SOLINPUT: A Computer Code to Create and Modify Input Files for the Geochemical Program SOLMINEQ.88

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CONTENTS

FIGURES

Page

TABLES

Page

CONVERSION FACTORS

Metric (International System) units are used in this report. For those readers who prefer to use inch-pound units, conversion factors for the terms used in this report are listed below:

Multiply metric unit	by	to obtain inch-pound unit
micrometer (μm)	0.03937	mil
centimeter	0.3937	inch
meter (m)	3.281	foot (ft)
square centimeter (cm^2)	0.1550	square inch (in^2)
cubic centimeter (cm^3)	0.06102	cubic inch (in^3)
cubic meter (m^3)	35.31	cubic feet (ft^3)
liter (ℓ)	0.03531	cubic feet (ft^3)
microgram (μg)	1.543×10^{-5}	grain (gr)
miligram (mg)	1.543×10^{-2}	grain (gr)
gram (g)	2.205×10^{-3}	pound (lb)
kilogram (kg)	2.205	pound (lb)
miligram/liter (mg/ℓ)	6.243×10^{-5}	pound/cubic foot (lb/ft^3)
atmosphere (atm)	14.70	pounds per square inch (psi)
bar	14.50	pounds per square inch (psi)
kilopascal (kPa)	0.1450	pounds per square inch (psi)
joule	9.478×10^{-5}	British thermal unit (Btu)
calorie (cal)	3.968×10^{-3}	British thermal unit (Btu)
kilocalorie (kcal)	3.968	British thermal unit (Btu)
degree Celcius (°C)	1.8 °C + 32	degree Fahrenheit (°F)
degree Kelvin (K)	1.8 (K - 273.15) + 32	degree Fahrenheit (°F)

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ABSTRACT

This report documents SOLINPUT, an interactive computer program designed to create and modify input files for the geochemical code SOLMINEQ.88. It details the construction of input files and specifies the computing environment needed to execute both programs. This manual also outlines the reactions, equations, and actual coding required to add aqueous and mineral components to both SOLMINEQ.88 and SOLINPUT.

Input files for SOLMINEQ.88 are created and edited by SOLINPUT using a menu-driven format. SOLINPUT is made up of a Main Menu, an Options Menu, and seven sub-menus. The Main Menu is concerned with reading and writing the input file, which may consist of up to 10 data sets, and is the only point from which SOLINPUT can be exited. The Options Menu directs the user to the appropriate sub-menu through which the basic physical and chemical data are entered and the modeling options are chosen. The items within each menu are arranged from top to bottom in the order in which they will be accessed. The last choice of each menu exits that menu and returns to the previous menu. SOLINPUT describes all of the chemical and physical parameters required for each run of SOLMINEQ.88 as well as the parameters needed for user selected options. SOLINPUT allows numeric data to be entered using several convenient formats. It also performs error checking on input entered and prompts the user to correct invalid entries.

INTRODUCTION

SOLMINEQ.88 (SOLution MINeral EQuilibrium, 1988) is the latest version of the 1973 computer program SOLMNEQ (Kharaka and Barnes, 1973) and its various updated versions. This program is general and comprehensive, but is particularly useful for modeling geochemical interactions in sedimentary basins and petroleum reservoirs. SOLMINEQ.88 can be used to study the effects of boiling, mixing of solutions, partitioning of gases between water, oil, and gas phases, ion exchange, adsorption/desorption, and dissolution/precipitation of solid phases.

This manual describes SOLINPUT, a computer code designed to generate input files for SOLMINEQ.88. In addition, it delineates the computing environment required to operate both of these codes. Finally, it describes the programming steps required to add minerals or new aqueous components with several species to SOLMINEQ.88 and SOLINPUT. A discussion of the theory, applications, and limitations of this code is given by Kharaka and others (1988). Another input code, SOLMINEQ.88 PC/SHELL, designed specifically for PC systems is available from Wiwchar and others (1988). This manual assumes the user has the knowledge to copy files and to compile and link FORTRAN-77 programs.

GETTING STARTED

SOLMINEQ.88 is consists of the following files:

File	# of Bytes
SOL1.FOR	211,594
SOL2.FOR	298,162
SOLINPUT.FOR	339,366
DATA.TBL	75,603
RXN.TBL	7,152
PIT.TBL	14,164

These files must be located in the same directory when they are loaded onto the computer system. In addition, a number of test case examples of input and output files are generally included on the distribution copy. This distribution copy 5 1/4" MS-DOS compatible, double-sided, double-density floppy disks. SOLMIN88.FOR is divided into two files, SOL1.FOR and SOL2.FOR. These two files should be concatenated when they are installed.

Once SOLMINEQ.88 is loaded onto a computer system, the next step is to compile the two files SOLMIN88.FOR and SOLINPUT.FOR using a FORTRAN-77 compiler conforming with the ANSI standard. The object files created must then be linked with the systems FORTRAN libraries. SOLMIN88.FOR and SOLINPUT.FOR may need to have their extensions changed (e.g. .FOR to .F77) in order for the compiler to recognize them.

SOLMIN88 is a large and complex code which requires some special considerations when using it on a personal computer (PC) using the MS-DOS operating system. The PC must have 640 kilobytes of RAM, a hard disk, and a math coprocessoring chip. When compiling the program, it is suggested the following options be used if the compiler supports them:

Generate 80286/80287 or 80386/80387 code
Do not check array bounds
Do not check subprogram interfaces
Store variables dynamically

The code can be linked using the standard DOS linker but an overlay linker will speed up execution and lower memory requirements. It is also suggested that the number of restart files opened by SOLMIN88 during any one run is kept to a minimum. All memory-resident programs must be purged from memory before executing SOLMIN88.

Portability

Two factors may affect portability of the codes. The first is the maximum and minimum double-precision numbers the computer can represent. The range of 10^{-35} to 10^{+35} has been assumed. If this range is too large (or if the computer allows a larger range) then the parameters CPUMIN and CPUMAX must be changed throughout both SOLMIN88 and SOLINPUT. It is best to assign a value a few orders of magnitude lower than the system's true range. For example, the default values shown above assume a true range of $10^{\pm 38}$.

The second factor that may affect portability is the unit numbers which are assigned by SOLMINEQ.88 to identify a particular file for use in input/output operations. This unit number may be in conflict with a unit number already assigned by the computer's operating system. The following units are used by SOLMINEQ.88:

Unit	Variable	Description
5	UNI	Input file to SOLMIN88
6	UNO	Output file from SOLMIN88
7	UNP	Data file of Pitzer parameters (PIT.TBL)
10	UND	Main data file (DATA.TBL)
12	UNR	Data file for dissolution reactions (RXN.TBL)
20	UN	Input file used by SOLINPUT
39	UNM	Mixing file used by SOLMIN88
40+	BASE	Input restart files created by SOLMIN88

If these file units conflict with operating system units, the problem can be solved either by externally assigning these file units with a command procedure, which will require writing the command procedure and modifying SOLMINEQ.88 to work with this procedure, or by changing the variable or parameter within SOLMINEQ.88 used to identify the conflicting unit to a new value.

SOLMINEQ.88 has been successfully run without the need to modify the source code on the following systems: DEC VAX series, Prime 50, and PC compatibles using the Lahey F77L compiler version 3[1].

Running the Code

SOLMIN88 requires the existence of an input data file before it can be executed. Input files created for previous versions of SOLMINEQ.88 (i.e. SOLMNEQ, SOLMNEQF, etc.) are incompatible with this version of the code. An input file may be created in two ways. One way is with an ASCII text editor using the formats given in table 1. The second method is to run SOLINPUT to create the input file. In general it will be easier to use SOLINPUT to create an input file. However, use of a text editor will make it easier to make small changes to the input file and to rearrange samples within an input file.

SOLMIN88 was designed to run interactively, although it can be modified to be run in the background or in a batch mode. SOLINPUT can only be run interactively. When run interactively, SOLMIN88 will prompt for the name of an input file to process and for the name of an output file to create. The code provides default filenames for both the input file and the output file. The defaults are chosen by entering a carriage return in response to each prompt.

The output file created by SOLMIN88 is about 130 characters wide and has imbedded FORTRAN printer control codes in it. This file can be examined on a terminal by setting the screen to 132 column mode. The output file can also be examined by printing it to a wide carriage printer and specifying FORTRAN printer control. (For example, one would specify the -FTN option of the SPOOL command on the PRIMOS operating system.) If the system does not support FORTRAN printer control codes the output will be unformatted with 1's and +'s in the first column but will otherwise be complete. The printer control codes used in SOLMIN88 can be changed to match a specific printer. The variable TOF contains the form feed printer control code while the variable CR instructs the printer to perform a carriage return without a linefeed.

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1. Note: Mention of brand names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

Table 1. -- Arrangement of data for input to SOLMINEQ.88

Line	Variable	Format
1	TITLE	A80
2	TEMP, HITEMP, DENS, PRESS	4E10.4
3	PH, EHM, EHMC, EMFZSC, UNITS	4E10.4, A5
4	Total aqueous concentration of [Na, K, Li, Ca, Mg, Fe, Al]	7E10.4
5	Total aqueous concentration of [SiO_2, Cl, SO_4, H_2S, HCO_3, CO_3, TIC]	7E10.4
6	Total aqueous concentration of [F, PO_4, NO_3, NH_3, B, Sr, Ba]	7E10.4
7	Total aqueous concentration of [Pb, Zn, Cu, Mn, Hg, Ag]	6E10.4
8	Total aqueous concentration of [As, U, V]	3E10.4
9	Total aqueous concentration of [Acetate, Oxalate, Succinate, CH_4]	4E10.4
10	Carbon, High Temperature Carbon Option	
	ALK, ITIC	2I2
11	Gas Addition Option	
	DCO2, DH2S, DNH3, DCH4	4E10.4
12	pH and CO2 Saturation Option	
	ICCSAT, IMCO3, FIXIT, FCCSAT	2I2, 2E10.4
13	Gas-Water-Oil Option	
	TCO2M, TCH4M, TH2SM, WROIL,	
	KCO2OL, KCH4OL, KH2SOL, DSEP	8E10.4
14	Ion Exchange Option	
	ADEX	A1
	if ADEX is "E" or "A", then	
	A. CEC, TAREA, SAREA, INSP	3E10.4, I3
	followed by INSP lines of	
	B. ISCHG(I), MBASE(I), SPN(I)	I4, E10.4, A10
	C. KRXN(I), ISCOMP(I),(COEF(I,J),IDN(I,J))	11(E10.4, I3)
15	Precipitation/Mixing/Boiling Options	
	IBMIX, ITMIX	2I2
	Dissolution/Precipitation Option:	
	If IBMIX = 1, then	
	(Dsl/Ppt a specific mineral amount)	
	If ITMIX < 0, then	
	A. IDDP, AMOL(1)	I4, E10.4
	(Dsl/Ppt a mineral to saturation)	
	Else If ITMIX = 0, then	
	A. IDSAT, IDDP, DP	2I4, E10.4
	(Add/Subtract aqueous species to saturation with a mineral)	
	If IDDP = 0, then	
	A. ITT	I4
	followed by ITT lines of	
	B. IRXDP(I), RXDP(I)	I4, E10.4
	(Add/Subtract a specific amount of aqueous species)	
	Else If ITMIX > 0, then ITMIX lines of	
	A. IDMIX(I), AMOL(I)	I4, E10.4

	Mixing Option:	
	Else If IBMIX = 2, then	
	A. INMIX, DFRAC1, DINC, MIXFLE	I4, 2E10.4, A80
	Boiling and Dilution Option:	
	Else If IBMIX = 3, then	
	A. FBOIL	E10.4
16	Optional User Defined Log K at TEMP	
	A. ODUM(I), NDUM(I), XDUM(I)	6(A1, I4, E10.4)
17	Optional User Defined Log K at HITEMP	
	B. ODUM(I), NDUM(I), XDUM(I)	6(A1, I4, E10.4)
18	Additional Anions Option	
	ANS1, ANS2	2I2
	Skip if both ANS1 = 0 and ANS2 = 0.	
	If ANS1 > 0 or ANS2 > 0, then	
	A. CUNITS, GFW, Z, DHA, PAGE1	2E10.4, I2, E10.4, A8
	followed by ANS1 lines of	
	B. INDEX, DHA, LOWKT, HIGHKT, NAME	I2, 3E10.4, A8
	If ANS1 > 0 and ANS2 > 0, then	
	A. CUNITS, GFW, Z, DHA, PAGE1	2E10.4, I2, E10.4, A8
	followed by ANS2 lines of	
	B. INDEX, DHA, LOWKT, HIGHKT, NAME	I2, 3E10.4, A8
19	Additional Cation Option	
	A. NUMCOM, Z, DHA, GFW, CUNITS, NAME	2I2, 3E10.4, A8
	followed by NUMCOM lines of	
	B. INDEX, DHA, LOWKT, HIGHKT, NAME	I2, 3E10.4, A8
20	Additional Minerals Option	
	NUMINS	I2
	followed by NUMINS lines of	
	A. LOWKT, HIGHKT, ADDACT, NAME	5E10.4, A8
	B. (COEFF(I), INDEX(I), I = 1, 8)	8(E10.4, I3)
21	NUFLAG, IPIT, (FLAGS(I), I = 1, 6)	8I2
22	INFORM, RATIO, GEOTH, IPRIN1, IPRIN2, OUTIN	5I2, A80
23	CONV1, CONV2	2E10.4

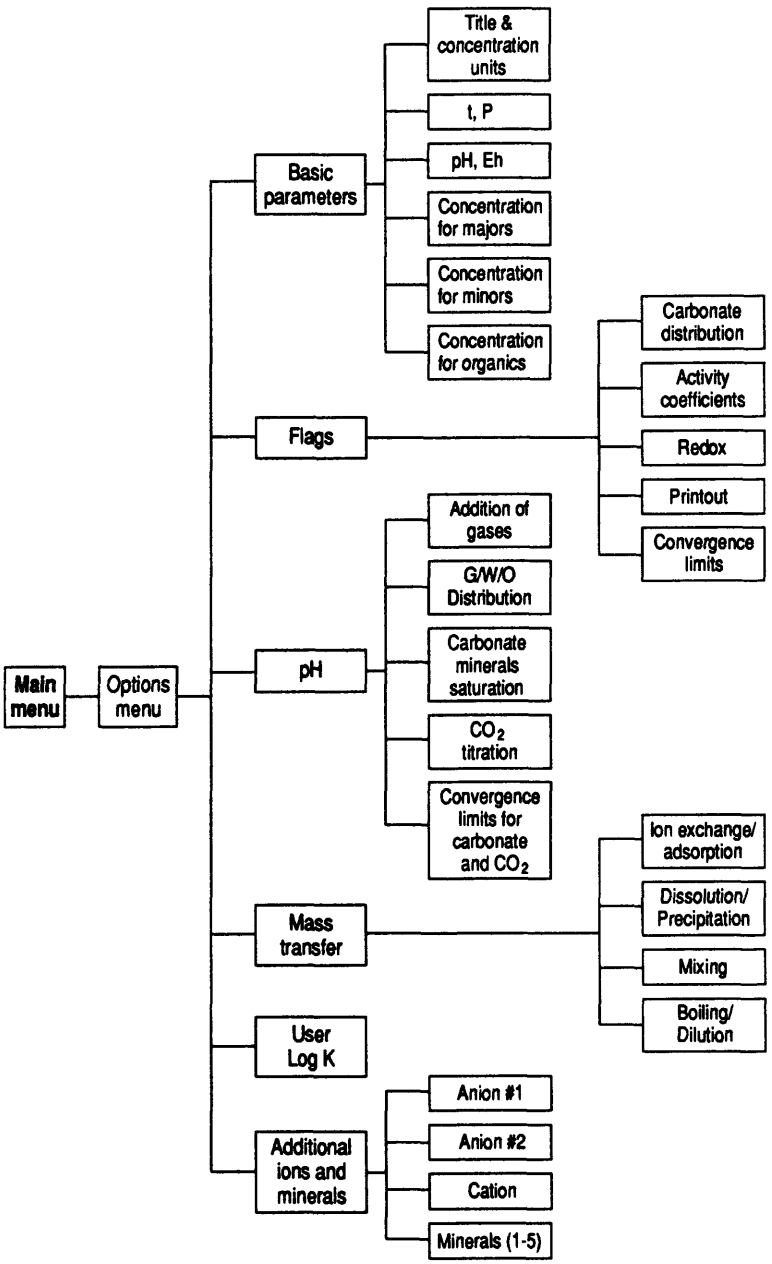

Figure 1. -- Menu Structure

MENU AND OPTION DESCRIPTIONS

General Comments

Data is input into SOLINPUT through a series of menus. The relation of these menus to one another is illustrated by figure 1. In general, the menus in SOLINPUT are arranged with the choices in the order in which they will be used. The last item on each menu will exit that menu and return to the previous menu. To choose a particular item in a menu, type the number of the selection followed by a carriage return (<CR>). Current values for each item are enclosed in square brackets "[ ]". If a <CR> is entered by itself in response to a prompt, the current value will be kept. The current value will be changed only if a new value is entered followed by a <CR>.

Numbers can be only entered to 5 digits of precision (although more are used in internal calculations). Commas cannot be used to separate groups of digits (for example, 1000 cannot be entered as 1,000). Aside from these restrictions, values can be entered in any format. The following are all acceptable ways of entering data:

0.0560 .056 5.6E-2 0.5600d-01

Regardless of how the value is entered, the program will display it using the format: [5.6000E-02]. If an invalid response is made to a prompt, the program will reject that response and continue to prompt the user until a valid response is entered. However, the program will make no attempt to determine whether a given value is creditable. SOLINPUT is case independent; values may be entered in either upper or lower case and the program will converting them where appropriate.

The Main Menu

When SOLINPUT is first started the Main Menu (fig. 2) will be displayed. Input files may be created, edited, or manipulated from this menu.

Input File Structure

SOLMINEQ.88 is designed so that several sets of chemical data can be written into one input file and processed all at once. A "sample" is one set of chemical data plus all of the information SOLMIN88 needs to process this data. SOLINPUT can create or edit an input file containing up to 10 samples (fig. 3). However, only one sample can be viewed or edited at a time. Whenever the Main Menu is displayed the current sample number is shown in the top right hand corner of the screen. To edit a sample different from the one shown, select Choice (3) to move to the next sample in the file or select Choice (4) to move to the previous sample in the file.

It is possible to change the maximum number of samples SOLINPUT can process. To increase or decrease this number, change the parameter MAX to the new value in the main program and in each subprogram where it occurs. If the number of samples allocated to SOLINPUT is increased, the program will require more memory from the system.

Creating and Editing a File

The process of creating a new input file or editing a previously created input file is essentially the same. To create a new input file select Choice (1) and enter the data for that sample as described below. To edit a pre-existing input file, the file must first be read into SOLINPUT through Choice (2) on the Main Menu. This will cause SOLINPUT to read the data stored in that file and replace its default values with this data. The file can then be edited by selecting Choice (1) on the Main Menu.

```
        SOLMINEQ_88  Input Data File Creation Program

                                                        Sample  1

    MAIN MENU


1)  Create/Edit Current Sample Data

2)  Read an Existing Input File

3)  Go to Next Sample

4)  Go to Previous Sample

5)  Write All Samples to an Input File

6)  Exit Program

    Enter Choice (1-6)
```

Figure 2. -- Main Menu

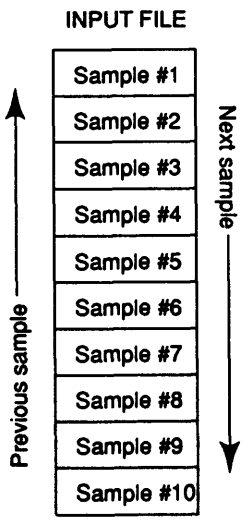

Figure 3. -- Relation of samples within an input file

Reading and Writing Input Files

When an input file is read into SOLINPUT by selecting Choice (2) on the Main Menu, all data currently stored in memory will be overwritten. SOLINPUT will display a warning if data are still in memory prior to reading the input file, allowing the user to prevent accidental deletion of the data. When data entry is completed the information must be saved. Selection of Choice (5) will cause SOLINPUT to ask for a filename in which to write the data. If the filename chosen already exists, SOLINPUT will display a warning before saving the data to that file allowing the user to abort the operation. Saving data to an already existing file will destroy any information stored in that file.

Exiting SOLINPUT

After writing the input file onto disk, select Choice (6) on the Main Menu to exit SOLINPUT. If Choice (6) is selected prior to saving the data in an input file, SOLINPUT will warn the user that the data will be lost unless it is saved before exiting the program. SOLINPUT will give the user a chance to go back and save the data before exiting the program. If the program is quit without saving the data, the original input file (if one exists) will remain unchanged.

The Options Menu

The Options Menu (fig. 4) is arranged into basic parameters, which are needed by SOLMIN88 to carry out speciation-saturation computations, and into options, which modify the way in which a water sample is processed. To reach the Options Menu select Choice (1) on the Main Menu. Once in the Options Menu select Choice (1) to enter the chemical and physical data for that sample and Choice (2) to control how SOLMIN88 interprets, processes, and displays these data. Choice (3) calculates pH at subsurface or experimental conditions (see below). Choice (4) selects the mass transfer capabilities of SOLMINEQ.88. Choice (5) is used to make temporary changes and extensions to the data bases whereas Choice (6) temporarily adds user defined ions and minerals to a particular simulation.

Basic Parameters Menu

The Basic Parameters Menu (fig. 5) is entered by selecting Choice (1) of the Options Menu. The physical and chemical properties of the current water sample are entered using the various choices from this menu.

Title

A title or short description may be entered for the current sample by selecting Choice (1) on this menu. Only the first 80 characters of the title are used. If no title is supplied, the program will use the default title of "Sample #xx", where xx is the current sample number (1 to 10).

Units

Five different units of concentration (mg/l, ppm, mol/l, mol/kg, meq/l) are available for the convenience of the user. Once the units have been chosen, ALL analytical values in that sample must be entered in those units. SOLMIN88 converts concentrations to molality (moles per kilogram of water) for internal calculations.

