.0
119
FEOH4-      400 -1.0      3.0       0.0                              2.0
-34.63    10.0
  8 1.0     3 4.0     1 -4.0    2 -1.0
120
FE2OH2+4    400 4.0       6.0       0.0                              0.0
-29.01    33.5
  8 2.0     3 2.0     1 -2.0    2 -2.0
```

```
121
FE3OH4+5     400 5.0        9.0        0.0                              0.0
-45.4      44.3
  8 3.0      3 4.0      1 -4.0     2 -3.0
122
FECL+2       300 2.0        3.0        0.0                              0.0
-11.55     15.6
  8 1.0      14 1.0     2 -1.0
123
FECL2+       300 1.0        3.0        0.0                              0.0
-10.90     10.0
  8 1.0      14 2.0     2 -1.0
124
FECL3        300 0.0        3.0        0.0                              0.0
-11.90     10.0
  8 1.0      14 3.0     2 -1.0
125
FESO4+       300 1.0        9.0        0.0                              0.0
-9.11      13.91
  8 1.0      16 1.0     2 -1.0
126
FESO42-      300 -1.0       15.0       0.0                              0.0
-7.61      14.60
  8 1.0      16 2.0     2 -1.0
127
FEHPO4+      400 1.0        3.0        0.0                              1.0
 4.74      12.23
  8 1.0      1 1.0     19 1.0     2 -1.0
128
FEH2P+2      400 2.0        3.0        0.0                              0.0
 11.95     5.48
  8 1.0      1 2.0     19 1.0     2 -1.0
129
FEF+2        300 2.0        3.0        0.0                              0.0
-6.8       12.7
  8 1.0      20 1.0     2 -1.0
130
FEF2+        300 1.0        3.0        0.0                              0.0
-2.2       14.7
  8 1.0      20 2.0     2 -1.0
131
FEF3         300 0.0        3.0        0.0                              0.0
0.97       15.4
  8 1.0      20 3.0     2 -1.0
135
MNOH+        300 1.0        2.0        0.0                              1.0
-10.59     14.40
  9 1.0      3 1.0      1 -1.0
136
MNOH3-       300 -1.0       2.0        0.0                              3.0
```

```
-34.80     0.0
  9 1.0      3 3.0      1 -3.0
137
MNCL+        200 1.0        2.0        0.0                          0.0
 0.607      0.0
  9 1.0     14 1.0
138
MNCL2        200 0.0        2.0        0.0                          0.0
 0.041      0.0
  9 1.0     14 2.0
139
MNCL3-       200 -1.0       2.0        0.0                          0.0
 -0.305     0.0
  9 1.0     14 3.0
140
MNHCO3+      300 1.0        2.0        0.0                          1.0
 11.60     -3.604
  9 1.0     15 1.0      1 1.0
141
MNSO4        200 0.0        8.0        0.0                          0.0
 2.26      2.17
  9 1.0     16 1.0
142
MN(NO3)2     200 0.0        12.0       0.0                          0.0
0.6         -0.396
  9 1.0     17 2.0
143
MNF+         200 1.0        2.0        0.0                          0.0
 0.85       0.0
  9 1.0     20 1.0
144
MN+3         200 3.0        3.0        0.0                          0.0
 -25.507    25.76
  9 1.0      2 -1.0
145
MNO4-2       400 -2.0       6.0        0.0                          0.0
 -118.440   150.02
  9 1.0      3 4.0      1 -8.0     2 -4.0
146
MNO4-        400 -1.0       7.0        3.5                          0.0
 -127.824   176.62
  9 1.0      3 4.0      1 -8.0     2 -5.0
150
ALOH+2       300 2.0        0.0        0.0                          0.0
-4.99      11.9
 10 1.0      3 1.0      1 -1.0
151
ALOH2+       300 1.0        0.0        0.0                          0.0
-10.1      0.0
 10 1.0      3 2.0      1 -2.0
```