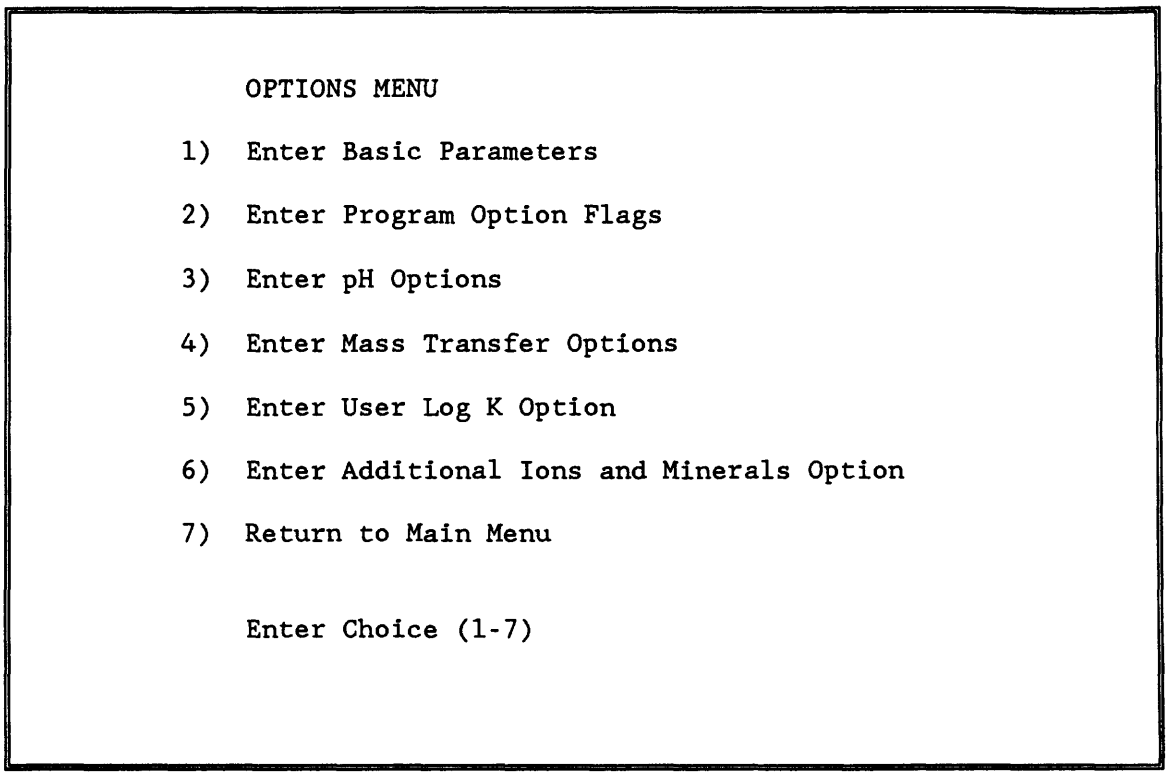

Figure 4. -- Options Menu

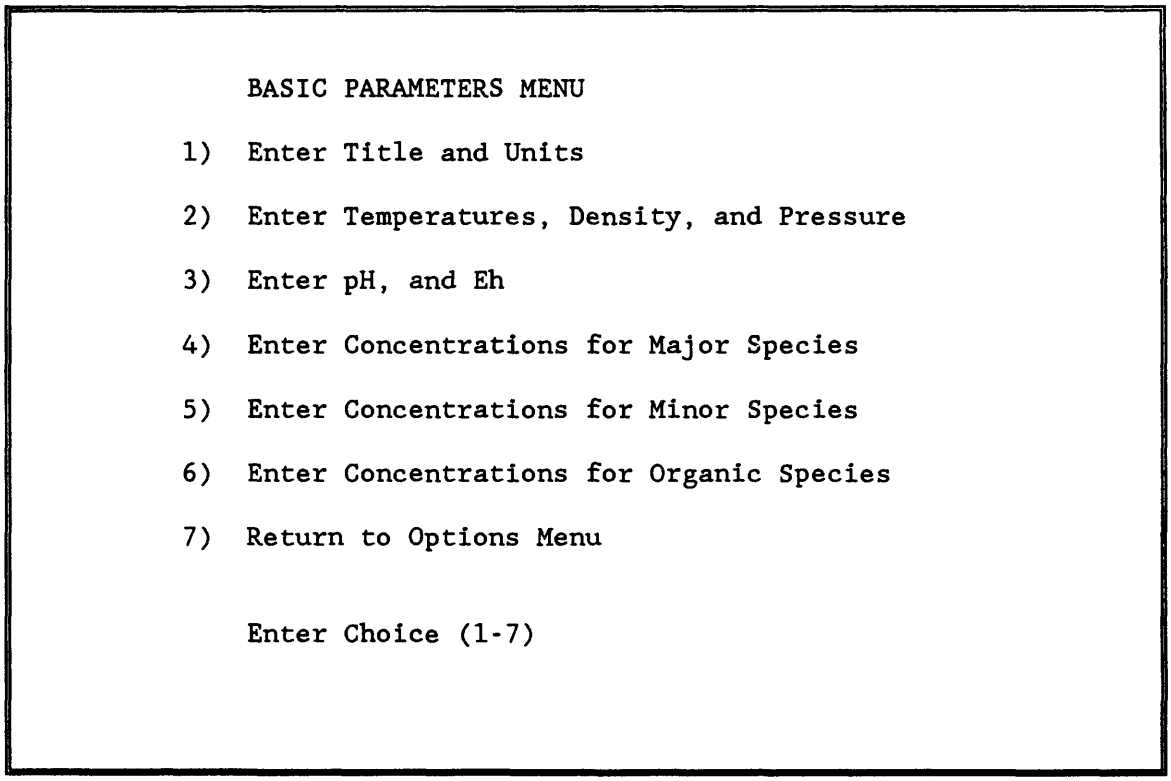

Figure 5. -- Basic Parameters Menu

Temperature

Temperatures are entered in °C and must be between 0 and 350 °C. The temperature at which the pH and Eh are measured is called the sampling temperature. The second temperature is the modeling temperature which can be the same, higher, or lower than the sampling temperature. SOLMIN88 will perform speciation and saturation calculations at both temperatures, if entered. However, it is not necessary to enter the modeling temperature if it is equal to the sampling temperature.

Density

Density is entered in g/cm^3 and is measured at the sampling temperature. If the default density of 0.0 is entered, SOLMIN88 will calculate the density of the sample based on the empirical equation (Kharaka and others, 1988):

$$\rho = 1 + (6.88 \times 10^{-7} * TDS), \quad (1)$$

where ρ is the density and TDS is the total dissolved solids (mg/ℓ) in the solution.

Pressure

Pressure is measured in bars and is the modeling or *in situ* pressure. (Currently SOLMINEQ.88 assumes an atmospheric pressure of 1 bar for the sampling pressure.) If the entered value for the pressure is 0.0, then SOLMIN88 will use one bar or the vapor pressure of water at the modeling temperature, which ever is greater, for its calculations. The entered pressure should not exceed 1,000 bars.

pH and Redox Potential

The values for pH and Eh must correspond to the sampling temperature. The redox potential is measured in volts and can be entered in one of three ways: (1) Eh, which is the measured or calculated redox potential using the hydrogen half cell as the reference electrode, (2) the redox potential using the calomel electrode for reference, and (3) or the redox potential using Zobell's solution to calibrate the cell. Only one of the three methods can be selected, the other two must be set to 9.0. The default value of 9.0 is outside the range for Eh in natural systems and is used to indicate that Eh was not determined.

Eh is used to speciate the multi-valent elements in SOLMINEQ.88. A negative Eh implies a reducing environment while a positive Eh suggests an oxidizing environment. The species to be distributed using Eh (see below) must be selected using the Flags Menu.

Species Concentrations

The analytical (total) concentrations of the various aqueous components found in solution are entered through Choices (4)-(6). All concentrations must be entered using the same units as those selected in Choice (1) of the Basic Parameters Menu. These values must be entered in terms of the master species. (See table 1, lines 4-9) Multivalent components are entered as totals. SOLMINEQ.88 distributes these components between all the redox states assuming redox equilibria if the user enters a value for the measured or calculated redox potential or values are entered for the concentration of SO_4, H_2S, and Fe (see below); otherwise, the program will distribute the entered values between the species with the redox states as the components in table 2. The uncertainties and limitations of redox computatuions in SOLMINEQ.88 and other geochemical codes are discusssed in detail by Kharaka and others (1988). For example, arsenic is entered as total As not as $H_2AsO_3^-$ or AsO_4^{-3}. The value of CH_4 represents the concentration of dissolved methane gas. The values entered for CO_3^{--} and HCO_3^- represent the alkalinity of the

solution. These values and total inorganic carbon (TIC) are used in conjunction with the Carbonate Distribution Flags (see below).

Table 2. -- List of aqueous components

No.	Species	No.	Species	No.	Species
0	Vacant**	14	Al^{+3}	31	$H_3BO_3(aq)$
1	Ca^{++}	15	Ba^{++}	32	$NH_3(aq)$
2	Mg^{++}	16	Cu^{+}	33	$H_2S(aq)$
3	Na^{+}	18	Fe^{++}	48	CH_3COO^{-}
4	K^{+}	21	Hg^{++}	98	CO_3^{--}
5	Cl^{-}	22	Li^{+}	136	NO_3^{-}
6	SO_4^{--}	23	Mn^{++}	169	UO_2^{++}
7	HCO_3^{-}	25	Pb^{++}	210	VO_4^{-3}
8	H^{+}	26	Sr^{++}	246	$C_2O_4^{--}$
9	OH^{-}	27	Zn^{++}	265	$C_4H_4O_4^{--}$
10	H_2O	28	$H_2AsO_3^{-}$	285	$CH_4(aq)$
12	$SiO_2(aq)$	29	PO_4^{-3}		
13	Ag^{+}	30	F^{-}		

The species numbers in the input refer to the index number of selected species in the data file which are organized above. The species (with the exception of H^{+} and OH^{-}) are those normally entered in the input data file for SOLMINEQ.88, and are the only species allowed to be used in the dissolution / precipitation options and ion exchange/adsorption options. Presently moles of H_2O is fixed in the program at 1 kilogram.

** For the ion exchange/adsorption options, vacant surface site is assigned the number zero.

The Flags Menu

The Flags Menu is entered by selecting (2) on the Options Menu. All information relating to the processing of the input file and the formatting of the output is entered through this menu. (fig. 6)

Carbonate Distribution

This sub-menu determines how the alkalinity is distributed at a given pH. The endpoint for alkalinity titrations is assumed to be 4.5. If Choice (0) is selected, then the concentrations entered for CO_3^{--} and/or HCO_3^- represent total alkalinity which is equal to:

$$\text{Alkalinity} = \sum m_{HCO_3^-} + \sum 2\, m_{CO_3^{--}} + \sum m_{OS} \qquad (2)$$

where the summation covers the species and complexes of the summed species and where OS represents other inorganic (e.g. HS^-, S^{--}, $Ca(OH)^+$) and organic (e.g. CH_3COO^-, $C_4H_4O_4^{--}$, $C_2O_4^{--}$) species which contribute to the alkalinity and have a pKa greater than or equal to 4.5. If Choice (1) is selected, then the concentrations entered for CO_3^{--} and/or HCO_3^- represent carbonate alkalinity only which is equal to:

$$\text{Alkalinity} = \sum m_{HCO_3^-} + \sum 2\, m_{CO_3^{--}} \qquad (3)$$

```
        FLAGS MENU

1)  Enter Carbonate Distribution

2)  Enter Activity Coefficient Control

3)  Enter Redox Equilibria

4)  Enter Printout Control

5)  Enter Iterative Convergence Limits

6)  Return to Options Menu

        Enter Choice (1-6)
```

Figure 6. -- Flags Menu

If Choice (2) is selected, then the carbonate species are entered in terms of TIC (Total Inorganic Carbon) which is given by:

$$m_{TIC} = m_{H_2CO_3^o} + \sum m_{HCO_3^-} + \sum m_{CO_3^{--}} \quad (4)$$

Whichever method is selected, the user will then be asked if TIC should be used to distribute the carbonate species at the modeling temperature. If a value for TIC is specified then SOLMIN88 will default to using TIC to distribute the carbonate species at the modeling temperature. However, if alkalinity is expressed as total alkalinity or carbonate alkalinity, then SOLMIN88 will default to distributing the carbonate species at the modeling temperature by holding the alkalinity constant. This default can be overridden by answering 'Y', which will force SOLMIN88 to use TIC for the distribution of carbonate species at the modeling temperature no matter how the alkalinity is expressed.

Activity Coefficients

To control how SOLMIN88 determines activity coefficients, select Choice (2) on the Flags Menu. The first selection determines how the activity coefficients of neutral species are calculated. The default is to set the activity coefficient of neutral species equal to the activity coefficient of CO_2(aq). This method has been described by Kharaka and others (1988). The user can also choose to set the activity coefficients of neutral species equal to one.

The second choice determines the method used to calculated the activity coefficients of charged species. The options include the $B^{\bullet}$ method (Helgeson, 1969), which is the default, and Pitzer's equations (Pitzer, 1981; Harvie and Weare, 1980; Kharaka and others, 1988). The $B^{\bullet}$ method provides good results for solutions with salinities up to 1 molal. The activity coefficients for solutions more concentrated than 1 molal will be more accurate if Pitzer's equations are used.

Redox Equilibria

SOLMINEQ.88 contains eight oxidation/reduction couples: Fe^{++}/Fe^{+3}, Cu^{+}/Cu^{++}, Hg^{+}/Hg^{++}, Mn^{++}/Mn^{+3}, U^{+4}/U^{+5}, U^{+5}/U^{+6}, V^{+3}/V^{+4}, and V^{+4}/V^{+5}. If an Eh measurement has been entered, then these redox couples can be distributed using equations (138-145) in table 3. When Choice (3) on the Flags Menu has been selected, the program will ask explicitly if a particular couple should be distributed based on Eh. If a 'Y' is entered then that specific couple will be distributed by SOLMIN88 using the Eh measurement. Otherwise, if values for H_2S, SO_4^{--}, and total Fe have been entered, then the above redox couples will be distributed based on the H_2S/SO_4^{--} and Fe^{++}/Fe^{+3} oxidation/reduction couples (Kharaka and others, 1988). In the absence of Eh values or concentrations of H_2S, SO_4^{--}, and total Fe, the components will be distributed between the redox states listed in table 2. If the distribution of species should only consider the ions in their reduced state then answer 'Y' for that couple and set Eh to 9.0. There is only one redox flag for uranium and one for vanadium; all couples of those species will be distributed by the same method.

Printout Control

Several options exist to enhance the output generated by SOLMIN88. They are accessed through Choice (4) of the Flags Menu. The first five print options are selected by answering 'Y' to the prompt or reset by answering 'N' to the prompt. The default ('N') is not to use any of these options, because they will increase the amount of output. These options are:

1) The log K values for the aqueous complexes in the data base can be printed at the pH and modeling temperatures.
2) The activity ratios and the log of the activity ratios for several of the major elements can be printed out.
3) Temperature estimates from several chemical geothermometers can be printed out.
4) Iteration data on the anion balance can be printed. This can be useful in solving convergence problems.
5) When a new pH is calculated, the hydrogen ion balance can be printed. This also is useful for samples with convergence problems.
6) A restart file can be created. This allows output from one SOLMIN88 run to be used as input for another run. This is useful in performing multiple operations on a given water sample. To select this option enter a filename in response to the prompt. If the filename is blank the restart file will not be created.

Tolerance Control

If the iteration flag is set (see Printout Control--Option 4) SOLMIN88 will print the convergence factor, Y_A of each anion given by

$$Y_A = 1 - \frac{m_{i,t}}{\Sigma\, n_{i,j}\, m_j} \quad , \tag{5}$$

where $m_{i,t}$, $n_{i,j}$, and m_j are, respectively, the analytical molality of the component i, the stoichiometric coefficient of component i in species j, and the computed molality of species j. When $|Y_A| \leq \delta$ that anion is considered to have converged. The default tolerance, δ, is 5.0×10^{-5}. This value can be changed through Choice (5) of this menu, but must be in the range $1.0 \times 10^{-2} > \delta > 1.0 \times 10^{-8}$. However, if δ is made too small, convergence may not take place in the 100 iterations allowed, resulting in incorrect speciation. On the other hand, if δ is too large the mass balance will carry a larger error resulting in decreased accuracy. The convergence value for the total hydrogen and hydroxide balance is treated in an analogous fashion.

Table 3. -- Dissociation reactions for aqueous complexes

ID # and Name	Reaction
1 HCO_3^-	$HCO_3^- \rightleftarrows H^+ + CO_3^{--}$
2 H_2O^0	$H_2O^0 \rightleftarrows H^+ + OH^-$
3 $H_4SiO_4^0$	$H_4SiO_4^0 \rightleftarrows H^+ + H_3SiO_4^-$
4 Cu^{++}	$Cu^{++} + Fe^{++} \rightleftarrows Cu^+ + Fe^{+3}$
5 Fe^{+3}	$Fe^{+3} + 0.5\ H_2O + 0.125\ HS^- \rightleftarrows Fe^{++} + 0.125\ SO_4^{--} + 1.125\ H^+$
6 Hg^{++}	$2Hg^{++} + 2Fe^{++} \rightleftarrows Hg_2^{++} + 2Fe^{+3}$
7 Mn^{+3}	$Mn^{+3} + Fe^{++} \rightleftarrows Mn^{++} + Fe^{+3}$
8 $H_2AsO_3^-$	$H_2AsO_3^- \rightleftarrows H^+ + HAsO_3^{--}$
9 AlF_5^{--}	$AlF_5^{--} \rightleftarrows Al^{+3} + 5F^-$
10 H_2S^0	$H_2S^0 \rightleftarrows H^+ + HS^-$
11 AlF^{++}	$AlF^{++} \rightleftarrows Al^{+3} + F^-$
12 AlF_2^+	$AlF_2^+ \rightleftarrows Al^{+3} + 2F^-$
13 AlF_3^0	$AlF_3^0 \rightleftarrows Al^{+3} + 3F^-$
14 AlF_4^-	$AlF_4^- \rightleftarrows Al^{+3} + 4F^-$
15 $Al(OH)^{++}$	$Al(OH)^{++} \rightleftarrows Al^{+3} + OH^-$
16 $Al(OH)_2^+$	$Al(OH)_2^+ \rightleftarrows Al^{+3} + 2OH^-$
17 $Al(OH)_4^-$	$Al(OH)_4^- \rightleftarrows Al^{+3} + 4OH^-$
18 $Al(SO_4)^+$	$Al(SO_4)^+ \rightleftarrows Al^{+3} + SO_4^{--}$
19 $Al(SO_4)_2^-$	$Al(SO_4)_2^- \rightleftarrows Al^{+3} + 2SO_4^{--}$
20 $AgCl^0$	$AgCl^0 \rightleftarrows Ag^+ + Cl^-$
21 $AgCl_2^-$	$AgCl_2^- \rightleftarrows Ag^+ + 2Cl^-$
22 $AgCl_3^{--}$	$AgCl_3^{--} \rightleftarrows Ag^+ + 3Cl^-$
23 $AgCl_4^{-3}$	$AgCl_4^{-3} \rightleftarrows Ag^+ + 4Cl^-$
24 $Ag(SO_4)^-$	$Ag(SO_4)^- \rightleftarrows Ag^+ + SO_4^{--}$
25 CH_3COOH^0	$CH_3COOH^0 \rightleftarrows H^+ + CH_3COO^-$
26 $BaCO_3^0$	$BaCO_3^0 \rightleftarrows Ba^{++} + CO_3^{--}$
27 $Ba(HCO_3)^+$	$Ba(HCO_3)^+ \rightleftarrows Ba^{++} + HCO_3^-$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
28 $Ba(OH)^{+}$	$Ba(OH)^{+} \rightleftarrows Ba^{++} + OH^{-}$
29 $BaSO_4^{o}$	$BaSO_4^{o} \rightleftarrows Ba^{++} + SO_4^{--}$
30 $CaCO_3^{o}$	$CaCO_3^{o} \rightleftarrows Ca^{++} + CO_3^{--}$
31 $Ca(HCO_3)^{+}$	$Ca(HCO_3)^{+} \rightleftarrows Ca^{++} + HCO_3^{-}$
32 $Ca(OH)^{+}$	$Ca(OH)^{+} \rightleftarrows Ca^{++} + OH^{-}$
33 $CaPO_4^{-}$	$CaPO_4^{-} \rightleftarrows Ca^{++} + PO_4^{-3}$
34 $CaHPO_4^{o}$	$CaHPO_4^{o} \rightleftarrows Ca^{++} + HPO_4^{--}$
35 $CaH_2PO_4^{+}$	$CaH_2PO_4^{+} \rightleftarrows Ca^{++} + H_2PO_4^{-}$
36 $CaSO_4^{o}$	$CaSO_4^{o} \rightleftarrows Ca^{++} + SO_4^{--}$
37 $CuCl^{o}$	$CuCl^{o} \rightleftarrows Cu^{+} + Cl^{-}$
38 $CuCl_2^{-}$	$CuCl_2^{-} \rightleftarrows Cu^{+} + 2Cl^{-}$
39 $CuCl_3^{--}$	$CuCl_3^{--} \rightleftarrows Cu^{+} + 3Cl^{-}$
40 $CuCl^{+}$	$CuCl^{+} \rightleftarrows Cu^{++} + Cl^{-}$
41 $CuCl_2^{o}$	$CuCl_2^{o} \rightleftarrows Cu^{++} + 2Cl^{-}$
42 $CuCl_3^{-}$	$CuCl_3^{-} \rightleftarrows Cu^{++} + 3Cl^{-}$
43 $CuCl_4^{--}$	$CuCl_4^{--} \rightleftarrows Cu^{++} + 4Cl^{-}$
44 $Cu(OH)^{+}$	$Cu(OH)^{+} \rightleftarrows Cu^{++} + OH^{-}$
45 $CuSO_4^{o}$	$CuSO_4^{o} \rightleftarrows Cu^{++} + SO_4^{--}$
46 $FeCl^{+}$	$FeCl^{+} \rightleftarrows Fe^{++} + Cl^{-}$
47 $FeCl_2^{o}$	$FeCl_2^{o} \rightleftarrows Fe^{++} + 2Cl^{-}$
48 $FeHPO_4^{o}$	$FeHPO_4^{o} \rightleftarrows Fe^{++} + HPO_4^{--}$
49 $H_3PO_4^{o}$	$H_3PO_4^{o} \rightleftarrows 3H^{+} + PO_4^{-3}$
50 $Fe(OH)^{+}$	$Fe(OH)^{+} \rightleftarrows Fe^{++} + OH^{-}$
51 $Fe(OH)_2^{o}$	$Fe(OH)_2^{o} \rightleftarrows Fe^{++} + 2OH^{-}$
52 $FeOOH^{-}$	$FeOOH^{-} + 3H^{+} \rightleftarrows Fe^{++} + 2H_2O$
53 $FeSO_4^{o}$	$FeSO_4^{o} \rightleftarrows Fe^{++} + SO_4^{--}$
54 $FeCl^{++}$	$FeCl^{++} \rightleftarrows Fe^{+3} + Cl^{-}$
55 $FeCl_2^{+}$	$FeCl_2^{+} \rightleftarrows Fe^{+3} + 2Cl^{-}$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
56 $FeCl_3^0$	$FeCl_3^0 \rightleftarrows Fe^{+3} + 3Cl^-$
57 $FeCl_4^-$	$FeCl_4^- \rightleftarrows Fe^{+3} + 4Cl^-$
58 $Fe(SO_4)^+$	$Fe(SO_4)^+ \rightleftarrows Fe^{+3} + SO_4^{--}$
59 $Fe(SO_4)_2^-$	$Fe(SO_4)_2^- \rightleftarrows Fe^{+3} + 2SO_4^{--}$
60 $Fe(OH)^{++}$	$Fe(OH)^{++} \rightleftarrows Fe^{+3} + OH^-$
61 $Fe(OH)_2^+$	$Fe(OH)_2^+ \rightleftarrows Fe^{+3} + 2OH^-$
62 $Fe(OH)_3^0$	$Fe(OH)_3^0 \rightleftarrows Fe^{+3} + 3OH^-$
63 $Fe(OH)_4^-$	$Fe(OH)_4^- \rightleftarrows Fe^{+3} + 4OH^-$
64 $B(OH)_4^-$	$B(OH)_4^- \rightleftarrows B(OH)_3^0 + OH^-$
65 AlF_6^{-3}	$AlF_6^{-3} \rightleftarrows Al^{+3} + 6F^-$
66 $H_3SiO_4^-$	$H_3SiO_4^- \rightleftarrows H^+ + H_2SiO_4^{--}$
67 $H_3AsO_3^0$	$H_3AsO_3^0 \rightleftarrows H^+ + H_2AsO_3^-$
68 $HAsO_4^{--}$	$HAsO_4^{--} \rightleftarrows H^+ + AsO_4^{-3}$
69 $H_2AsO_4^-$	$H_2AsO_4^- \rightleftarrows 2H^+ + AsO_4^{-3}$
70 $H_3AsO_4^0$	$H_3AsO_4^0 \rightleftarrows 3H^+ + AsO_4^{-3}$
71 HF^0	$HF^0 \rightleftarrows H^+ + F^-$
72 $H_2CO_3^0$	$H_2CO_3^0 \rightleftarrows H^+ + HCO_3^-$
73 HPO_4^{--}	$HPO_4^{--} \rightleftarrows H^+ + PO_4^{-3}$
74 $H_2PO_4^-$	$H_2PO_4^- \rightleftarrows 2H^+ + PO_4^{-3}$
75 HS^-	$HS^- \rightleftarrows H^+ + S^{--}$
76 HSO_4^-	$HSO_4^- \rightleftarrows H^+ + SO_4^{--}$
77 HNO_3^0	$HNO_3^0 \rightleftarrows H^+ + NO_3^-$
78 $HgCl^+$	$HgCl^+ \rightleftarrows Hg^{++} + Cl^-$
79 $HgCl_2^0$	$HgCl_2^0 \rightleftarrows Hg^{++} + 2Cl^-$
80 $HgCl_3^-$	$HgCl_3^- \rightleftarrows Hg^{++} + 3Cl^-$
81 $HgCl_4^{--}$	$HgCl_4^{--} \rightleftarrows Hg^{++} + 4Cl^-$
82 $HgSO_4^0$	$HgSO_4^0 \rightleftarrows Hg^{++} + SO_4^{--}$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
83 $HgS(H_2S)_2^o$	$HgS(H_2S)_2^o + H^+ \rightleftarrows Hg^{++} + 2H_2S^o + HS^-$
84 $Hg(HS)_3^-$	$Hg(HS)_3^- \rightleftarrows Hg^{++} + 3HS^-$
85 Hg^o	$Hg^o + 2Fe^{+3} \rightleftarrows Hg^{+2} + 2Fe^{++}$
86 KCl^o	$KCl^o \rightleftarrows K^+ + Cl^-$
87 KCO_3^-	$KCO_3^- \rightleftarrows K^+ + CO_3^{--}$
88 $KHSO_4^o$	$KHSO_4^o \rightleftarrows K^+ + HSO_4^-$
89 KSO_4^-	$KSO_4^- \rightleftarrows K^+ + SO_4^{--}$
90 $KHPO_4^-$	$KHPO_4^- \rightleftarrows K^+ + HPO_4^{--}$
91 $LiOH^o$	$LiOH^o \rightleftarrows Li^+ + OH^-$
92 $LiSO_4^-$	$LiSO_4^- \rightleftarrows Li^+ + SO_4^{--}$
93 $MgCO_3^o$	$MgCO_3^o \rightleftarrows Mg^{++} + CO_3^{--}$
94 $MgHCO_3^+$	$MgHCO_3^+ \rightleftarrows Mg^{++} + HCO_3^-$
95 MgF^+	$MgF^+ \rightleftarrows Mg^{++} + F^-$
96 $MgOH^+$	$MgOH^+ \rightleftarrows Mg^{++} + OH^-$
97 $MgSO_4^o$	$MgSO_4^o \rightleftarrows Mg^{++} + SO_4^{--}$
98 $MgPO_4^-$	$MgPO_4^- \rightleftarrows Mg^{++} + PO_4^{-3}$
99 $MgHPO_4^o$	$MgHPO_4^o \rightleftarrows Mg^{++} + HPO_4^{--}$
100 $MgH_2PO_4^+$	$MgH_2PO_4^+ \rightleftarrows Mg^{++} + H_2PO_4^-$
101 $MnCl^+$	$MnCl^+ \rightleftarrows Mn^{++} + Cl^-$
102 $MnCl_2^o$	$MnCl_2^o \rightleftarrows Mn^{++} + 2Cl^-$
103 $MnCl_3^-$	$MnCl_3^- \rightleftarrows Mn^{++} + 3Cl^-$
104 $MnCl_4^{--}$	$MnCl_4^{--} \rightleftarrows Mn^{++} + 4Cl^-$
105 $MnHCO_3^+$	$MnHCO_3^+ \rightleftarrows Mn^{++} + HCO_3^-$
106 $MnSO_4^o$	$MnSO_4^o \rightleftarrows Mn^{++} + SO_4^{--}$
107 $MnCl^{++}$	$MnCl^{++} \rightleftarrows Mn^{+3} + Cl^-$
108 $MnHPO_4^o$	$MnHPO_4^o \rightleftarrows Mn^{++} + HPO_4^{--}$
109 $MnOH^+$	$MnOH^+ \rightleftarrows Mn^{++} + OH^-$
110 $NaCl^o$	$NaCl^o \rightleftarrows Na^+ + Cl^-$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
111 $NaCO_3^-$	$NaCO_3^- \rightleftarrows Na^+ + CO_3^{--}$
112 $NaHCO_3^0$	$NaHCO_3^0 \rightleftarrows Na^+ + HCO_3^-$
113 $Na_2CO_3^0$	$Na_2CO_3^0 \rightleftarrows 2Na^+ + CO_3^{--}$
114 $Na_2SO_4^0$	$Na_2SO_4^0 \rightleftarrows 2Na^+ + SO_4^{--}$
115 $NaSO_4^-$	$NaSO_4^- \rightleftarrows Na^+ + SO_4^{--}$
116 $NaHPO_4^-$	$NaHPO_4^- \rightleftarrows Na^+ + HPO_4^{--}$
117 $HgOH^+$	$HgOH^+ \rightleftarrows Hg^{++} + OH^-$
118 NH_4OH^0	$NH_4OH^0 \rightleftarrows NH_4^+ + OH^-$
119 $NaHS^0$	$NaHS^0 \rightleftarrows Na^+ + HS^-$
120 NaF^0	$NaF^0 \rightleftarrows Na^+ + F^-$
121 $PbCl^+$	$PbCl^+ \rightleftarrows Pb^{++} + Cl^-$
122 $PbCl_2^0$	$PbCl_2^0 \rightleftarrows Pb^{++} + 2Cl^-$
123 $PbCl_3^-$	$PbCl_3^- \rightleftarrows Pb^{++} + 3Cl^-$
124 $PbCl_4^{--}$	$PbCl_4^{--} \rightleftarrows Pb^{++} + 4Cl^-$
125 $PbSO_4^0$	$PbSO_4^0 \rightleftarrows Pb^{++} + SO_4^{--}$
126 $Zn(CH_3COO)_2^0$	$Zn(CH_3COO)_2^0 \rightleftarrows Zn^{++} + 2CH_3COO^-$
127 $SrOH^+$	$SrOH^+ \rightleftarrows Sr^{++} + OH^-$
128 $SrCO_3^0$	$SrCO_3^0 \rightleftarrows Sr^{++} + CO_3^{--}$
129 $SrHCO_3^+$	$SrHCO_3^+ \rightleftarrows Sr^{++} + HCO_3^-$
130 $SrSO_4^0$	$SrSO_4^0 \rightleftarrows Sr^{++} + SO_4^{--}$
131 $ZnCl^+$	$ZnCl^+ \rightleftarrows Zn^{++} + Cl^-$
132 $ZnCl_2^0$	$ZnCl_2^0 \rightleftarrows Zn^{++} + 2Cl^-$
133 $ZnCl_3^-$	$ZnCl_3^- \rightleftarrows Zn^{++} + 3Cl^-$
134 $ZnCl_4^{--}$	$ZnCl_4^{--} \rightleftarrows Zn^{++} + 4Cl^-$
135 $ZnSO_4^0$	$ZnSO_4^0 \rightleftarrows Zn^{++} + SO_4^{--}$
136 AsO_4^{-3}	$AsO_4^{-3} + 4H^+ + 2Fe^{++} \rightleftarrows H_2AsO_3^- + 2Fe^{+3} + H_2O$
137 $Hg(OH)_2^0$	$Hg(OH)_2^0 \rightleftarrows Hg^{++} + 2OH^-$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
138 Fe^{++} to Fe^{+3}	$Fe^{++} \rightleftarrows Fe^{+3} + e^-$
139 Cu^{+} to Cu^{++}	$Cu^{+} \rightleftarrows Cu^{++} + e^-$
140 Hg_2^{++} to Hg^{++}	$Hg_2^{++} \rightleftarrows 2Hg^{++} + 2e^-$
141 Mn^{++} to Mn^{+3}	$Mn^{++} \rightleftarrows Mn^{+3} + e^-$
142 U^{+4} to UO_2^{+}	$U^{+4} + 2H_2O \rightleftarrows UO_2^{+} + 4H^{+} + e^-$
143 UO_2^{+} to UO_2^{++}	$UO_2^{+} \rightleftarrows UO_2^{++} + e^-$
144 V^{+3} to VO^{++}	$V^{+3} + H_2O \rightleftarrows VO^{++} + 2H^{+} + e^-$
145 VO^{++} to VO_4^{-3}	$VO^{++} + 3H_2O \rightleftarrows VO_4^{-3} + 6H^{+} + e^-$
146 $CaCl^{+}$	$CaCl^{+} \rightleftarrows Ca^{++} + Cl^-$
147 $CaCl_2^{o}$	$CaCl_2^{o} \rightleftarrows Ca^{++} + 2Cl^-$
148 UOH^{+3}	$UOH^{+3} \rightleftarrows U^{+4} + OH^-$
149 $U(OH)_2^{++}$	$U(OH)_2^{++} \rightleftarrows U^{+4} + 2OH^-$
150 $U(OH)_3^{+}$	$U(OH)_3^{+} + 3H^{+} \rightleftarrows U^{+4} + 3H_2O$
151 $U(OH)_4^{o}$	$U(OH)_4^{o} + 4H^{+} \rightleftarrows U^{+4} + 4H_2O$
152 $U(OH)_5^{-}$	$U(OH)_5^{-} + 5H^{+} \rightleftarrows U^{+4} + 5H_2O$
153 UF^{+3}	$UF^{+3} \rightleftarrows U^{+4} + F^-$
154 UF_2^{++}	$UF_2^{++} \rightleftarrows U^{+4} + 2F^-$
155 UF_3^{+}	$UF_3^{+} \rightleftarrows U^{+4} + 3F^-$
156 UF_4^{o}	$UF_4^{o} \rightleftarrows U^{+4} + 4F^-$
157 UF_5^{-}	$UF_5^{-} \rightleftarrows U^{+4} + 5F^-$
158 UF_6^{--}	$UF_6^{--} \rightleftarrows U^{+4} + 6F^-$
159 UCl^{+3}	$UCl^{+3} \rightleftarrows U^{+4} + Cl^-$
160 $U(HPO_4)^{++}$	$U(HPO_4)^{++} \rightleftarrows U^{+4} + HPO_4^{--}$
161 $U(HPO_4)_2^{o}$	$U(HPO_4)_2^{o} \rightleftarrows U^{+4} + 2HPO_4^{--}$
162 $U(HPO_4)_3^{--}$	$U(HPO_4)_3^{--} + 3H^{+} \rightleftarrows U^{+4} + 3H_2PO_4^-$
163 $U(HPO_4)_4^{-4}$	$U(HPO_4)_4^{-4} + 4H^{+} \rightleftarrows U^{+4} + 4H_2PO_4^-$
164 $U(SO_4)^{++}$	$U(SO_4)^{++} \rightleftarrows U^{+4} + SO_4^{--}$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
165 $U(SO_4)_2^0$	$U(SO_4)_2^0 \rightleftarrows U^{+4} + 2SO_4^{--}$
166 $U_6(OH)_{15}^{+9}$	$U_6(OH)_{15}^{+9} + 12H^+ \rightleftarrows 6U^{+4} + 30H^- + 12H_2O$
167 $(UO_2)(OH)^+$	$(UO_2)(OH)^+ \rightleftarrows UO_2^{++} + OH^-$
168 $(UO_2)(OH)_2^0$	$(UO_2)(OH)_2^0 \rightleftarrows UO_2^{++} + 2OH^-$
169 $(UO_2)_2(OH)_2^{++}$	$(UO_2)_2(OH)_2^{++} \rightleftarrows 2UO_2^{++} + 2OH^-$
170 $(UO_2)_3(OH)_5^+$	$(UO_2)_3(OH)_5^+ + 5H^+ \rightleftarrows 3UO_2^{++} + 5H_2O$
171 $(UO_2)_3(OH)_7^-$	$(UO_2)_3(OH)_7^- + 7H^+ \rightleftarrows 3UO_2^{++} + 7H_2O$
172 $UO_2(SO_4)^0$	$UO_2(SO_4)^0 \rightleftarrows UO_2^{++} + SO_4^{--}$
173 $UO_2(SO_4)_2^{--}$	$UO_2(SO_4)_2^{--} \rightleftarrows UO_2^{++} + 2SO_4^{--}$
174 UO_2F^+	$UO_2F^+ \rightleftarrows UO_2^{++} + F^-$
175 $UO_2F_2^0$	$UO_2F_2^0 \rightleftarrows UO_2^{++} + 2F^-$
176 $UO_2F_3^-$	$UO_2F_3^- \rightleftarrows UO_2^{++} + 3F^-$
177 $UO_2F_4^{--}$	$UO_2F_4^{--} \rightleftarrows UO_2^{++} + 4F^-$
178 UO_2Cl^+	$UO_2Cl^+ \rightleftarrows UO_2^{++} + Cl^-$
179 $UO_2H_3SiO_4^+$	$UO_2H_3SiO_4^+ + H^+ \rightleftarrows UO_2^{++} + H_4SiO_4^0$
180 $UO_2(HPO_4)^0$	$UO_2(HPO_4)^0 \rightleftarrows UO_2^{++} + HPO_4^{--}$
181 $UO_2(HPO_4)_2^{--}$	$UO_2(HPO_4)_2^{--} \rightleftarrows UO_2^{++} + 2HPO_4^{--}$
182 $UO_2(H_2PO_4)^+$	$UO_2(H_2PO_4)^+ \rightleftarrows UO_2^{++} + HPO_4^{--} + H^+$
183 $UO_2(H_2PO_4)_2^0$	$UO_2(H_2PO_4)_2^0 \rightleftarrows UO_2^{++} + 2HPO_4^{--} + 2H^+$
184 $UO_2(H_2PO_4)_3^-$	$UO_2(H_2PO_4)_3^- \rightleftarrows UO_2^{++} + 3HPO_4^{--} + 3H^+$
185 $UO_2(CO_3)^0$	$UO_2(CO_3)^0 \rightleftarrows UO_2^{++} + CO_3^{--}$
186 $UO_2(CO_3)_2^{--}$	$UO_2(CO_3)_2^{--} \rightleftarrows UO_2^{++} + 2CO_3^{--}$
187 $UO_2(CO_3)_3^{-4}$	$UO_2(CO_3)_3^{-4} \rightleftarrows UO_2^{++} + 3CO_3^{--}$
188 HVO_4^{-2}	$HVO_4^{--} \rightleftarrows VO_4^{-3} + H^+$
189 $H_2VO_4^{-1}$	$H_2VO_4^- \rightleftarrows VO_4^{-3} + 2H^+$
190 $H_3VO_4^0$	$H_3VO_4^0 \rightleftarrows VO_4^{-3} + 3H^+$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
191 $H_4VO_4^+$	$H_4VO_4^+ \rightleftarrows VO_4^{-3} + 4H^+$
192 $NaHVO_4^-$	$NaHVO_4^- \rightleftarrows Na^+ + VO_4^{-3} + H^+$
193 VO_2F^0	$VO_2F^0 \rightleftarrows VO_2^+ + F^-$
194 $VO_2F_2^-$	$VO_2F_2^- \rightleftarrows VO_2^+ + 2F^-$
195 $V(OH)^{++}$	$V(OH)^{++} \rightleftarrows V^{+3} + OH^-$
196 $V(OH)_2^+$	$V(OH)_2^+ \rightleftarrows V^{+3} + 2OH^-$
197 $V(OH)_3^0$	$V(OH)_3^0 \rightleftarrows V^{+3} + 3OH^-$
198 $VOOH^+$	$VOOH^+ \rightleftarrows VO^{++} + OH^-$
199 $VOSO_4^0$	$VOSO_4^0 \rightleftarrows VO^{++} + SO_4^{--}$
200 $VOCl^+$	$VOCl^+ \rightleftarrows VO^{++} + Cl^-$
201 VOF^+	$VOF^+ \rightleftarrows VO^{++} + F^-$
202 VOF_2^0	$VOF_2^0 \rightleftarrows VO^{++} + 2F^-$
203 $UO_2CH_3COO^+$	$UO_2CH_3COO^+ \rightleftarrows UO_2^{++} + CH_3COO^-$
204 $UO_2(CH_3COO)_2^0$	$UO_2(CH_3COO)_2^0 \rightleftarrows UO_2^{++} + 2CH_3COO^-$
205 UO_2^+	$UO_2^+ + Fe^{+3} \rightleftarrows UO_2^{++} + Fe^{++}$
206 U^{+4}	$U^{+4} + Fe^{+3} + 2H_2O \rightleftarrows UO_2^+ + Fe^{++} + 4H^+$
207 V^{+3}	$V^{+3} + Fe^{+3} + H_2O \rightleftarrows VO^{++} + Fe^{++} + 2H^+$
208 VO^{++}	$VO^{++} + Fe^{+3} + 3H_2O \rightleftarrows VO_4^{-3} + Fe^{++} + 6H^+$
209 $AlCH_3COO^{++}$	$AlCH_3COO^{++} \rightleftarrows Al^{+3} + CH_3COO^-$
210 $BaCH_3COO^+$	$BaCH_3COO^+ \rightleftarrows Ba^{++} + CH_3COO^-$
211 $CaCH_3COO^+$	$CaCH_3COO^+ \rightleftarrows Ca^{++} + CH_3COO^-$
212 $CuCH_3COO^0$	$CuCH_3COO^0 \rightleftarrows Cu^+ + CH_3COO^-$
213 $FeCH_3COO^+$	$FeCH_3COO^+ \rightleftarrows Fe^{++} + CH_3COO^-$
214 $Fe(CH_3COO)_2^0$	$Fe(CH_3COO)_2^0 \rightleftarrows Fe^{++} + 2CH_3COO^-$
215 KCH_3COO^0	$KCH_3COO^0 \rightleftarrows K^+ + CH_3COO^-$
216 $MgCH_3COO^+$	$MgCH_3COO^+ \rightleftarrows Mg^{++} + CH_3COO^-$
217 $NaCH_3COO^0$	$NaCH_3COO^0 \rightleftarrows Na^+ + CH_3COO^-$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
218 $PbCH_3COO^+$	$PbCH_3COO^+ \rightleftarrows Pb^{++} + CH_3COO^-$
219 $Pb(CH_3COO)_2^0$	$Pb(CH_3COO)_2^0 \rightleftarrows Pb^{++} + 2CH_3COO^-$
220 $Pb(CH_3COO)_3^-$	$Pb(CH_3COO)_3^- \rightleftarrows Pb^{++} + 3CH_3COO^-$
221 $SrCH_3COO^+$	$SrCH_3COO^+ \rightleftarrows Sr^{++} + CH_3COO^-$
222 $ZnCH_3COO^+$	$ZnCH_3COO^+ \rightleftarrows Zn^{++} + CH_3COO^-$
223 $HC_2O_4^-$	$HC_2O_4^- \rightleftarrows H^+ + C_2O_4^{--}$
224 $H_2C_2O_4^0$	$H_2C_2O_4^0 \rightleftarrows 2H^+ + C_2O_4^{--}$
225 $AlC_2O_4^+$	$AlC_2O_4^+ \rightleftarrows Al^{+3} + C_2O_4^{--}$
226 $Al(C_2O_4)_2^-$	$Al(C_2O_4)_2^- \rightleftarrows Al^{+3} + 2C_2O_4^{--}$
227 $BaC_2O_4^0$	$BaC_2O_4^0 \rightleftarrows Ba^{++} + C_2O_4^{--}$
228 $CaC_2O_4^0$	$CaC_2O_4^0 \rightleftarrows Ca^{++} + C_2O_4^{--}$
229 $FeC_2O_4^0$	$FeC_2O_4^0 \rightleftarrows Fe^{++} + C_2O_4^{--}$
230 $FeC_2O_4^+$	$FeC_2O_4^+ \rightleftarrows Fe^{+3} + C_2O_4^{--}$
231 $KC_2O_4^-$	$KC_2O_4^- \rightleftarrows K^+ + C_2O_4^{--}$
232 $MgC_2O_4^0$	$MgC_2O_4^0 \rightleftarrows Mg^{++} + C_2O_4^{--}$
233 $MnC_2O_4^0$	$MnC_2O_4^0 \rightleftarrows Mn^{++} + C_2O_4^{--}$
234 $Mn(C_2O_4)_2^{--}$	$Mn(C_2O_4)_2^{--} \rightleftarrows Mn^{++} + 2C_2O_4^{--}$
235 $Mn(C_2O_4)_3^{-4}$	$Mn(C_2O_4)_3^{-4} \rightleftarrows Mn^{++} + 3C_2O_4^{--}$
236 $MnC_2O_4^+$	$MnC_2O_4^+ \rightleftarrows Mn^{+3} + C_2O_4^{--}$
237 $NaC_2O_4^-$	$NaC_2O_4^- \rightleftarrows Na^+ + C_2O_4^{--}$
238 $PbC_2O_4^0$	$PbC_2O_4^0 \rightleftarrows Pb^{++} + C_2O_4^{--}$
239 $SrC_2O_4^0$	$SrC_2O_4^0 \rightleftarrows Sr^{++} + C_2O_4^{--}$
240 $ZnC_2O_4^0$	$ZnC_2O_4^0 \rightleftarrows Zn^{++} + C_2O_4^{--}$
241 $H(C_4H_4O_4)^-$	$H(C_4H_4O_4)^- \rightleftarrows H^+ + C_4H_4O_4^{--}$
242 $H_2(C_4H_4O_4)^0$	$H_2(C_4H_4O_4)^0 \rightleftarrows 2H^+ + C_4H_4O_4^{--}$
243 $AlC_4H_4O_4^+$	$AlC_4H_4O_4^+ \rightleftarrows Al^{+3} + C_4H_4O_4^{--}$