```
152
ALOH3        300 0.0        0.0        0.0                              1.0
-16.0      0.0
 10 1.0      3 3.0      1 -3.0
153
ALOH4-       300 -1.0       0.0        0.0                              2.0
-23.000    44.06
 10 1.0      3 4.0      1 -4.0
154
ALSO4+       200 1.0        6.0        0.0                              0.0
 3.02       2.15
 10 1.0     16 1.0
155
ALSO42-      200 -1.0       12.0       0.0                              0.0
 4.92       2.84
 10 1.0     16 2.0
156
ALF+2        200 2.0        0.0        0.0                              0.0
 7.01       0.0
 10 1.0     20 1.0
157
ALF2+        200 1.0        0.0        0.0                              0.0
 12.75      20.0
 10 1.0     20 2.0
158
ALF3         200 0.0        0.0        0.0                              0.0
 17.02      2.50
 10 1.0     20 3.0
159
ALF4-        200 -1.0       0.0        0.0                              0.0
 19.72      0.0
 10 1.0     20 4.0
163
BAOH+        300 1.0        0.0        0.0                              1.0
 -13.358    15.095
 11 1.0      3 1.0      1 -1.0
165
SROH+        300 1.0        0.0        5.0                              1.0
 -13.178    14.495
 12 1.0      3 1.0      1 -1.0
166
SRHCO3+      310        1.0        4.0        5.4                              1.0
 11.513     2.486     104.6389     0.04739549  -5151.79     -38.92561    563713.9
 12    1.0 15    1.0  1    1.0
167
SRCO3        210        0.0        4.0        0.0                              2.0
 2.805      5.217     -1.019       0.012826
 12    1.0 15    1.0
168
SRSO4        200        0.0        6.0
```

```
 2.55      1.6
 12    1.0 16    1.0
170
H3SIO4-      210 -1.0       0.0        0.0                              1.0
 -9.929     8.936      6.368        -0.016346    -3405.9
 13 1.0      1 -1.0
171
H2SIO4-2     210 -2.0       0.0        0.0                              2.0
 -21.617    29.717     39.478       -0.065927    -12355.1
 13 1.0      1 -2.0
172
SIF6-2       400 -2.0       0.0        0.0                              0.0
 30.18      -16.26
 13 1.0      1 4.0     20 6.0      3 -4.0
181
LISO4-       200 -1.0       6.0        0.0                              0.0
0.640      0.0
 21 1.0     16 1.0

LOOK MIN
CALCITE    2   4.0        -8.480     -2.297          1
  15 1.0           4 1.0
-171.9065   -.077993     2839.319       71.595
ARAGONIT   2   4.0        -8.336     -2.589          1
  15 1.0           4 1.0
-171.9773   -.077993     2903.293       71.595
DOLOMITE   3   8.0        -17.09     -9.436          0
   4 1.0           5 1.0          15 2.0
SIDERITE   2   6.0        -10.57     -6.14           0
   8 1.0          15 1.0
RHODOCHR   2   6.0        -10.41     -2.079          0
   9 1.0          15 1.0
STRONTIT   2          4.0     -9.271     -0.40       1
  12         1.0  15         1.0
155.0305                  -7239.594    -56.58638
GYPSUM     3   6.0        -4.602     -0.028          1
   4 1.0          16 1.0           3 2.0
82.090                    -3853.936    -29.8115
ANHYDRITE  2   6.0        -4.384     -4.3            0
   4 1.0          16 1.0
CELESTIT   2   6.0        -6.578     0.228           0
  12 1.0          16 1.0
BARITE     2   6.0        -9.978     6.141           0
  11 1.0          16 1.0
HYDROXAP   4   0.0        -3.421     -36.155         0
   3 1.0          65 3.0           4 5.0          1 -4.0
FLUORITE   2   0.0        -10.96     4.71            0
   4 1.0          20 2.0
CHALCEDY   2   0.0        -3.523     4.615           0
  13 1.0           3 -2.0
```

```
QUARTZ      2    0.0         -4.006     6.22            0
  13 1.0           3 -2.0
GIBBSITE    3           0.0      8.77     -22.8         0
  10         1.0    3          3.0    1        -3.0
KAOLINIT    4           0.0    -36.921     49.150      0
   3        -7.0    1          2.0   13          2.0 153          2.0
SEPIOLIT    4    0.0         -40.079    26.532          0
   5 2.0           13 3.0           31 4.0           3 -4.5
HEMATITE    3    3.0         -4.008     -30.845         0
 115 2.0           3 3.0            1 -6.0
GOETHITE    3    3.0         0.486      -14.48          0
 115 1.0           3 2.0            1 -3.0
FEOH3A      3    3.0         4.891      0.0             0
 115 1.0           3 3.0            1 -3.0
PYRITE      4       0.0      -18.48      11.3           0
   1  -2.0          2  -2.0          8  1.0          42  2.0
FES PPT     3    0.0         -3.915     0.0             0
   8 1.0           42 1.0           1 -1.0
VIVIANIT    3    6.0         -36.000    0.0             0
   8 3.0           19 2.0           3 8.0
PCO2        1       4.0       -1.468     -4.776         1
  35  1.0
108.3865     0.01985076   -6919.53     -40.45154     669365.0
O2 GAS      1       4.0        -2.96       -1.844        0
  32  1.0
H2 GAS      1      -2.0        -3.15       -1.759        0
  33  1.0

END
```