Table 3. -- Dissociation Reactions for Aqueous Complexes -- (Continued)

ID # and Name	Reaction
244 $Al(C_4H_4O_4)_2^-$	$Al(C_4H_4O_4)_2^- \rightleftarrows Al^{+3} + 2C_4H_4O_4^{--}$
245 $BaC_4H_4O_4^o$	$BaC_4H_4O_4^o \rightleftarrows Ba^{++} + C_4H_4O_4^{--}$
246 $CaC_4H_4O_4^o$	$CaC_4H_4O_4^o \rightleftarrows Ca^{++} + C_4H_4O_4^{--}$
247 $FeC_4H_4O_4^o$	$FeC_4H_4O_4^o \rightleftarrows Fe^{++} + C_4H_4O_4^{--}$
248 $FeC_4H_4O_4^+$	$FeC_4H_4O_4^+ \rightleftarrows Fe^{+3} + C_4H_4O_4^{--}$
249 $KC_4H_4O_4^-$	$KC_4H_4O_4^- \rightleftarrows K^+ + C_4H_4O_4^{--}$
250 $MgC_4H_4O_4^o$	$MgC_4H_4O_4^o \rightleftarrows Mg^{++} + C_4H_4O_4^{--}$
251 $MnC_4H_4O_4^o$	$MnC_4H_4O_4^o \rightleftarrows Mn^{++} + C_4H_4O_4^{--}$
252 $NaC_4H_4O_4^-$	$NaC_4H_4O_4^- \rightleftarrows Na^+ + C_4H_4O_4^{--}$
253 $PbC_4H_4O_4^o$	$PbC_4H_4O_4^o \rightleftarrows Pb^{++} + C_4H_4O_4^{--}$
254 $SrC_4H_4O_4^o$	$SrC_4H_4O_4^o \rightleftarrows Sr^{++} + C_4H_4O_4^{--}$
255 $ZnC_4H_4O_4^o$	$ZnC_4H_4O_4^o \rightleftarrows Zn^{++} + C_4H_4O_4^{--}$
256 FeF^{++}	$FeF^{++} \rightleftarrows Fe^{+3} + F^-$
257 SiF_6^{--}	$SiF_6^{--} + 4OH^- \rightleftarrows H_4SiO_4^o + 6F^-$
258 $Pb(HS)_2^o$	$Pb(HS)_2^o \rightleftarrows Pb^{++} + 2HS^-$
259 $Pb(HS)_3^-$	$Pb(HS)_3^- \rightleftarrows Pb^{++} + 3HS^-$
260 $PbCO_3^o$	$PbCO_3^o \rightleftarrows Pb^{++} + CO_3^{--}$
261 $PbOH^+$	$PbOH^+ \rightleftarrows Pb^{++} + OH^-$
262 $Zn(HS)_2^o$	$Zn(HS)_2^o \rightleftarrows Zn^{++} + 2HS^-$
263 $Zn(HS)_3^-$	$Zn(HS)_3^- \rightleftarrows Zn^{++} + 3HS^-$
264 $ZnHCO_3^+$	$ZnHCO_3^+ \rightleftarrows Zn^{++} + HCO_3^-$
265 $ZnOH^+$	$ZnOH^+ \rightleftarrows Zn^{++} + OH^-$
266 $Zn(OH)_2^o$	$Zn(OH)_2^o \rightleftarrows Zn^{++} + 2OH^-$
267 $Zn(HS)(OH)^o$	$Zn(HS)(OH)^o \rightleftarrows Zn^{++} + HS^- + OH^-$

The pH Options Menu

The pH Option Menu (fig. 7) is selected through Choice (3) of the Options Menu.

Gas Addition Option

Choice (1) is the gas addition option which allows the user to titrate gases lost during production and sampling, prior to the pH measurement, back into the solution. The lost gases are added back at the sampling temperature. SOLINPUT will prompt for the total amounts each gas lost in moles per kilogram of water. Currently the only gases SOLMINEQ.88 considers are: CO_2, H_2S, NH_3, and CH_4.

Gas-Water-Oil Distribution Option

Gases that have separated from a solution containing oil, water, and gas phases can be added back into the solution by selecting Choice (2). To use this option the amount in moles per kilogram of the gases lost and their Henry's law coefficients for solubility in oil are required. Also, the weight ratio of oil to water must be known. SOLINPUT also will prompt for the density of the oil at 15 °C. This information is not currently used by SOLMINEQ.88 and is only included for future modifications. Only the gases CO_2, CH_4, and H_2S can be partitioned back into the solution. Currently NH_3 cannot be partitioned back into the solution.

```
        pH OPTIONS

   1)   Gas Addition Option

   2)   Gas-Water-Oil Distribution Option

   3)   Carbonate Mineral Saturation Option

   4)   CO2 Option

   5)   Tolerance factor for Mineral and CO2 Options

   6)   Return to Options Menu

        Enter Choice (1-6)
```

Figure 7. -- pH Options Menu

This option assumes the gases to be in equilibrium with water and oil at the sampling temperature and pressure. If the samples were collected from a test separator which was at a pressure greater than one bar, then two runs of SOLMIN88 are required to determine the *in situ* conditions. For the first run, the sampling temperature should be entered as normal and the separator temperature and pressure should be entered for the modeling temperature and pressure. In addition, the restart file option should be selected. After the run the restart file should be edited and the separator temperature should be entered for the sampling temperature and the normal modeling temperature and pressure should be entered. If a test separator was not used then a single run will suffice.

Carbonate Mineral Saturation Option

This option allows the user to determine the pH of a solution which is in equilibrium with calcite, dolomite, or siderite. To use this option, Choice (3) must be selected under this menu. The carbonate mineral to equilibrate with formation water is then selected. The pH entered in the Basic Parameters Menu will be used as the starting pH for this option. The closer this value is to the final value, the faster this option will be processed.

CO_2 Option

Choice (4) under the pH Options Menu selects the CO_2 option. This option is used to titrate CO_2 into or out of solution until a specified pH, P_{CO_2} or equilibrium with calcite, siderite, or dolomite is reached.

This option will calculate the concentration of dissolved carbon dioxide by equilibrating the solution with either calcite, dolomite, or siderite when selection 1 through 3 is chosen. Selection 4 will allow the recalculation of solution parameters by specifying a fixed molality of H_2CO_3. Selection 5 will fix the pH of the solution forcing the addition and/or subtraction of CO_2 until a specified pH is reached. Finally, selection 6 will calculate the amount of dissolved carbon by fixing the value of P_{CO_2} specified in bars. If selections 4-6 are chosen SOLINPUT will prompt for the designated value.

Tolerance

Both the Caronated Mineral Saturation option and the CO_2 option require a tolerance value to determine when equilibrium has been achieved. This default value is 0.05 log units. Refer to the discussion of the CO_2 Saturation Option and pH Option in Kharaka and others (1988). The tolerance is changed through Choice (5) on the pH Options Menu.

The Mass Transfer Menu

The mass transfer capabilities of SOLMINEQ.88 are selected through this menu (fig. 8) by entering Choice (4) on the Options Menu. Currently, the Dissolution / Precipitation Option, the Mixing Option, and the Boiling and Dilution Option cannot be selected simultaneously; selection of one precludes the use of another. In addition, selection of one will also reset the variables used in the other two options to their default values.

Ion Exchange and Adsorption Option

The Ion Exchange and Adsorption option is entered by selecting Choice (1) on the Mass Transfer Menu. Choice (1) under the Ion Exchange and Adsorption Option indicates adsorption, Choice (2) selects ion exchange, and Choice (3) resets this option to its default values.

For both ion exchange and adsorption the Cation Exchange Capacity (CEC) in milli-equivalents per kilogram must be entered. If the CEC is not known, SOLMINEQ.88 can calculate it from (see Kharaka and others, 1988):

(a) A_T, the total area of the exchanging surface per kilogram of water [units: cm^2] and

(b) N_s, the site density per unit area of the surface [units: sites / cm^2].

SOLINPUT will prompt for all three of these values. However, if the CEC entered is greater than zero then SOLMIN88 will ignore A_T and N_s in its calculations.

The aqueous species which interact with the surface are defined next. The total number of species to interact with the surface must be entered (maximum of 10). If the surface has vacant sites they must also be included as one of the species. For each species the following information must be entered:

(a) its name,

(b) the fraction of surface sites initially occupied by that species (expressed as a decimal),

(c) the charge of the surface complex, and

(d) the selectivity constant for the association reaction of the surface site with the aqueous species.

The concentrations of the surface complexes should be expressed as equivalent fractions in the selectivity constant.

For each surface species defined above it is necessary to define its reaction with the surface. The number of components in the association reaction are entered. Then for each component the index number and the reaction coefficient are defined. The index numbers are found in table 2. Vacant sites are referenced with an index number of 0. A negative reaction coefficient indicates the component is a reactant and a positive reaction coefficient indicates the component is a product.

Dissolution / Precipitation Option

The Dissolution / Precipitation Menu (fig. 9) is entered through Choice (2) on the Mass Transfer Menu (fig. 8).

1) Dissolve / precipitate a mineral to saturation.--This choice will equilibrate the solution with one of the minerals in the data base. The ID of the mineral must be specified using table 4.

2) Dissolve / precipitate a specific mineral amount.--This option will titrate the solution with one of the mineral in the data base. The ID of the mineral from table 4 must be specified along with the number of moles of the mineral per kilogram of water.

3) Equilibrate solution with a mineral from the dissolution / precipitation of another mineral.--The solution may be titrated with one mineral until a second mineral is saturated. The ID of the mineral with which the solution is to be equilibrated and the ID of the mineral to be dissolved / precipitated must be specified.

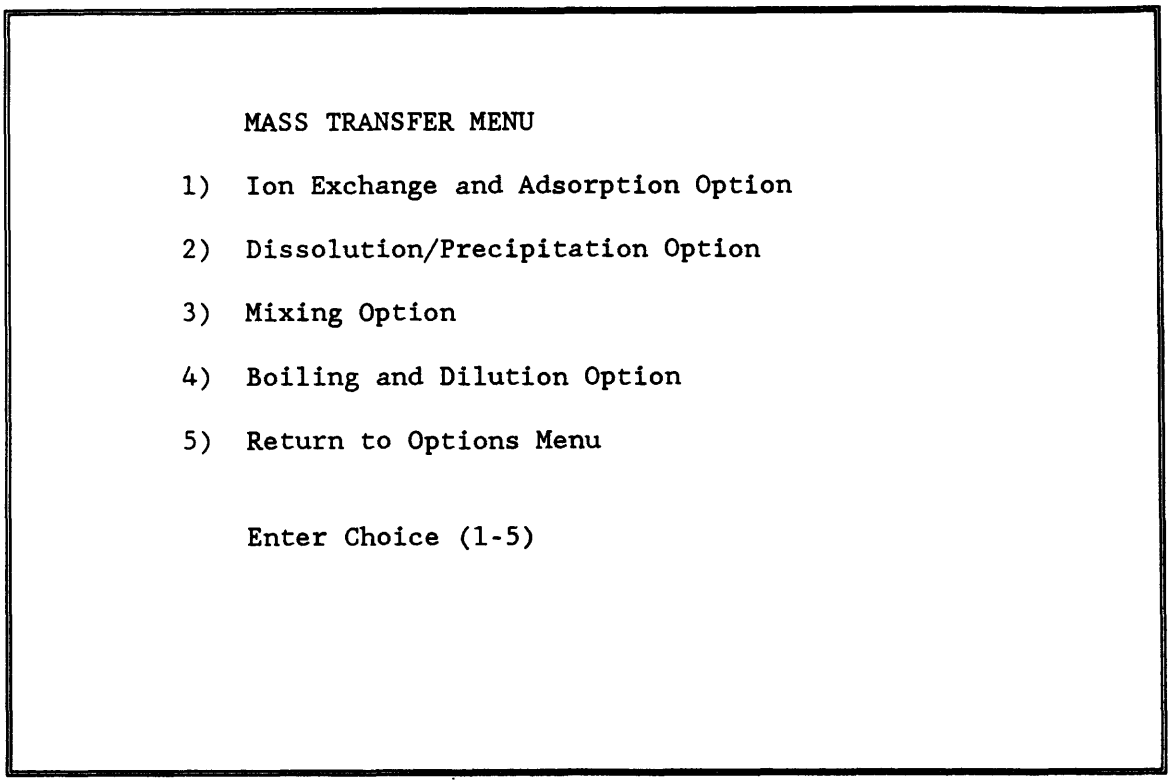

Figure 8. -- Mass Transfer Menu

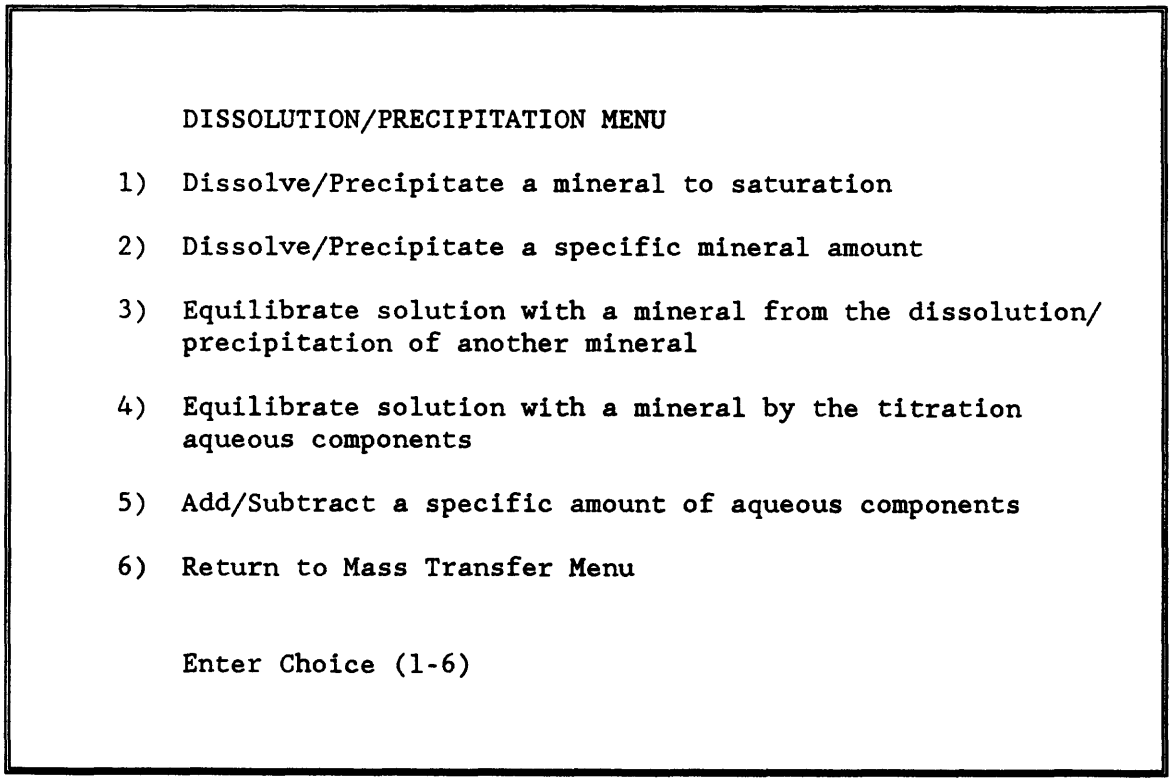

Figure 9. -- Dissolution / Precipitation Menu

4) Equilibrate the solution with a mineral by the titration of aqueous components.--The solution may be equilibrated with a mineral through the titration of aqueous components. The ID of the mineral to be equilibrated, the total number of aqueous components to be added (subtracted) to the solution, the ID of each aqueous component, its reaction coefficient, and the dissolution / precipitation (DP) (see below) switch must be entered. Only the aqueous components listed in table 2 may be used. If more than one component is added (subtracted), the reaction coefficient represents relative proportions only. If the DP switch is positive, SOLMIN88 will dissolve minerals or add aqueous components into the solution. If the DP switch is negative, SOLMIN88 will precipitate minerals or subtract aqueous components out of solution. If the DP switch is set to zero, then SOLMIN88 will determine the direction necessary to equilibrate the solution with the mineral. Otherwise, the magnitude of the DP switch acts as a scaling factor for the default step size (0.01) in log units. The magnitude of the DP switch should normally be 1.0 unless the step size is too large or too small for proper the convergence.

5) Add/subtract a specific amount of aqueous components.--This choice will add/subtract aqueous components into/from the solution based upon a congruent, incongruent, or net reaction. The number of aqueous components, the ID (from table 2) and molality (moles / kg of H_2O) of each component must be entered.

Mixing Option

The Mixing Option, Choice (3) on the Mass Transfer Menu, will isobarically mix two water samples. Data for these two samples may reside in the same or in different files. If in the same file, the second sample must directly follow the first. If in different files, the second sample must be by itself. The mixing option must be chosen for both samples. The first sample must contain the mixing instructions; any parameters set in the second sample will be ignored. SOLMIN88 first processes each sample completely to create end-member solutions. It then mixes these two end-members to create the daughter mixtures.

Four parameters in the first sample instruct SOLMINEQ.88 how to mix the two solutions. The first parameter specifies the total number of mixtures to create from the two solutions. The second value indicates the starting fraction of the first sample to be mixed with the second. The third parameter specifies the fractional increment of the first sample to be added for each mixture created. The final entry is the filename in which the second sample resides. If the second sample is in the same input file as the first, leave this value blank.

Example: To make 6 solutions starting with 100 percent of Sample 2 and going to 100 percent of Sample 1 at 20 percent increments, specify the following parameters:

Total number of mixtures:	4
Smallest fraction of Sample 1:	0.2
Increment of Sample 1 to be added:	0.2

SOLMIN88 will automatically calculate the end-member compositions for the two samples. The above values will then create the following solutions:

Solution	Sample 1	Sample 2
2	20%	80%
3	40%	60%
4	60%	40%
5	80%	20%

Boiling and Dilution Option

The Boiling and Dilution Option is selected by Choice (4) on the Mass Transfer Menu. This option will boil up to 99 percent of the water out of a sample or allow dilution of that sample with pure water. The only parameter this option requires is the fraction of water to be removed to the gas phase or to be diluted with. This fraction must be expressed as a decimal and is positive to indicate boiling and negative to indicate dilution.

Table 4. -- Reactions for the Congruent Dissolution of Minerals

ID # and Name	Reaction
1 Adularia	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$
2 Akermanite	$Ca_2MgSi_2O_7 + 6H^+ + H_2O \rightleftarrows 2Ca^{++} + Mg^{++} + 2H_4SiO_4^0$
3 Albite	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$
4 Albite, Low	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$
5 Albite, High	$NaAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows Na^+ + Al^{+3} + 3H_4SiO_4^0$
6 Alunite	$KAl_3(SO_4)_2(OH)_6 + 6H^+ \rightleftarrows K^+ + 3Al^{+3} + 2SO_4^{--} + 6H_2O$
7 Amesite, 14A	$Mg_2Al_2SiO_5(OH)_4 + 10H^+ \rightleftarrows 2Mg^{++} + 2Al^{+3} + H_4SiO_4^0 + 5H_2O$
8 Analcime	$NaAlSi_2O_6 \cdot H_2O + 4H^+ + H_2O \rightleftarrows Na^+ + Al^{+3} + 2H_4SiO_4^0$
9 Andalusite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^0 + H_2O$
10 Andesine	$Ca_{.4}Na_{.6}Al_{1.4}Si_{2.6}O_8 \rightleftarrows .4CaAl_2Si_2O_8 + .6NaAlSi_3O_8$
11 Anhydrite	$CaSO_4 \rightleftarrows Ca^{++} + SO_4^{--}$
12 Annite	$KFe_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Fe^{++} + Al^{+3} + 3H_4SiO_4^0$
13 Anorthite	$CaAl_2Si_2O_8 + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + 2H_4SiO_4^0$
14 Apatite, Cl	$Ca_5(PO_4)_3Cl \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + Cl^-$
15 Apatite, F	$Ca_5(PO_4)_3F \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + F^-$
16 Apatite, OH	$Ca_5(PO_4)_3OH \rightleftarrows 5Ca^{++} + 3PO_4^{-3} + OH^-$
17 Aragonite	$CaCO_3 \rightleftarrows Ca^{++} + CO_3^{--}$
18 Augite	$CaAl_2SiO_6 + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + H_4SiO_4^0 + 2H_2O$
19 Azurite	$Cu_3(CO_3)_2(OH)_2 \rightleftarrows 3Cu^{++} + 2CO_3^{--} + 2OH^-$
20 Barite	$BaSO_4 \rightleftarrows Ba^{++} + SO_4^{--}$
21 Boehmite	$AlO(OH) + 3H^+ \rightleftarrows Al^{+3} + 2H_2O$
22 Brucite	$Mg(OH)_2 \rightleftarrows Mg^{++} + 2OH^-$
23 Bytownite	$Ca_{.8}Na_{.2}Al_{1.8}Si_{2.2}O_8 \rightleftarrows .8CaAl_2Si_2O_8 + .2NaAlSi_3O_8$
24 Calcite	$CaCO_3 \rightleftarrows Ca^{++} + CO_3^{--}$
25 Celestite	$SrSO_4 \rightleftarrows Sr^{++} + SO_4^{--}$
26 Chalcedony	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^0$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
27 Chamosite, 7A	$Fe_2Al_2SiO_5(OH)_4 + 10H^+ \rightleftarrows 2Fe^{++} + 2Al^{+3} + H_4SiO_4^o + 5H_2O$
28 Chlorite, 7A	$Mg_5Al_2Si_3O_{10}(OH)_8 + 16H^+ \rightleftarrows 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4^o + 6H_2O$
29 Chlorite, 14A	$Mg_5Al_2Si_3O_{10}(OH)_8 + 16H^+ \rightleftarrows 5Mg^{++} + 2Al^{+3} + 3H_4SiO_4^o + 6H_2O$
30 Chrysotile	$Mg_3Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 3Mg^{++} + 2H_4SiO_4^o + H_2O$
31 Clinoenstatite	$MgSiO_3 + 2H^+ + H_2O \rightleftarrows Mg^{++} + H_4SiO_4^o$
32 Clinoptilolite, Sodium	$Na_2Al_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows 2Na^+ + 2Al^{+3} + 10H_4SiO_4^o$
33 Clinoptilolite, Potassium	$K_2Al_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows 2K^+ + 2Al^{+3} + 10H_4SiO_4^o$
34 Clinoptilolite, Calcium	$CaAl_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 10H_4SiO_4^o$
35 Clinoptilolite, Magnesium	$MgAl_2Si_{10}O_{24}\cdot 8H_2O + 8H^+ + 8H_2O \rightleftarrows Mg^{++} + 2Al^{+3} + 10H_4SiO_4^o$
36 Corundum	$Al_2O_3 + 6H^+ \rightleftarrows 2Al^{+3} + 3H_2O$
37 Cristobalite,α	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^o$
38 Cristobalite,β	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^o$
39 Dickite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^o + H_2O$
40 Diopside	$CaMgSi_2O_6 + 4H^+ + 2H_2O \rightleftarrows Ca^{++} + Mg^{++} + 2H_4SiO_4^o$
41 Dolomite	$CaMg(CO_3)_2 \rightleftarrows Ca^{++} + Mg^{++} + 2CO_3^{--}$
42 Dolomite, DSORD	$CaMg(CO_3)_2 \rightleftarrows Ca^{++} + Mg^{++} + 2CO_3^{--}$
43 Enstatite	$MgSiO_3 + 2H^+ + H_2O \rightleftarrows Mg^{++} + H_4SiO_4^o$
44 Epidote	$Ca_2FeAl_2Si_3O_{12}(OH) + 13H^+ \rightleftarrows 2Ca^{++} + Fe^{+3} + 2Al^{+3} + 3H_4SiO_4^o + H_2O$
45 Fayalite	$Fe_2SiO_4 + 4H^+ \rightleftarrows 2Fe^{++} + H_4SiO_4^o$
46 Fluorite	$CaF_2 \rightleftarrows Ca^{++} + 2F^-$
47 Forsterite	$Mg_2SiO_4 + 4H^+ \rightleftarrows 2Mg^{++} + H_4SiO_4^o$
48 Gibbsite, Am	$Al(OH)_3 \rightleftarrows Al^{+3} + 3OH^-$
49 Gibbsite	$Al(OH)_3 \rightleftarrows Al^{+3} + 3OH^-$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
50 Greenalite	$Fe_3Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 3Fe^{++} + 2H_4SiO_4^0 + H_2O$
51 Gypsum	$CaSO_4 \cdot 2H_2O \rightleftarrows Ca^{+2} + SO_4^{-2} + 2H_2O$
52 Halite	$NaCl \rightleftarrows Na^+ + Cl^-$
53 Halloysite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^0 + H_2O$
54 Heulandite	$CaAl_2Si_7O_{18} \cdot 6H_2O + 8H^+ + 4H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 7H_4SiO_4^0$
55 Huntite	$CaMg_3(CO_3)_4 \rightleftarrows Ca^{++} + 3Mg^{++} + 4CO_3^{--}$
56 Hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 3H_2O \rightleftarrows 5Mg^{++} + 4CO_3^{--} + 2OH^- + 3H_2O$
57 Hydrophilite	$CaCl_2 \rightleftarrows Ca^{++} + 2Cl^-$
58 Illite	$K_{.6}Mg_{.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 8H^+ + 2H_2O \rightleftarrows .6K^+ + .25Mg^{++} + 2.3Al^{+3} + 3.5H_4SiO_4^0$
59 Kaolinite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftarrows 2Al^{+3} + 2H_4SiO_4^0 + H_2O$
60 Kenyaite	$NaSi_{11}O_{20.5}(OH)_4 \cdot 3H_2O + H^+ + 16.5H_2O \rightleftarrows Na^+ + 11H_4SiO_4^0$
61 K-Feldspar	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$
62 Kyanite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^0 + H_2O$
63 Labradorite	$Ca_{.6}Na_{.4}Al_{1.6}Si_{2.4}O_8 \rightleftarrows .6CaAl_2Si_2O_8 + .4NaAlSi_3O_8$
64 Larnite	$Ca_2SiO_4 + 4H^+ \rightleftarrows 2Ca^{++} + H_4SiO_4^0$
65 Laumontite	$CaAl_2Si_4O_{12} \cdot 4H_2O + 8H^+ \rightleftarrows Ca^{++} + 2Al^{+3} + 4H_4SiO_4^0$
66 Leucite	$KAlSi_2O_6 + 4H^+ + 2H_2O \rightleftarrows K^+ + Al^{+3} + 2H_4SiO_4^0$
67 Lime	$CaO + 2H^+ \rightleftarrows Ca^{++} + H_2O$
68 Magadite	$NaSi_7O_{13}(OH)_3 \cdot 3H_2O + H^+ + 9H_2O \rightleftarrows Na^+ + 7H_4SiO_4^0$
69 Magnesio-ferrite	$MgFe_2O_4 + 8H^+ \rightleftarrows Mg^{++} + 2Fe^{+3} + 4H_2O$
70 Magnesite	$MgCO_3 \rightleftarrows Mg^{++} + CO_3^{--}$
71 Chloro-magnesite	$MgCl_2 \rightleftarrows Mg^{++} + 2Cl^-$
72 Marialite	$(NaAlSi_3O_8)_3 \cdot NaCl + 12H^+ + 12H_2O \rightleftarrows 4Na^+ + 3Al^{+3} + Cl^- + 9H_4SiO_4^0$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
73 Merwinite	$Ca_3MgSi_2O_8 + 8H^+ \rightleftarrows 3Ca^{++} + Mg^{++} + 2H_4SiO_4^0$
74 Microcline	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^0$
75 Meionite	$(CaAl_2Si_2O_8)_3 \cdot CaCO_3 + 24H^+ \rightleftarrows 4Ca^{++} + 6Al^{+3} + CO_3^{--} + 6H_4SiO_4^0$
76 Mirabilite	$Na_2SO_4 \cdot 10H_2O \rightleftarrows 2Na^+ + SO_4^{--} + 10H_2O$
77 Monticellite	$CaMgSiO_4 + 4H^+ \rightleftarrows Ca^{++} + Mg^{++} + H_4SiO_4^0$
78 Mordenite, Na	$NaAlSi_5O_{12} \cdot 3H_2O + 4H^+ + 5H_2O \rightleftarrows Na^+ + Al^{+3} + 5H_4SiO_4^0$
79 Mordenite, K	$KAlSi_5O_{12} \cdot 3H_2O + 4H^+ + 5H_2O \rightleftarrows K^+ + Al^{+3} + 5H_4SiO_4^0$
80 Muscovite	$KAl_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Al^{+3} + 3H_4SiO_4^0$
81 Nahcolite	$NaHCO_3 \rightleftarrows Na^+ + HCO_3^-$
82 Nathermite	$Na_2CO_3 \cdot H_2O \rightleftarrows 2Na^+ + CO_3^{--} + H_2O$
83 Natron	$Na_2CO_3 \cdot 10H_2O \rightleftarrows 2Na^+ + CO_3^{--} + 10H_2O$
84 Nepheline	$NaAlSiO_4 + 4H^+ \rightleftarrows Na^+ + Al^{+3} + H_4SiO_4^0$
85 Nesquehonite	$MgCO_3 \cdot 3H_2O \rightleftarrows Mg^{++} + CO_3^{--} + 3H_2O$
86 Nontronite, Na	$Na_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33Na^+ + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$
87 Nontronite, K	$K_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33K^+ + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$
88 Nontronite, H	$H_{.33}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 6.99H^+ + 2.68H_2O \rightleftarrows 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$
89 Nontronite, Ca	$Ca_{.165}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Ca^{++} + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$
90 Nontronite, Mg	$Mg_{.165}Fe_2Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Mg^{++} + 2Fe^{+3} + 0.33Al^{+3} + 3.67H_4SiO_4^0$
91 Oldhamite	$CaS + H^+ \rightleftarrows Ca^{++} + HS^-$
92 Oligoclase	$Ca_{.2}Na_{.8}Al_{1.2}Si_{2.8}O_8 \rightleftarrows .2CaAl_2Si_2O_8 + .8NaAlSi_3O_8$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
93 Paragonite	$NaAl_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows Na^+ + 3Al^{+3} + 3H_4SiO_4$
94 Pargasite	$NaCa_2Mg_4Al_3Si_6O_{22}(OH)_2 + 22H^+ \rightleftarrows Na^+ + 2Ca^{++} + 4Mg^{++} + 3Al^{+3} + 6H_4SiO_4^o$
95 Periclase	$MgO + 2H^+ \rightleftarrows Mg^{++} + H_2O$
96 Phillipsite	$Na_{.5}K_{.5}AlSi_3O_8 \cdot H_2O + 4H^+ + 3H_2O \rightleftarrows .5Na^+ + .5K^+ + Al^{+3} + 3H_4SiO_4^o$
97 Phlogopite, OH	$KMg_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftarrows K^+ + 3Mg^{++} + Al^{+3} + 3H_4SiO_4^o$
98 Fluor-phlogopite	$KMg_3AlSi_3O_{10}F_2 + 8H^+ + 2H_2O \rightleftarrows K^+ + 3Mg^{++} + Al^{+3} + 2F^- + 3H_4SiO_4^o$
99 Portlandite	$Ca(OH)_2 \rightleftarrows Ca^{++} + 2OH^-$
100 Potassium Oxide	$K_2O + 2H^+ \rightleftarrows 2K^+ + H_2O$
101 Prehnite	$Ca_2Al_2Si_3O_{10}(OH)_2 + 10H^+ \rightleftarrows 2Ca^{++} + 2Al^{+3} + 3H_4SiO_4^o$
102 Pyrophyllite	$Al_2Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftarrows 2Al^{+3} + 4H_4SiO_4^o$
103 Quartz	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^o$
104 Sanidine, High	$KAlSi_3O_8 + 4H^+ + 4H_2O \rightleftarrows K^+ + Al^{+3} + 3H_4SiO_4^o$
105 Saponite, Na	$Na_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33Na^+ + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^o$
106 Saponite, K	$K_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.33K^+ + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^o$
107 Saponite, H	$H_{.33}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 6.99H^+ + 2.68H_2O \rightleftarrows 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^o$
108 Saponite, Ca	$Ca_{.165}Mg_3Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Ca^{++} + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^o$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
109 Saponite, Mg	$Mg_{3.165}Al_{.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows 0.165Mg^{++} + 3Mg^{++} + 0.33Al^{+3} + 3.67H_4SiO_4^o$
110 Sepiolite	$Mg_4Si_6O_{15}(OH)_2 \cdot 6H_2O + 8H^+ + H_2O \rightleftarrows 4Mg^{++} + 6H_4SiO_4^o$
111 Silica, Amorphous	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^o$
112 Silica Gel	$SiO_2 + 2H_2O \rightleftarrows H_4SiO_4^o$
113 Sillimanite	$Al_2SiO_5 + 6H^+ \rightleftarrows 2Al^{+3} + H_4SiO_4^o + H_2O$
114 Smectite, Ca	$Ca_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .167Ca^{++} + 2.33Al^{+3} + 3.67H_4SiO_4^o$
115 Smectite, K	$K_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .33K^+ + 2.33Al^{+3} + 3.67H_4SiO_4^o$
116 Smectite, Mg	$Mg_{.167}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .167Mg^{++} + 2.33Al^{+3} + 3.67H_4SiO_4^o$
117 Smectite, Na	$Na_{.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 7.32H^+ + 2.68H_2O \rightleftarrows .33Na^+ + 2.33Al^{+3} + 3.67H_4SiO_4^o$
118 Sodium Monoxide	$Na_2O + 2H^+ \rightleftarrows 2Na^+ + H_2O$
119 Spinel	$MgAl_2O_4 + 8H^+ \rightleftarrows Mg^{++} + 2Al^{+3} + 4H_2O$
120 Stilbite	$CaAl_2Si_7O_{18} \cdot 7H_2O + 8H^+ + 3H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 7H_4SiO_4^o$
121 Strengite	$FePO_4 \cdot 2H_2O \rightleftarrows Fe^{+3} + PO_4^{-3} + 2H_2O$
122 Strontianite	$SrCO_3 \rightleftarrows Sr^{++} + CO_3^{--}$
123 Sylvite	$KCl \rightleftarrows K^+ + Cl^-$
124 Talc	$Mg_3Si_4O_{10}(OH)_2 + 6H^+ + 4H_2O \rightleftarrows 3Mg^{++} + 4H_4SiO_4^o$
125 Thenardite	$Na_2SO_4 \rightleftarrows 2Na^+ + SO_4^{--}$
126 Tremolite	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 14H^+ + 8H_2O \rightleftarrows 2Ca^{++} + 5Mg^{++} + 8H_4SiO_4^o$
127 Trona	$Na_2CO_3NaHCO_3 \cdot 2H_2O \rightleftarrows 3Na^+ + CO_3^{--} + HCO_3^- + 2H_2O$
128 Vivianite	$Fe_3(PO_4)_2 \cdot 8H_2O \rightleftarrows 3Fe^{++} + 2PO_4^{-3} + 8H_2O$
129 Wairakite	$CaAl_2Si_4O_{12} \cdot 2H_2O + 8H^+ + 2H_2O \rightleftarrows Ca^{++} + 2Al^{+3} + 4H_4SiO_4^o$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
130 Witherite	$BaCO_3 \rightleftarrows Ba^{++} + CO_3^{--}$
131 Wollastonite	$CaSiO_3 + 2H^+ + H_2O \rightleftarrows Ca^{++} + H_4SiO_4^o$
132 Zoisite	$Ca_2Al_3Si_3O_{12}(OH) + 13H^+ \rightleftarrows 2Ca^{++} + 3Al^{+3} + 3H_4SiO_4^o + H_2O$
133 Silver	$Ag + Fe^{+3} \rightleftarrows Ag^+ + Fe^{++}$
134 Cerargyrite	$AgCl \rightleftarrows Ag^+ + Cl^-$
135 Acanthite	$Ag_2S + H^+ \rightleftarrows 2Ag^+ + HS^-$
136 Copper, Native	$Cu + Fe^{+3} \rightleftarrows Cu^+ + Fe^{++}$
137 Malachite	$Cu_2CO_3(OH)_2 \rightleftarrows 2Cu^{++} + CO_3^{--} + 2OH^-$
138 Tenorite	$CuO + 2H^+ \rightleftarrows Cu^{++} + H_2O$
139 Cuprite	$Cu_2O + 2H^+ \rightleftarrows 2Cu^+ + H_2O$
140 Covellite	$CuS + H^+ \rightleftarrows Cu^{++} + HS^-$
141 Chalcocite	$Cu_2S + H^+ \rightleftarrows 2Cu^+ + HS^-$
142 Chalcopyrite	$CuFeS_2 + 2H^+ \rightleftarrows Cu^{++} + Fe^{++} + 2HS^-$
143 Bornite	$Cu_5FeS_4 + 4H^+ \rightleftarrows 4Cu^+ + Cu^{++} + Fe^{++} + 4HS^-$
144 Lawrencite	$FeCl_2 \rightleftarrows Fe^{++} + 2Cl^-$
145 Molysite	$FeCl_3 \rightleftarrows Fe^{+3} + 3Cl^-$
146 Siderite	$FeCO_3 \rightleftarrows Fe^{++} + CO_3^{--}$
147 Ferrous Oxide	$FeO + 2H^+ \rightleftarrows Fe^{++} + H_2O$
148 Hematite	$Fe_2O_3 + 6H^+ \rightleftarrows 2Fe^{+3} + 3H_2O$
149 Maghemite	$Fe_2O_3 + 6H^+ \rightleftarrows 2Fe^{+3} + 3H_2O$
150 Magnetite	$Fe_3O_4 + 8H^+ \rightleftarrows 2Fe^{+3} + Fe^{++} + 4H_2O$
151 $Fe(OH)_3$	$Fe(OH)_3 \rightleftarrows Fe^{+3} + 3OH^-$
152 Goethite	$FeO(OH) + 3H^+ \rightleftarrows Fe^{+3} + 2H_2O$
153 Pyrrotite	$FeS + H^+ \rightleftarrows Fe^{++} + HS^-$
154 Troilite	$FeS + H^+ \rightleftarrows Fe^{++} + HS^-$
155 Pyrite	$FeS_2 + H_2O \rightleftarrows Fe^{++} + 1.75HS^- + 0.25SO_4^{--} + 0.25H^+$
156 Greigite	$Fe_3S_4 + 4H^+ \rightleftarrows 2Fe^{+3} + Fe^{++} + 4HS^-$
157 Mercury (L)	$Hg + 2Fe^{+3} \rightleftarrows Hg^{++} + 2Fe^{++}$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
158 Mercurous Chloride	$HgCl_2 \rightleftarrows Hg^{++} + 2Cl^-$
159 Calomel	$Hg_2Cl_2 \rightleftarrows Hg_2^{++} + 2Cl^-$
160 Montroydite	$HgO + 2H^+ \rightleftarrows Hg^{++} + H_2O$
161 Cinnabar	$HgS + H^+ \rightleftarrows Hg^{++} + HS^-$
162 Cinnabar, Meta-	$HgS + H^+ \rightleftarrows Hg^{++} + HS^-$
163 Scacchite	$MnCl_2 \rightleftarrows Mn^{++} + 2Cl^-$
164 Rhodochrosite	$MnCO_3 \rightleftarrows Mn^{++} + CO_3^{--}$
165 Manganosite	$MnO + 2H^+ \rightleftarrows Mn^{++} + H_2O$
166 Pyrolusite	$MnO_2 + Mn^{++} + 4H^+ \rightleftarrows 2Mn^{+3} + 2H_2O$
167 Alabandite	$MnS + H^+ \rightleftarrows Mn^{++} + HS^-$
168 Cotunnite	$PbCl_2 \rightleftarrows Pb^{++} + 2Cl^-$
169 Cerussite	$PbCO_3 \rightleftarrows Pb^{++} + CO_3^{--}$
170 Litharge	$PbO + 2H^+ \rightleftarrows Pb^{++} + H_2O$
171 Massicot	$PbO + 2H^+ \rightleftarrows Pb^{++} + H_2O$
172 Galena	$PbS + H^+ \rightleftarrows Pb^{++} + HS^-$
173 Anglesite	$PbSO_4 \rightleftarrows Pb^{++} + SO_4^{--}$
174 Smithsonite	$ZnCO_3 \rightleftarrows Zn^{++} + CO_3^{--}$
175 Zincite	$ZnO + 2H^+ \rightleftarrows Zn^{++} + H_2O$
176 Sphalerite	$ZnS + H^+ \rightleftarrows Zn^{++} + HS^-$
177 Zincosite	$ZnSO_4 \rightleftarrows Zn^{++} + SO_4^{--}$
178 Rutherfordine	$UO_2CO_3 \rightleftarrows UO_2^{++} + CO_3^{--}$
179 Uramphite	$(NH_4)_2(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows 2NH_4^+ + 2UO_2^{++} + 2HPO_4^{--}$
180 Przhevalskite	$Pb(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Pb^{++} + 2UO_2^{++} + 2HPO_4^{--}$
181 Torbernite	$Cu(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Cu^{++} + 2UO_2^{++} + 2HPO_4^{--}$
182 Saleeite	$Mg(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Mg^{++} + 2UO_2^{++} + 2HPO_4^{--}$
183 Autunite, Sr	$Sr(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Sr^{++} + 2UO_2^{++} + 2HPO_4^{--}$
184 Uranocircite	$Ba(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Ba^{++} + 2UO_2^{++} + 2HPO_4^{--}$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
185 Bassetite	$Fe(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Fe^{++} + 2UO_2^{++} + 2HPO_4^{--}$
186 Clarkeite	$UO_3 + 2H^+ \rightleftarrows UO_2^{++} + H_2O$
187 Gummite	$UO_3 + 2H^+ \rightleftarrows UO_2^{++} + H_2O$
188 $UO_2(OH)_2$	$UO_2(OH)_2 \rightleftarrows UO_2^{++} + 2OH^-$
189 $UF_4 \cdot 2.5H_2O$	$UF_4 \cdot 2.5H_2O \rightleftarrows U^{+4} + 4F^- + 2.5H_2O$
190 $U(HPO_4)_2 \cdot 4H_2O$	$U(HPO_4)_2 \cdot 4H_2O \rightleftarrows U^{+4} + 2HPO_4^{--} + 4H_2O$
191 Ningyoite	$CaU(HPO_4)_2 \cdot 2H_2O + 2H^+ \rightleftarrows Ca^{++} + U^{+4} + 2HPO_4^{--} + 2H_2O$
192 U_3O_8	$U_3O_8 + 4H^+ \rightleftarrows UO_2^{++} + 2UO_2^+ + 2H_2O$
193 Uraninite, Amorphous	$UO_2 + 4H^+ \rightleftarrows U^{+4} + 2H_2O$
194 Uraninite	$UO_2 + 4H^+ \rightleftarrows U^{+4} + 2H_2O$
195 U_4O_9	$U_4O_9 + 10H^+ \rightleftarrows 2U^{+4} + 2UO_2^+ + 5H_2O$
196 Coffinite	$USiO_4 + 4H^+ \rightleftarrows U^{+4} + H_4SiO_4^o$
197 Autunite, H	$H_2(UO_2)_2(PO_4)_2 \rightleftarrows 2UO_2^{++} + 2HPO_4^{--}$
198 Autunite, Na	$Na_2(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows 2Na^+ + 2UO_2^{++} + 2HPO_4^{--}$
199 Autunite, K	$K_2(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows 2K^+ + 2UO_2^{++} + 2HPO_4^{--}$
200 Autunite	$Ca(UO_2)_2(PO_4)_2 + 2H^+ \rightleftarrows Ca^{++} + 2UO_2^{++} + 2HPO_4^{--}$
201 Carnotite	$K_2(UO_2)_2(VO_4)_2 \rightleftarrows 2K^+ + 2UO_2^{++} + 2VO_4^{-3}$
202 Tyuyamunite	$Ca(UO_2)_2(VO_4)_2 \rightleftarrows Ca^{++} + 2UO_2^{++} + 2VO_4^{-3}$
203 Uranophane	$Ca(UO_2)_2(HSiO_4)_2 + 6H^+ \rightleftarrows Ca^{++} + 2UO_2^{++} + 2H_4SiO_4^o$
204 Schoepite	$UO_2(OH)_2 \cdot H_2O \rightleftarrows UO_2^{++} + 2OH^- + H_2O$
205 $MgUO_4$	$MgUO_4 + 4H^+ \rightleftarrows Mg^{++} + UO_2^{++} + 2H_2O$
206 $CaUO_4$	$CaUO_4 + 4H^+ \rightleftarrows Ca^{++} + UO_2^{++} + 2H_2O$
207 $BaUO_4$	$BaUO_4 + 4H^+ \rightleftarrows Ba^{++} + UO_2^{++} + 2H_2O$
208 UO_2F_2	$UO_2F_2 \rightleftarrows UO_2^{++} + 2F^-$
209 US_3	$US_3 + 2H_2O \rightleftarrows UO_2^{++} + 3HS^- + H^+$
210 Karelianite	$V_2O_3 + 6H^+ \rightleftarrows 2V^{+3} + 3H_2O$

Table 4. -- Congruent Dissolution of Minerals -- (Continued)

ID # and Name	Reaction
211 Vanadium Tetro-	$V_2O_4 + 4H^+ \rightleftarrows 2VO^{++} + 2H_2O$
212 Vanadium Pento-	$V_2O_5 + 3H_2O \rightleftarrows 2VO_4^{-3} + 6H^+$
213 $VOSO_4 \cdot 6H_2O$	$VOSO_4 \cdot 6H_2O \rightleftarrows VO^{++} + SO_4^{--} + 6H_2O$
214 $Pb_3(VO_4)_2$	$Pb_3(VO_4)_2 \rightleftarrows 3Pb^{++} + 2VO_4^{-3}$

User Log K Option

The User Log K Option allows the replacement of dissociation and dissolution equilibrium constants in the data base with those defined by the user. These changes only apply to the selected sample in the input file. If the user wants the changes to apply to more than the selected sample, the data base should be modified. Up to 6 equilibrium constants may be replaced at the sampling temperature and up to 6 may be replaced at the modeling temperature. To use this option select Choice (5) on the Options Menu.

Each log K entered must be identified as (A)queous or (M)ineral. If (Q)uit is selected for this prompt, SOLINPUT will keep the previous values entered and prompt for values at the modeling temperature if it exists or exit to the Options Menu otherwise. If an aqueous log K is to be replaced, the identification number from table 3 must be entered. If a mineral log K is to be replaced, the identification number from table 4 must be entered. Finally, the new log K for that temperature must be input. After the 6th entry for either temperature, the program will move to the next temperature or exit to the Options Menu.

Additional Ions and Minerals Option

SOLMINEQ.88 allows the user to add two additional anions, one cation, and up to 5 minerals for a particular simulation. This option is selected through Choice (6) of the Options Menu (fig. 4). Figure 10 displays the Additional Ions and Minerals Menu.

Adding Ions

The steps involved in adding a new ion to the sample are: (1) define the component species, and (2) define the complexes which form with that species.

Definition of the component species.--Select Choice (1) or (3) to define the additional anion component or Choice (5) to define the additional cation component. SOLINPUT will then prompt for the name (up to 8 characters), the charge, the hydrated radius, the gram formula weight and the concentration. It is currently not possible to specify a redox relationship for the additional ion, nor can a reaction be defined for the oxidized forms of the cation species. If a zero is entered for the ion size parameter then the program will assign it a value of 0, 4, 6, 9, or 12 based on its charge of 0, 1, 2, 3, or ≥ 4, respectively. The concentration must be entered in the same units in which the rest of the chemical analyses have been input.

Definition of the complexes.--To define the complexes, select Choice (2) or (4) for the anions or Choice (6) for the cation. A menu will display the possible components that may form complexes with the ion. Table 5 lists the dissociation reactions defined for each additional ion complex in SOLMINEQ.88. For each component selected, SOLINPUT will prompt for the ion size parameter of the complex (if not a neutral complex) and the log of the constant for the dissociation reaction at each temperature. Again, if a zero is entered for the ion size parameter it will be assigned as above.

```
    ADDITIONAL IONS AND MINERALS MENU

1)  Enter Anion #1

2)  Enter Complexes for Anion #1

3)  Enter Anion #2

4)  Enter Complexes for Anion #2

5)  Enter Additional Cation

6)  Enter Cation Complexes

7)  Enter Additional Minerals

8)  Return to Options Menu

    Enter Choice (1-8)
```

Figure 10. -- Additional Ions and Minerals Menu

```
    Choose Mineral

1)  Min # 1

2)  Min # 2

3)  Min # 3

4)  Min # 4

5)  Min # 5

6)  Return to previous menu

    Enter Choice (1-6)
```

Figure 11. -- Mineral Selection Menu

Table 5. -- Additional ion reactions

1) $HAn^{-z+1} \rightleftarrows H^{+} + An^{-z}$

2) $H_2An^{-z+2} \rightleftarrows 2H^{+} + An^{-z}$

3) $AlAn^{-z+3} \rightleftarrows Al^{+3} + An^{-z}$

4) $BaAn^{-z+2} \rightleftarrows Ba^{++} + An^{-z}$

5) $CaAn^{-z+2} \rightleftarrows Ca^{++} + An^{-z}$

6) $CuAn^{-z+1} \rightleftarrows Cu^{+} + An^{-z}$

7) $FeAn^{-z+2} \rightleftarrows Fe^{++} + An^{-z}$

8) $KAn^{-z+1} \rightleftarrows K^{+} + An^{-z}$

9) $MgAn^{-z+2} \rightleftarrows Mg^{++} + An^{-z}$

10) $MnAn^{-z+2} \rightleftarrows Mn^{++} + An^{-z}$

11) $NaAn^{-z+1} \rightleftarrows Na^{+} + An^{-z}$

12) $PbAn^{-z+2} \rightleftarrows Pb^{++} + An^{-z}$

13) $SrAn^{-z+2} \rightleftarrows Sr^{++} + An^{-z}$

14) $ZnAn^{-z+2} \rightleftarrows Zn^{++} + An^{-z}$

$CatCl^{z-1} \rightleftarrows Cat^{z} + Cl^{-}$

$CatSO_4^{z-2} \rightleftarrows Cat^{z} + SO_4^{--}$

$CatHCO_3^{z-1} \rightleftarrows Cat^{z} + HCO_3^{-}$

$CatOH^{z-1} \rightleftarrows Cat^{z} + OH^{-}$

$CatPO_4^{z-3} \rightleftarrows Cat^{z} + PO_4^{-3}$

$CatF^{z-1} \rightleftarrows Cat^{z} + F^{-}$

$CatCH_3COO^{z-1} \rightleftarrows Cat^{z} + CH_3COO^{-}$

$CatCO_3^{z-2} \rightleftarrows Cat^{z} + CO_3^{--}$

$CatHS^{z-1} \rightleftarrows Cat^{z} + HS^{-}$

$CatC_2O_4^{z-2} \rightleftarrows Cat^{z} + C_2O_4^{--}$

$CatC_4H_4O_4^{z-2} \rightleftarrows Cat^{z} + C_4H_4O_4^{--}$

$CatAn\#1^{zc-za} \rightleftarrows Cat^{zc} + An\#1^{-za}$

$CatAn\#2^{zc-za} \rightleftarrows Cat^{zc} + An\#2^{-za}$

Adding Minerals

The additional minerals are added through Choice (7) of the Additional Ions and Minerals Menu. The minerals sub-menu (fig. 11) will display the currently defined minerals. Select Choice (1-5) to add or modify a mineral. For each mineral added the following must be defined: its name, its dissolution reaction, and the log of its equilibrium constant for the reaction at both the sampling and modeling temperatures. Each reaction may contain up to 9 components. Each component must have its ID specified (from table 2) and its reaction coefficient defined. A positive reaction coefficient indicates a product; a negative reaction coefficient indicates a reactant. If a zero is entered for an ID, SOLINPUT will stop prompting for components. A 10th component can be defined for the minerals, the additional activity parameter. The additional activity parameter represents a constant value for one or more aqueous species that are not currently in the SOLMINEQ.88 data base. This parameter is added to the activity product of the mineral reaction. The additional activity parameter is not currently used by the dissolution / precipitation option in its calculations.

Adding New Minerals and Ions

New minerals, cations, and anions can be added permanently to SOLMINEQ.88 using the detailed steps outlined in Appendices I, II, and III, respectively. The additions and modifications to the source code as well as the data tables are given. To illustrate by example, the addition of the mineral ankerite is described in Appendix I, a selected number of Cd species are given in Appendix II and a number of Br species are used in Appendix III. Cd and Br minerals, of course, can be added using the same steps described in Appendix I for ankerite.

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APPENDIX I. Programming Notes: Adding a Mineral.

Adding a mineral not currently in the data base to SOLMINEQ.88 is relatively simple. Only two of the data bases need to be modified, DATA.TBL and RXN.TBL. The first change is to modify the third value of the first line of DATA.TBL to reflect the new maximum number of minerals (MXMNK). The second change is to add the log K values for the selected mineral, from 0 to 350 °C, to the bottom of the current list of mineral log K values in the file DATA.TBL. The log K values in the table are at the following temperature increments: 0, 25, 50, 75, 100, 125, 150, 200, 250, 300, 350 °C. The values entered should be between -300 and +300 or they will be ignored. Line up entries with the decimal points of previous entries. A value must be entered for each temperature increment or the interpolation scheme used by SOLMIN88 will produce incorrect values. The last change is to modify RXN.TBL to include the dissolution reaction for which the log K values correspond. The reaction must be a congruent dissolution reaction and can only include those components listed in table 3. For each reaction the ID of each component along with its reaction coefficient must be defined. For example, to add the mineral Ankerite, $Ca(Fe_{0.5}Mg_{0.5})(CO_3)_2$, to RXN.TBL the following entry would be added to the end of the table:

```
215,
1.0,1,0.5,18,0.5,2,2.0,98
```

which would represent the reaction

$$Ca(Fe_{0.5}Mg_{0.5})(CO_3)_2 \rightleftarrows Ca^{++} + 0.5\,Fe^{++} + 0.5\,Mg^{++} + 2\,CO_3^{--} \qquad \text{(AI.1)}$$

If a component in the reaction does not exist in SOLMINEQ.88 then the mineral must be added using the additional mineral option or the component must be defined as discussed in Appendixes II and III.

APPENDIX II. Programming Notes: Adding a Cation.

Currently, adding a cation component or an additional cation complex involves modifying SOLMIN88, SOLINPUT, and DATA.TBL. Cadmium will be used as an example of how to add a cation component. The following steps describe the procedure.

(i) Define the component to be added

The component must be defined according to its index number, name, charge, ion size parameter, and atomic mass. This data must be placed in the appropriate format in the first section of the file DATA.TBL. This section corresponds to table IA of Kharaka and others (1988). The entry for cadmium would be as follows:

```
296 Cd ++      2 6.0 112.410
```

The index number should follow the number of the last aqueous species in the data base. The parameter NMAX in the code SOLMIN88 must be large enough to accommodate all of the aqueous species plus the user defined aqueous species (of which there are currently 44). Therefore,

$$NMAX = MXSP + 44$$

and all occurrences of NMAX in the code SOLMIN88 must be changed.

(ii) Define the complexes which will form with the component

Each anion currently in SOLMINEQ.88 which will complex with the cation to be added must be defined in DATA.TBL as in section (i) above. If cadmium forms complexes with Cl^-, SO_4^{--}, HCO_3^-, OH^-, and CO_3^{--} then the following data would be entered into section 1 of DATA.TBL:

```
297 CdCl +     1 4.0   147.863
298 CdCl2      0 0.0   183.316
299 CdSO4      0 0.0   208.468
300 CdHCO3 +   1 6.0   173.427
301 CdOH +     1 6.0   129.417
302 Cd(OH)2    0 0.0   146.425
303 CdCO3      0 0.0   172.419
```

MXSP, the number of aqueous species, must now be changed. This is the first value on the first line of DATA.TBL and, in this case, would be changed from 295 to 303.

(iii) Define equations for each complex

The dissociation reaction for each complex needs to be defined (see table IIa). From the dissociation reactions the mass action equations are written (see table IIb). Each mass action equation defines an equilibrium constant for that reaction. The log K for each of these equations must be defined at the temperature of interest or at the following temperatures: 0, 25, 50, 75, 100, 125, 150, 200, 250, 300, 350 °C. A value must be entered for each temperature increment (the same value can be used for all temperatures) or the interpolation scheme used by SOLMIN88 will produce incorrect results. These values should be between ±35 (Log CPUMIN ≤ Log K ≤ Log CPUMAX). Any value outside of this range will be set to the appropriate boundary. Once the log K values have been defined they must be entered in section 2 of DATA.TBL which corresponds to table IB in Kharaka and others (1988) (see table IIc). In addition, the value MXAQK on the first line of DATA.TBL must be changed to include the new number of aqueous complexes. The second value on the line, in this case 267, would be changed to 274.

Table IIa. -- Dissociation reactions of cadmium

$CdCl^+ \rightleftarrows Cd^{++} + Cl^-$	(AIIa.1)
$CdCl_2 \rightleftarrows Cd^{++} + 2Cl^-$	(AIIa.2)
$CdSO_4 \rightleftarrows Cd^{++} + SO_4^{--}$	(AIIa.3)
$CdHCO_3^+ \rightleftarrows Cd^{++} + HCO_3^-$	(AIIa.4)
$CdOH^+ \rightleftarrows Cd^{++} + OH^-$	(AIIa.5)
$Cd(OH)_2 \rightleftarrows Cd^{++} + 2OH^-$	(AIIa.6)
$CdCO_3 \rightleftarrows Cd^{++} + CO_3^{--}$	(AIIa.7)

Table IIb. -- Rewritten mass equations for cadmium

$$m_{CdCl^+} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m_{Cl^-}\ \gamma_{Cl^-})}{(K_{CdCl^+})\ (\gamma_{CdCl^+})} \qquad \text{(AIIb.1)}$$

$$m_{CdCl_2} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m^2_{Cl^-}\ \gamma^2_{Cl^-})}{(K_{CdCl_2})\ (\gamma_{CdCl_2})} \qquad \text{(AIIb.2)}$$

$$m_{CdSO_4} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m_{SO_4^{--}}\ \gamma_{SO_4^{--}})}{(K_{CdSO_4})\ (\gamma_{CdSO_4})} \qquad \text{(AIIb.3)}$$

$$m_{CdHCO_3^+} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m_{HCO_3^-}\ \gamma_{HCO_3^-})}{(K_{CdHCO_3^+})\ (\gamma_{CdHCO_3^+})} \qquad \text{(AIIb.4)}$$

$$m_{CdOH^+} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m_{OH^-}\ \gamma_{OH^-})}{(K_{CdOH^+})\ (\gamma_{CdOH^+})} \qquad \text{(AIIb.5)}$$

$$m_{Cd(OH)_2} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m^2_{OH^-}\ \gamma^2_{OH^-})}{(K_{Cd(OH)_2})\ (\gamma_{Cd(OH)_2})} \qquad \text{(AIIb.6)}$$

$$m_{CdCO_3} = \frac{(m_{Cd^{++}}\ \gamma_{Cd^{++}})\ (m_{CO_3^{--}}\ \gamma_{CO_3^{--}})}{(K_{CdCO_3})\ (\gamma_{CdCO_3})} \qquad \text{(AIIb.7)}$$

(iv) Write the mass balance equation

The mass balance equation

$$m_{i,t} = \sum_{1}^{j} n_{i,j} m_j \quad , \tag{AII.1}$$

where $m_{i,t}$, $n_{i,j}$, and m_j are, respectively, the analytical molality of the component i, the stoichiometric coefficient of component i in species j, and the computed molality of species j, must be written for the added cation. For cadmium the equation is

$$m_{Cd,t} = m_{Cd^{++}} + m_{CdCl^{+}} + m_{CdCl_2} + m_{CdSO_4} + m_{CdHCO_3^{+}} + m_{CdOH^{+}} + m_{Cd(OH)_2} + m_{CdCO_3} \tag{AII.2}$$

If the mass action equations are solved for the molality of the complex (see table IIb) using the relationship

$$a = \gamma m \quad , \tag{AII.3}$$

then they can be substituted into equation (AII.2). Equation (AII.2) can then be solved for $m_{Cd^{++}}$ giving

$$m_{Cd^{++}} = \frac{m_{Cd,\,t}}{1 + (\gamma_{Cd^{++}})\ \Omega} \tag{AII.4}$$

where

$$\Omega = \frac{(m_{Cl^-}\ \gamma_{Cl^-})}{(K_{CdCl^+})\ (\gamma_{CdCl^+})} + \frac{(m^2_{Cl^-}\ \gamma^2_{Cl^-})}{(K_{CdCl_2})\ (\gamma_{CdCl_2})} + \frac{(m_{SO_4^{--}}\ \gamma_{SO_4^{--}})}{(K_{CdSO_4})\ (\gamma_{CdSO_4})} + \frac{(m_{HCO_3^-}\ \gamma_{HCO_3^-})}{(K_{CdHCO_3^+})\ (\gamma_{CdHCO_3^+})} +$$

$$\frac{(m_{OH^-}\ \gamma_{OH^-})}{(K_{CdOH^+})\ (\gamma_{CdOH^+})} + \frac{(m^2_{OH^-}\ \gamma^2_{OH^-})}{(K_{Cd(OH)_2})\ (\gamma_{Cd(OH)_2})} +$$

$$\frac{(m_{CO_3^{--}}\ \gamma_{CO_3^{--}})}{(K_{CdCO_3})\ (\gamma_{CdCO_3})}$$

Table IIc. -- Sample format for the equilibrium constants of dissociation for cadmium complexes*

	0/200	25/250	50/300	75/350	100	125	150
268 CdCl +	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
269 CdCl2	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
270 CdSO4	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
271 CdHCO3 +	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
272 CdOH+	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
273 Cd(OH)2	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
274 CdCO3	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			

*The correct values for the dissociation contants at each temperature or the value at the temperature of interest should replace the dummy values.

(v) Begin Coding

The molality of Cd^{++} in equation (AII.4) would be coded as follows:

```
C ------------------------------------------------------------------|
C     Cadmium Species                                               |
C ------------------------------------------------------------------|

      IF (EXELT(36) .GT. CPUMIN) THEN
        M(297) = ALFA(5)     / KT1(268) * GAMMA(297)
        M(298) = ALFA(5)**2  / KT1(269) * GAMMA(298)
        M(299) = ALFA(6)     / KT1(270) * GAMMA(299)
        M(300) = ALFA(7)     / KT1(271) * GAMMA(300)
        M(301) = ALFA(9)     / KT1(273) * GAMMA(302)
        M(302) = ALFA(9)**2  / KT1(274) * GAMMA(303)
        M(303) = ALFA(98)    / KT1(275) * GAMMA(304)

        M(296) = EXELT(36) / (1.0D0 + GAMMA(296) * (M(297) + M(298) +
                 M(299) + M(300) + M(301) + M(302) + M(303)))
        ALFA(296) = M(296) * GAMMA(296)

        DO ## I = 297, 303
          M(I)    = M(I) * ALFA(296)
          ALFA(I) = M(I) * GAMMA(I)
        END DO
   ## CONTINUE
```

An appropriate statement label should be substituted for ## in the DO loop. This section of code should be placed in subroutine DISTRB anywhere after line DIS 6480 and before DIS 18600. The variable EXELT will need to be redimensioned throughout the code, in this case from EXELT(35) to EXELT(36). In addition, the statement

EXELT(36) = ANALM(296)

will have to be added to the code to correctly initialize EXELT in the following places: ADS 6735, CAL 2100, MIX 2635, MIX 5265, MIX 7675, and MIX 8225. The other variables should be dimensioned correctly if NMAX has been set correctly (see (i) above).

For each anion the added cation component is coupled with, the molality of the complex must be added to the anion summation. For species such as $CdCl_2$, twice the molality of the complex must be added to the chlorine summation. The summation of the anion species is located in subroutine DISTRB starting at line DIS18610. The summation vector, S, is mapped as follows:

S(1)	$HCO_3^- + CO_3^{--}$
S(2)	SO_4^{--}
S(3)	F^-
S(4)	PO_4^{-3}
S(5)	Cl^-
S(6)	CH_3COO^-
S(7)	S^{--}
S(8)	$C_2O_4^{--}$

S(9)	$C_4H_4O_4^{--}$
S(10)	User Defined Anion #1
S(11)	User Defined Anion #2

For cadmium the original code fragments from Kharaka and others (1988) would be changed as follows:

```
S(1) =     M(7)   + 2.0*M(98)  + 2.0*M(51)  +     M(52)  +        DIS18650
.       2.0*M(55)  +     M(56)  + 2.0*M(114) + 2.0*M(120) +        DIS18660
.           M(121) +     M(132) + 2.0*M(138) +     M(139) +        DIS18670
.       2.0*M(140) + 2.0*M(155) +     M(156) + 2.0*M(207) +        DIS18680
.       4.0*M(208) + 6.0*M(209) + 2.0*M(288) +     M(292) +        DIS18690
.           M(300) + 2.0*M(301) + 2.0*M(303) +                     DIS18695
.           M(MXSP+34)          + 2.0*M(MXSP+39)                   DIS18700
                                                                   DIS18710
S(2) =     M(6)   +     M(41)  + 2.0*M(42)  +     M(47)  +        DIS18720
.          M(54)  +     M(61)  +     M(70)  +     M(78)  +        DIS18730
.          M(83)  + 2.0*M(84)  +     M(103) +     M(109) +        DIS18740
.          M(115) +     M(116) +     M(119) +     M(124) +        DIS18750
.          M(133) +     M(141) +     M(142) +     M(152) +        DIS18760
.          M(157) +     M(162) +     M(186) + 2.0*M(187) +        DIS18770
.          M(194) + 2.0*M(195) +     M(224) +     M(299) +        DIS18775
.          M(MXSP+33)                                            DIS18780

S(5) = S(5)       +                                              DIS19010
.       2.0*M(129) + 3.0*M(130) + 4.0*M(131) +     M(137) +     DIS19020
.           M(148) + 2.0*M(149) + 3.0*M(150) + 4.0*M(151) +     DIS19030
.           M(153) +     M(158) + 2.0*M(159) + 3.0*M(160) +     DIS19040
.       4.0*M(161) +     M(181) +     M(200) +     M(225) +     DIS19050
.           M(281) + 2.0*M(282) +     M(297) + 2.0*M(298) +     DIS19055
.           M(MXSP+32)                                          DIS19060
                                                                DIS19070
```

If the species added will complex with either carbonate or bicarbonate then it must be included in the carbonate summation according to how much carbon it contributes. For the cadmium complexes being considered only $CdHCO_3^+$ and $CdCO_3$ would contribute to the CO_2 summation. The original code fragment from Kharaka and others (1988) would be changed as follows:

```
SCO2 =     M(7)   +     M(51)  +     M(52)  +     M(55)  +        DIS19400
.          M(56)  +     M(97)  +     M(98)  +     M(114) +        DIS19410
.          M(120) +     M(121) +     M(132) +     M(138) +        DIS19420
.          M(139) +     M(140) +     M(155) +     M(156) +        DIS19430
.          M(207) + 2.0*M(208) + 3.0*M(209) +     M(288) +        DIS19440
.          M(292) +     M(300) +     M(303) +                     DIS19450
.          M(MXSP+34) + M(MXSP+39)                               DIS19460
```

The non-carbonate species which contribute to the measured alkalinity must be subtracted from the measured alkalinity to calculate the amount of inorganic carbon present. Of the cadmium species considered only $Cd(OH)^+$ and $Cd(OH)_2$ could contribute to an alkalinity titration. The subroutine DISTRB would be modified as follows to account for the presence of these two species:

```
   ANALCO = ANALCO      -                                                    DIS19710
.           2.0*M(265) -      M(266) -      M(269) -      M(289) -          DIS19720
.              M(293) - 2.0*M(294) -      M(295) - 2.0*M(296) -             DIS19730
.              M(301) - 2.0*M(302)                                          DIS19735
```

In addition, the subroutine PRINTR also needs to be modified,

```
 SUM2 = M(7)  + M(52)  + M(56)  + M(121) +   M(132) +   M(139)     PRI 1800
.             + M(156) + M(300) + M(MXSP+34)                      PRI 1810
 SUM3 = M(98) + M(51)  + M(55)  + M(114) +   M(120) +   M(138)     PRI 1820
.             + M(140) + M(155) + M(207) + 2*M(208) + 3*M(209)     PRI 1830
              + M(303) + M(MXSP+39)                               PRI 1840

 ALK7 = ALK7        +                                              PRI 2100
.        2.0*M(265) +     M(266) +     M(269) +     M(289) +      PRI 2110
.            M(293) + 2.0*M(294) +     M(295) +     M(296) ±      PRI 2120
.            M(301) + 2.0*M(302)                                  PRI 2125
```

Finally, the added complexes must be accounted for in the hydrogen and hydroxide summations. Sources of hydrogen must be added to the hydrogen summation in accordance to their stoichiometry. Sinks for hydrogen must be added to the hydroxide summation in accordance to the stoichiometery of the complex. In the case of cadmium, the molality of $CdHCO_3^+$ would be added to the hydrogen balance and the molality of $CdOH^+$ and twice the molality of $Cd(OH)_2$ would be added to the hydroxide balance. SOLMIN88 would be modified as follows:

```
 HTOT  = HTOT   +                                                     DIS22900
.          M(145) +                    M(156) +     M(182) +         DIS22910
.      2.0*M(183) + 3.0*M(184) + 4.0*M(185) +     M(202) +         DIS22920
.      2.0*M(203) + 2.0*M(204) + 4.0*M(205) + 6.0*M(206) +         DIS22930
.          M(213) + 2.0*M(214) + 3.0*M(215) + 4.0*M(216) +         DIS22940
.          M(217) +     M(228) +     M(247) + 2.0*M(248) +         DIS22950
.          M(266) + 2.0*M(267) + 2.0*M(286) + 3.0*M(287) +         DIS22960
.      2.0*M(290) + 3.0*M(291) +     M(292) +     M(295) +         DIS22970
.          M(300) +     M(MXSP+34)          +     M(MXSP+40)       DIS22980

 OHTOT = OHTOT  +                                                    DIS23060
.      2.0*M(171) + 3.0*M(172) + 4.0*M(173) + 5.0*M(174) +         DIS23070
.     15.0*M(188) +     M(189) + 2.0*M(190) + 2.0*M(191) +         DIS23080
.      5.0*M(192) + 7.0*M(193) +     M(220) + 2.0*M(221) +         DIS23090
.      3.0*M(222) +     M(223) +     M(289) +     M(293) +         DIS23100
.      2.0*M(294) +     M(295) +     M(301) + 2.0*M(302) +         DIS23110
.          M(MXSP+35)                                              DIS23115
```

(vi) Finishing Touches

After the geochemistry is programed, the subroutines INPUT, STORE, and the program SOLINPUT must be modified. The first step is to decide where in the input file the concentration of the added cation component will be located. Examination of table 1 shows line 7 can hold one more minor species, line 8 can hold four more trace species, and line 9 can hold three more organic species. If the cation is a major species, it will either have to be added to line 7 or line 8 or another line can be added to the input file to accommodate it. If several components are to be added then another line will have to be added to the input file. For this example cadmium will be added to line 7 after silver. To do this, subroutine INPUT would be modified as follows:

```
      DATA ILP /3, 4, 22, 1, 2, 18, 14, 12, 5, 6, 33, 7, 98, 30, 29,     INP 1900
     .          136, 32, 31, 26, 15, 25, 27, 16, 23, 21, 13, 269, 28,    INP 1910
     .          169, 210, 48, 246, 265, 285/                             INP 1920

      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 21, 27)           INP 2860
      WRITE (UNO, 9080) 'Pb      ', 'Zn      ', 'Cu      ', 'Mn      ',  INP 2870
     .                  'Hg      ', 'Ag      ', 'Cd      '               INP 2880
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 21, 27)                     INP 2890
      IPGLN = IPGLN + 2                                                  INP 2900
                                                                         INP 2910
      LINE = LINE + 1                                                    INP 2920
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 28, 30)           INP 2930
      WRITE (UNO, 9080) 'As      ', 'U       ', 'V       '               INP 2940
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 28, 30)                     INP 2950
      IPGLN = IPGLN + 2                                                  INP 2960
                                                                         INP 2970
      LINE = LINE + 1                                                    INP 2980
      READ (UNI, 9070, ERR = 150) (CUNITS(ILP(I)), I = 31, 34)           INP 2990
      WRITE (UNO, 9080) 'Acetate ', 'Oxalate ', 'Succinate', 'CH4'       INP 3000
      WRITE (UNO, 9050) (CUNITS(ILP(I)), I = 31, 34)                     INP 3010
      IPGLN = IPGLN + 2                                                  INP 3020
```

Subroutine STORE would have these changes:

```
      DATA PTR /3, 4, 22, 1, 2, 18, 14, 12, 5, 6, 33, 7, 98, 30, 29,     STO 1740
     &          136, 32, 31, 26, 15, 25, 27, 16, 23, 21, 13, 269, 28,    STO 1750
     &          169, 210, 48, 246, 265, 285/                             STO 1760

      WRITE (UN, 9080) (ANALM(PTR(I)), I = 21, 27)                       STO 2020
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 28, 30)                       STO 2030
      WRITE (UN, 9080) (ANALM(PTR(I)), I = 31, 34)                       STO 2040
```

SOLINPUT currently can accept two more components before any variables need to be redimensioned. If more than two components are added, then the size of the variable CUNITS will have to be increased in size throughout the program. The subroutine READFL, STORE, LINE## (where ## corresponds to the number of the line on which the component is to be added) and the menu subroutine MAJORS or MINORS if the component is non-organic.

To modify subroutine LINE##, the name of the component must be added to the variable HOLD and the index limits on the DO loops must be changed in that subroutine and the following subroutines which contain

concentrations. The corresponding changes for cadmium from above would be to modify subroutine LINE07 as follows:

```
      DATA HOLD /'Pb', 'Zn', 'Cu', 'Mn', 'Hg', 'Ag', 'Cd'/                L07 0220
                                                                          L07 0230
C ========================================================================|L07 0240
                                                                          L07 0250
      CALL CLEAR (SCREEN)                                                 L07 0260
                                                                          L07 0270
      DO 10 I = 21, 27                                                    L07 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-20),               L07 0290

      DO 10 I = 28, 30                                                    L08 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-27),               L08 0290

      DO 10 I = 31, 34                                                    L09 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-30),               L09 0290
```

The subroutine MINORS would have the menu line changed as follows:

```
      PRINT OPTION, '2)  ENTER: Pb, Zn, Cu, Mn, Hg, Ag, Cd'               MIN 0290
```

Subroutine READFL would need to have the indexing updated in the read statements.

```
      READ (UN, 9080) (CUNITS(I,SAMP), I = 21, 27)                        REA 1100
      READ (UN, 9080) (CUNITS(I,SAMP), I = 28, 30)                        REA 1110
      READ (UN, 9080) (CUNITS(I,SAMP), I = 31, 34)                        REA 1120
```

Finally, subroutine STORE would also need to have the indexing updated in the write statements.

```
        WRITE (UN, 9080) (CUNITS(I,L), I = 21, 27)                        STO 1250
        WRITE (UN, 9080) (CUNITS(I,L), I = 28, 30)                        STO 1260
        WRITE (UN, 9080) (CUNITS(I,L), I = 31, 34)                        STO 1270
```

APPENDIX III. Programming Notes: Adding an Anion.

The procedure for adding an anion component is essentially the same as adding a cation component. Bromine with three complexes will be used as an example for this section.

(i) Define the component to be added

This is the same as section (i) of Appendix II. The entry for bromine would be as follows:

```
304 Br -      -1 3.5    79.904
```

(ii) Define the complexes which will form with the component

This section is the same as section (ii) of Appendix II. If bromine forms complexes with H^+, Na^+, and Ca^{++} then the following data would be entered into section 1 of DATA.TBL:

```
305 HBr         0 0.0    80.912
306 NaBr        0 0.0   102.894
307 CaBr2       0 0.0   199.888
```

MXSP would be changed to 307.

(ii) Define equations for each complex

The dissociation reactions for bromine are:

$$HBr \rightleftarrows H^+ + Br^- \qquad \text{(AIII.1)}$$

$$NaBr \rightleftarrows Na^+ + Br^- \qquad \text{(AIII.2)}$$

$$CaBr_2 \rightleftarrows Ca^{++} + 2Br^- \qquad \text{(AIII.3)}$$

The mass action equations for bromine are:

$$K_{HBr} = \frac{(a_{H^+})\ (a_{Br^-})}{a_{HBr}} \qquad \text{(AIII.4)}$$

$$K_{NaBr} = \frac{(a_{Na^+})\ (a_{Br^-})}{a_{NaBr}} \qquad \text{(AIII.5)}$$

$$K_{CaBr_2} = \frac{(a_{Ca}{}^{++})\ (a_{Br}{}^{-})^2}{a_{CaCl_2}} \qquad \text{(AIII.6)}$$

The equilibrium constants for the dissociation reactions of bromine would be placed in section 2 of DATA.TBL and the variable MXAQK would be changed to 277.

	0/200	25/250	50/300	75/350	100	125	150
275 HBr	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
276 NaBr	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			
277 CaBr2	999.99	999.99	999.99	999.99	999.99	999.99	999.99
	999.99	999.99	999.99	999.99			

(iv) Write the mass balance equations

A mass balance equation must be written for the complex or complexes the anion forms with hydrogen. In the case of bromine the equation would be

$$m_{Br,t} = m_{Br}{}^{-} + m_{HBr} \qquad \text{(AIII.7)}$$

In addition, the cation complexes of the anion must be added to the mass balance equations for each cation. Solving the mass action equations (AIII.4-6) for the molality of the complexes using equation (AII.3) gives the following equations:

$$m_{HBr}{}^{+} = \frac{(m_{H}{}^{+}\ \gamma_{H}{}^{+})\ (m_{Br}{}^{-}\ \gamma_{Br}{}^{-})}{(K_{HBr}{}^{+})\ (\gamma_{HBr}{}^{+})} \qquad \text{(AIII.8)}$$

$$m_{NaBr} = \frac{(m_{Na}{}^{+}\ \gamma_{Na}{}^{+})\ (m_{Br}{}^{-}\ \gamma_{Br}{}^{-})}{(K_{NaBr})\ (\gamma_{NaBr})} \qquad \text{(AIII.9)}$$

$$m_{CaBr_2} = \frac{(m_{Ca}{}^{++}\ \gamma_{Ca}{}^{++})\ (m_{Br}^{2}{}^{-}\ \gamma_{Br}^{2}{}^{-})}{(K_{CaCl_2})\ (\gamma_{CaCl_2})} \qquad \text{(AIII.10)}$$

Combing equation (AIII.7) with equation (AIII.8) and solving for $m_{Br}{}^{-}$ gives

$$m_{Br}{}^{-} = \frac{m_{Br,\,t}}{1 + ((\gamma_{Br}{}^{-}\ a_{H}{}^{+}) / (K_{HBr}\ \gamma_{HBr}))} \qquad \text{(AIII.11)}$$

(v) Begin coding

The solution of equation (AIII.11) would be coded as follows:

```
C ------------------------------------------------------------------|
C     Bromide species                                               |
C ------------------                                               |

      IF (EXELT(37) .GT. CPUMIN) THEN
        M(304)     = TITR(12) / (1.0D0 + ((GAMMA(304) * ALFA(8)) /
                                 (KT1(275) * GAMMA(305))))
        ALFA(304)  = M(304) * GAMMA(304)

        M(305)     = (ALFA(304) * ALFA(8)) / (KT1(275) * GAMMA(305))
        ALFA(305)  = M(305) * GAMMA(305)
      END IF
```

This code fragment may be placed anywhere between line DIS 2950 and line DIS 6130. The variable EXELT will need to be redimensioned throughout the code, in this case to EXELT(37). In addition, the variable TITR will need to be redimensioned throughout the code, in this case from TITR(11) to TITR(12). The statements,

EXELT(37) = ANALM(304)
TITR(12) = EXELT(37)

will have to be added to the code to correctly initialize EXELT and TITR in the following places: ADS 6738 and 6855, CAL 2105 and 2225, MIX 5268 and 5385, MIX 7678 and 7785, MIX 8228 and 8345.

If complexes with hydrogen are not included or do not exist then the initial molality of the species needs to be initialized instead. The above code fragment would be replaced with

```
C ------------------------------------------------------------------|
C     Bromide species                                               |
C ------------------                                               |


      IF (EXELT(37) .GT. CPUMIN) THEN
        M(304)     = TITR(12)
      ' ALFA(304)  = M(304) * GAMMA(304)
      END IF
```

The anion must be included in the mass balance equation for each cation with which it is coupled. For NaBr equation (AIII.9) and $CaBr_2$ (AIII.10) would be coded as

```
        M(307) = ALFA(304)**2 / (KT1(277) * GAMMA(307))                  DIS 6665
        M(MXSP+ 6) = ALFA(MXSP+ 1) / (KT1(MXAQK+ 5) * GAMMA(MXSP+ 6))   DIS 6670
        M(MXSP+21) = ALFA(MXSP+16) / (KT1(MXAQK+19) * GAMMA(MXSP+21))   DIS 6680
                                                                         DIS 6690
        M(1) = EXELT(1) / (1.0D0 + GAMMA(1) * (M(55) + M(56) + M(57) +   DIS 6700
     .         M(58) + M(59) + M(60) + M(61) + M(231) + M(252) +        DIS 6710
     .         M(271) + M(281) + M(282) + M(307) + M(MXSP+6) +          DIS 6720
```

```
          M(MXSP+21)))                                                    DIS 6725


      M(307)          = M(307) * ALFA(1)                                  DIS 7002
      ALFA(307)       = M(307) * GAMMA(307)                               DIS 7004
```

and

```
      M(306) = ALFA(304) / (KT1(277) * GAMMA(306)                         DIS 8155
      M(MXSP+12) = ALFA(MXSP+ 1) / (KT1(MXAQK+11) * GAMMA(MXSP+12))       DIS 8160
      M(MXSP+27) = ALFA(MXSP+16) / (KT1(MXAQK+25) * GAMMA(MXSP+27))       DIS 8170
                                                                          DIS 8180
      M(3)     = EXELT(3) / (1.0D0 + GAMMA(3) * (M(137) + M(138) +        DIS 8190
     .             M(139) + 2.0D0*M(140) + 2.0D0*M(141)   + M(142) +      DIS 8200
     .             M(143) + M(144) + M(145) + M(237) + M(261) +           DIS 8210
     .             M(277) + M(306) + M(MXSP+12) + M(MXSP+27)))            DIS 8220

      M(306)          = M(306) * ALFA(3)                                  DIS 8425
      ALFA(306)       = M(306) * GAMMA(306)                               DIS 8427
```

Next the mass balance of the added anion must be computed. This is the sum of all the species which contain that anion. The variable S must be redimensioned in subroutine DISTRB, in this case from 11 to 12. The following line of code (for bromine) is then added starting at line DIS19390

```
      S(12) = M(304) + M(305) + M(306) + 2.0*M(307)                       DIS19395
```

If the anion added would affect the alkalinity titration, as in the case of organic ligands, then the appropriate complexes would need to be included in the alkalinity calculation. (See the discussion in Appendix II, section v). In this case bromine and its complexes will not affect the alkalinity.

Next the iteration test for the anion must be determined. A complete discussion can be found in Kharaka and others, 1988 (Iteration Techniques). Two more variables will need to be redimensioned to the new number of anions, DIFF and FACTOR. The code for bromine would start at line DIS22340 as follows:

```
      IF (EXELT(37) .GE. CPUMIN) THEN
        X = (S(12) - EXELT(37)) / EXELT(37)
        CROSS = .FALSE.
        IF ((X * DIFF(12)) .LT. 0.0)  CROSS = .TRUE.
        DIFF(12) = X
        IF (DABS(DIFF(12)) .GE. CONV1) DONE = .FALSE.
        IF (DONE) THEN
            FACTOR(12) = 1.0
        ELSE IF (ITER .GT. 7) THEN
          X = EXELT(37) / S(12)
          CALL AITLIM (FACTOR(12), X, CROSS)
        END IF
        X = FACTOR(12)
        IF (S(12) .GT. CPUMIN) THEN
          TITR(12) = TITR(12) - (X * (1.0 - (EXELT(37) / S(12))) *
          TITR(12))
```

```
    ELSE
      TITR(12) = EXELT(37)
    END IF
  END IF
```

Finally, the added complexes must be added to the hydrogen and hydroxide summations. For this example only HBr would contribute and would be added to HTOT as was shown in Appendix II.

(vi) Finishing Touches

The changes required for the input are completely analogous to those detailed in Appendix II.

APPENDIX IV. Listing of SOLINPUT

```
      PROGRAM SOLINP                                                    SOL 0010
C ================================================================== |SOL 0020
C     Writen by:                                                      |SOL 0030
C                     J.D. DeBraal (U.S. Geological Survey) 6/1/89    |SOL 0040
C                                                                     |SOL 0050
C     This program creates and modifies input files for SOLMINEQ.88   |SOL 0060
C     with up to MAX samples per file.  This program uses file unit   |SOL 0070
C     UN and assumes CPUMIN is the smallest double precision number   |SOL 0080
C     the computer can represent.  It also assumes the terminal screen|SOL 0090
C     is SCREEN vertical lines.  These parameters should be altered   |SOL 0100
C     to fit the computing environment.  Otherwise, the code should be|SOL 0110
C     completely portable to any machine using an ANSI standard       |SOL 0120
C     conforming FORTRAN-77 compiler.                                 |SOL 0130
C ------------------------------------------------------------------ |SOL 0140
C     Declare variables                                               |SOL 0150
C ---------------------                                               |SOL 0160
C     ACTLEN    INT   The actual length of a string variable          |SOL 0170
C     ACTUAL    INT   Used as a pointer to reference the added ions   |SOL 0180
C     ADEX      INT   Flag for surface chemistry option               |SOL 0190
C     ALK       INT   Flag for distribution of carbonate species      |SOL 0200
C     AMOL      DBL   Molality of aqueous/mineral species added       |SOL 0210
C     ANHOLD    CHA   Names of the anions used with the added cations |SOL 0220
C     ANS       CHA   Returned answer from a program control prompt   |SOL 0230
C     ANSR      INT   Number of complexes used for the added ions     |SOL 0240
C     ANSWR     CHA   Temporary test for character input              |SOL 0250
C     CEC       DBL   Cation exchange capacity                        |SOL 0260
C     CHOICE    INT   Menu selection and pointer                      |SOL 0270
C     COEF      DBL   Stoichiometric coefficient and ID number        |SOL 0280
C     CONC      DBL   Analytical concentration of the added ions      |SOL 0290
C     CONV1     DBL   Tolerance factor for convergence of anions      |SOL 0300
C     CONV2     DBL   Tolerance factor for hydronium mass-balance     |SOL 0310
C     CPUMIN    DBL   Smallest real number the program will recognize |SOL 0320
C     CUNITS    DBL   Analytical input concentration                  |SOL 0330
C     DA        DBL   Temporary variable used to figure out DHA       |SOL 0340
C     DCH4      DBL   Concentration of CH4 lost before pH measurment  |SOL 0350
C     DCO2      DBL   Concentration of CO2 lost before pH measurment  |SOL 0360
C     DH2S      DBL   Concentration of H2S lost before pH measurment  |SOL 0370
C     DNH3      DBL   Concentration of NH3 lost before pH measurment  |SOL 0380
C     DEFALT    INT   Return value                                    |SOL 0390
C     DENS      DBL   Density                                         |SOL 0400
C     DFRAC1    DBL   Smallest fraction of soln 1 mixed with soln 2   |SOL 0410
C     DHA       DBL   Ion size parameter                              |SOL 0420
C     DNA       DBL   Temporary ion size parameter for added ions     |SOL 0430
C     DP        DBL   Dissolution/precipitation switch                |SOL 0440
C     DSEP      DBL   Density of oil at 15 degrees C                  |SOL 0450
C     EHM       DBL   Measured Eh in volts                            |SOL 0460
C     EHMC      DBL   Measured Eh using the Calomel electrode         |SOL 0470
C     EMFZSC    DBL   Measured Eh using the Zobell's solution         |SOL 0480
C     FBOIL     DBL   Fraction of solution boiled-off as steam        |SOL 0490
C     FCCSAT    DBL   Tolerance factor for pH and CO2 options         |SOL 0500
C     FIXIT     DBL   Fixing value in the CO2 option                  |SOL 0510
C     FLAGS     INT   Selection flags for calculation of redox equil. |SOL 0520
```

```
C     FLNAME    CHA   Name of the input file                                  |SOL 0530
C     GEOTH     INT   Flag to select geothermometer                           |SOL 0540
C     GFW       DBL   Gram formula weight of aqueous species                  |SOL 0550
C     HERE      LOG   Determines if the file to be opened exists              |SOL 0560
C     HIGHKT    DBL   Temp variable to read the high log K value              |SOL 0570
C     HITEMP    DBL   In-situ temperature                                     |SOL 0580
C     HOLD      CHA   Names of the cations used with the added anions         |SOL 0590
C     I         INT   Loop and counting variable                              |SOL 0600
C     IBMIX     INT   Switch for mixing option                                |SOL 0610
C     ICCSAT    INT   Switch for pH option                                    |SOL 0620
C     IDDP      INT   Id number of the mineral to be dissolved/ppt            |SOL 0630
C     IDMIX     INT   Id number of the aqueous species to be added            |SOL 0640
C     IDN       INT   Id numbers of the ISCOMP components adsorption          |SOL 0650
C     IDSAT     INT   Id number of the mineral to be equilibrated             |SOL 0660
C     ILQ       INT   Charge of the complexes in the added ions               |SOL 0670
C     IMCO3     INT   Selects CO2 option                                      |SOL 0680
C     INC       DBL   Increment of solution 1 to be added                     |SOL 0690
C     INDEX     INT   Read in index number of the added ions                  |SOL 0700
C     INFORM    INT   Flag to print all the log K values in data base         |SOL 0710
C     INMIX     INT   Total number of mixtures of two solution mixed          |SOL 0720
C     INSP      INT   Total number of surface sites for adsorption            |SOL 0730
C     IPIT      INT   Flag to use pitzer activity coefficients                |SOL 0740
C     IPRIN1    INT   Flag for printing iteration of anions                   |SOL 0750
C     IPRIN2    INT   Flag for printing hydronium balance                     |SOL 0760
C     IRXDP     INT   Id number of the aqueous species to be added            |SOL 0770
C     ISCHG     INT   Charge of each surface site for adsorption              |SOL 0780
C     ISCOMP    INT   Total number of components in dissociation              |SOL 0790
C     ITIC      INT   Hitemp distribution of carbonate species                |SOL 0800
C     ITMIX     INT   Switch for the mineral saturation option                |SOL 0810
C     ITT       INT   Number of aqueous species to add/sub with water         |SOL 0820
C     J         INT   Loop and counting variable                              |SOL 0830
C     KCH4OL    DBL   Henry's law coefficient for CH4 in oil                  |SOL 0840
C     KCO2OL    DBL   Henry's law coefficient for CO2 in oil                  |SOL 0850
C     KH2SOL    DBL   Henry's law coefficient for H2S in oil                  |SOL 0860
C     KRXN      DBL   K for dissociation reaction of surface species          |SOL 0870
C     L         INT   Loop variable used to represent sample number           |SOL 0880
C     LCHAR     CHA   Single character used to test boundary conditions       |SOL 0890
C     LEN       INT   Length of a character variable                          |SOL 0900
C     LOWKT     DBL   Read in value of low log K                              |SOL 0910
C     MAX       INT   The maximum number of samples a file can have           |SOL 0920
C     MAXSAM    INT   The number of samples in the file curently              |SOL 0930
C     MBASE     DBL   Mole fraction of each surface species                   |SOL 0940
C     MINAME    CHA   Name of the added minerals                              |SOL 0950
C     MINCO     DBL   Stoichiometric coefficient for added minerals           |SOL 0960
C     MININD    INT   Index number of the added mineral                       |SOL 0970
C     MINLOG    DBL   Log K values for added minerals                         |SOL 0980
C     MIXFLE    CHA   Name of the mixing file                                 |SOL 0990
C     NAME      CHA   Read in name of the added ion                           |SOL 1000
C     NANS      CHA   Input varible to prevent a crash                        |SOL 1010
C     ND        INT   Index value of the added ion complexes                  |SOL 1020
C     NDUM      INT   Id of mineral/aqueous complex with K(T) changed         |SOL 1030
C     NL        INT   Number of blank lines to print for screen formats       |SOL 1040
C     NLINES    INT   Formal argument for number of lines                     |SOL 1050
C     NUFLAG    INT   Sets the activity coefficients of neutral species       |SOL 1060
```

```
C     NUM       INT   Flag used to point to one of the added ions       |SOL 1070
C     NUMINS    INT   Number of minerals defined in input file          |SOL 1080
C     ODUM      CHA   Switch to indicate a mineral/aqueous comples      |SOL 1090
C     OPTION    CHA   Formating variable                                |SOL 1100
C     OUTIN     CHA   Name of restart file                              |SOL 1110
C     PAGE      CHA   Name of the added ions                            |SOL 1120
C     PH        DBL   Measured pH of the solution                       |SOL 1130
C     PRESS     DBL   Total pressure                                    |SOL 1140
C     RATIO     INT   Flag for printing activity ratios of elements     |SOL 1150
C     REDION    CHA   Names of the redox ions                           |SOL 1160
C     RXDP      DBL   Molal amount of the aqueous species added         |SOL 1170
C     SAMP      INT   Current sample number                             |SOL 1180
C     SAREA     DBL   Total surface area per kilogram of solvent        |SOL 1190
C     SCREEN    INT   Number of printable lines on the screen           |SOL 1200
C     SPN       CHA   Name of each surface species adsorption           |SOL 1210
C     STRING    CHA   Used to calculate the length of a string          |SOL 1220
C     TAREA     DBL   Site density per unit area adsorption             |SOL 1230
C     TCH4M     DBL   Moles CH4 distributed bewteen oil, water, vapor   |SOL 1240
C     TCO2M     DBL   Moles CO2 distributed between oil, water, vapor   |SOL 1250
C     TH2SM     DBL   Moles H2S distributed between oil, water, vapor   |SOL 1260
C     TEMP      DBL   Temperature of the solution when pH was measured  |SOL 1270
C     TIC       DBL   Concentration of total inorganic carbon           |SOL 1280
C     TITLE     CHA   Name of the sample                                |SOL 1290
C     TMPVAL    INT   Value used to protect real value for wrong input  |SOL 1300
C     TNUM      CHA   Sample number converted to a character            |SOL 1310
C     UN        INT   The file unit of the input file                   |SOL 1320
C     UNITS     CHA   Units of concentration                            |SOL 1330
C     USING     CHA   Formating variable                                |SOL 1340
C     USING1    CHA   Formating variable                                |SOL 1350
C     WROIL     DBL   Oil to water weight ratio                         |SOL 1360
C     WRTFLE    INT   Determines if the file has been edited            |SOL 1370
C     XD        DBL   Holds Log K's for additional anions & cations     |SOL 1380
C     XDUM      DBL   New log K(T) value                                |SOL 1390
C     Z         INT   Charge of aqueous species                         |SOL 1400
C     ZCOM      INT   Calculated charge for the added ions              |SOL 1410
C ---------------------------------------------------------------------|SOL 1420
                                                                        SOL 1430
      INTEGER MAX, SCREEN                                               SOL 1440
      PARAMETER (MAX = 10, SCREEN = 24)                                 SOL 1450
                                                                        SOL 1460
      INTEGER ALK(MAX), ANSR(3,MAX), CHOICE, FLAGS(6,MAX), GEOTH(MAX)   SOL 1470
      INTEGER IBMIX(MAX), ICCSAT(MAX), IDDP(MAX), IDMIX(50,MAX)         SOL 1480
      INTEGER IDN(10,10,MAX), IDSAT(MAX), IMCO3(MAX)                    SOL 1490
      INTEGER INFORM(MAX), INMIX(MAX), INSP(MAX), IPIT(MAX)             SOL 1500
      INTEGER IPRIN1(MAX), IPRIN2(MAX), IRXDP(10,MAX), ISCHG(10,MAX)    SOL 1510
      INTEGER ISCOMP(10,MAX), ITIC(MAX), ITMIX(MAX), ITT(MAX), MAXSAM   SOL 1520
      INTEGER MININD(10,5,MAX), ND(2,45,MAX), NDUM(12,MAX), NL          SOL 1530
      INTEGER NUFLAG(MAX), RATIO(MAX), SAMP, WRTFLE, Z(3,MAX)           SOL 1540
                                                                        SOL 1550
      CHARACTER *  1 ADEX(MAX), ANS, ODUM(12,MAX)                       SOL 1560
      CHARACTER *  5 UNITS(MAX)                                         SOL 1570
      CHARACTER *  8 PAGE(45,MAX), MINAME(5,MAX)                        SOL 1580
      CHARACTER * 10 SPN(10,MAX)                                        SOL 1590
      CHARACTER * 80 FLNAME, MIXFLE(MAX), OUTIN(MAX), TITLE(MAX)        SOL 1600
```

```
                                                                      SOL 1610
      DOUBLE PRECISION AMOL(50,MAX), CEC(MAX), COEF(10,10,MAX)        SOL 1620
      DOUBLE PRECISION CONC(3,MAX), CONV1(MAX), CONV2(MAX)            SOL 1630
      DOUBLE PRECISION CUNITS(35,MAX), DCH4(MAX), DCO2(MAX)           SOL 1640
      DOUBLE PRECISION DENS(MAX), DFRAC1(MAX), DH2S(MAX)              SOL 1650
      DOUBLE PRECISION DHA(3,MAX), DNA(45,MAX), DNH3(MAX), DP(MAX)    SOL 1660
      DOUBLE PRECISION EHM(MAX), EHMC(MAX), EMFZSC(MAX), FBOIL(MAX)   SOL 1670
      DOUBLE PRECISION FCCSAT(MAX), FIXIT(MAX), GFW(3,MAX), HITEMP(MAX) SOL 1680
      DOUBLE PRECISION INC(MAX), KCH4OL(MAX), KCO2OL(MAX), KH2SOL(MAX) SOL 1690
      DOUBLE PRECISION KRXN(10,MAX), MBASE(10,MAX), MINCO(10,5,MAX)   SOL 1700
      DOUBLE PRECISION MINLOG(2,5,MAX), PH(MAX), DSEP(MAX), PRESS(MAX) SOL 1710
      DOUBLE PRECISION RXDP(10,MAX), SAREA(MAX), TAREA(MAX), TCH4M(MAX) SOL 1720
      DOUBLE PRECISION TCO2M(MAX), TEMP(MAX), TH2SM(MAX), TIC(MAX)    SOL 1730
      DOUBLE PRECISION WROIL(MAX), XD(2,45,MAX), XDUM(12,MAX)         SOL 1740
                                                                      SOL 1750
      EXTERNAL CLEAR, OPTION, EXIT, INIT, MAMENU, NSAMP, PSAMP        SOL 1760
      EXTERNAL READFL, STORE                                          SOL 1770
                                                                      SOL 1780
      COMMON           SAMP                                           SOL 1790
      COMMON /COM1  / TITLE, UNITS, FLNAME                            SOL 1800
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                       SOL 1810
      COMMON /COM3  / PH, EHM, EHMC, EMFZSC                           SOL 1820
      COMMON /COM4  / CUNITS, TIC                                     SOL 1830
      COMMON /COM5  / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2           SOL 1840
      COMMON /COM6  / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,   SOL 1850
     &                FCCSAT                                         SOL 1860
      COMMON /COM7  / TCO2M, TCH4M, TH2SM, WROIL,                     SOL 1870
     &                KCO2OL, KCH4OL, KH2SOL, DSEP                   SOL 1880
      COMMON /COM8  / ADEX, SPN                                       SOL 1890
      COMMON /COM9  / CEC, TAREA, SAREA, INSP, ISCHG, MBASE, KRXN,    SOL 1900
     &                ISCOMP, COEF, IDN                              SOL 1910
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,      SOL 1920
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL   SOL 1930
      COMMON /COM11 / ODUM                                            SOL 1940
      COMMON /COM12 / NDUM, XDUM                                      SOL 1950
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2            SOL 1960
      COMMON /COM14 / FLAGS                                           SOL 1970
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                         SOL 1980
      COMMON /COM16 / PAGE                                            SOL 1990
      COMMON /COM17 / ND, XD, DNA                                     SOL 2000
      COMMON /COM18 / MINAME                                          SOL 2010
      COMMON /COM19 / MINCO, MININD, MINLOG                           SOL 2020
      COMMON /COM20 / MIXFLE, OUTIN                                   SOL 2030
                                                                      SOL 2040
C ======================================================================|SOL 2050
C     Main program.  Sets up variables, controls files, and samples     |SOL 2060
C ----------------------------------------------------------------------|SOL 2070
                                                                      SOL 2080
      CALL CLEAR (SCREEN)                                             SOL 2090
                                                                      SOL 2100
      PRINT '(18X, A)', 'SOLMINEQ_88  Input Data File Creation Program' SOL 2110
      PRINT *                                                         SOL 2120
                                                                      SOL 2130
      CALL INIT (MAXSAM, WRTFLE)                                      SOL 2140
```

```
   NL = 0                                                                SOL 2150
                                                                         SOL 2160
10 CONTINUE                                                              SOL 2170
   CALL CLEAR (NL)                                                       SOL 2180
   CALL MAMENU (CHOICE)                                                  SOL 2190
                                                                         SOL 2200
   IF      (CHOICE .EQ. 1) THEN                                          SOL 2210
     CALL OPTION                                                         SOL 2220
     WRTFLE = 0                                                          SOL 2230
   ELSE IF (CHOICE .EQ. 2) THEN                                          SOL 2240
     IF (WRTFLE .NE. 1) THEN                                             SOL 2250
       PRINT *, 'Existing data will be destroyed.'                       SOL 2260
       PRINT *, 'Do you wish to continue [<CR> = No] ?'                  SOL 2270
       ANS = 'N'                                                         SOL 2280
                                                                         SOL 2290
       READ '(A1)', ANS                                                  SOL 2300
                                                                         SOL 2310
       IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                          SOL 2320
         CALL INIT (MAXSAM, WRTFLE)                                      SOL 2330
         CALL READFL (MAXSAM)                                            SOL 2340
       END IF                                                            SOL 2350
     ELSE                                                                SOL 2360
       CALL READFL (MAXSAM)                                              SOL 2370
     END IF                                                              SOL 2380
   ELSE IF (CHOICE .EQ. 3) THEN                                          SOL 2390
     CALL NSAMP (MAXSAM)                                                 SOL 2400
   ELSE IF (CHOICE .EQ. 4) THEN                                          SOL 2410
     CALL PSAMP                                                          SOL 2420
   ELSE IF (CHOICE .EQ. 5) THEN                                          SOL 2430
     CALL STORE (MAXSAM, WRTFLE)                                         SOL 2440
   ELSE IF (CHOICE .EQ. 6) THEN                                          SOL 2450
     IF (WRTFLE .NE. 1) THEN                                             SOL 2460
       PRINT *, 'You are quitting the program without saving your',      SOL 2470
  &             ' file!'                                                 SOL 2480
       PRINT *, 'Do you wish to save your file [<CR> = Y] ? '            SOL 2490
                                                                         SOL 2500
       ANS = 'Y'                                                         SOL 2510
       READ '(A1)', ANS                                                  SOL 2520
                                                                         SOL 2530
       IF (ANS .NE. 'N' .AND. ANS .NE. 'n') THEN                         SOL 2540
         NL = SCREEN - 22                                                SOL 2550
         GOTO 10                                                         SOL 2560
       END IF                                                            SOL 2570
     END IF                                                              SOL 2580
     GOTO 20                                                             SOL 2590
   END IF                                                                SOL 2600
                                                                         SOL 2610
   NL = SCREEN - 22                                                      SOL 2620
   GOTO 10                                                               SOL 2630
                                                                         SOL 2640
20 CONTINUE                                                              SOL 2650
                                                                         SOL 2660
   END                                                                   SOL 2670
```

```
      SUBROUTINE ACTIVE (NUFLAG, IPIT)                                  ACT 0010
C ================================================================== |ACT 0020
C     This routine determines which method will be used to calculate   |ACT 0030
C     the activity coefficients of the aqueous species.                |ACT 0040
C ------------------------------------------------------------------ |ACT 0050
                                                                        ACT 0060
      INTEGER MAX, SCREEN                                               ACT 0070
      CHARACTER * 15 USING                                              ACT 0080
      PARAMETER (MAX = 10, SCREEN = 24, USING = '(1X, A, I2, A)')       ACT 0090
                                                                        ACT 0100
      INTEGER NL, NUFLAG(MAX), IPIT(MAX), SAMP, TMPVAL                  ACT 0110
                                                                        ACT 0120
      CHARACTER * 1 ANS                                                 ACT 0130
                                                                        ACT 0140
      EXTERNAL CLEAR, IANSWR                                            ACT 0150
                                                                        ACT 0160
      COMMON           SAMP                                             ACT 0170
                                                                        ACT 0180
C ================================================================== |ACT 0190
                                                                        ACT 0200
      NL = SCREEN                                                       ACT 0210
                                                                        ACT 0220
   10 CONTINUE                                                          ACT 0230
                                                                        ACT 0240
      CALL CLEAR (NL)                                                   ACT 0250
      PRINT *, 'Do you want to set the activity coefficient of neutral',ACT 0260
     &         ' species:'                                              ACT 0270
      PRINT *, '     0)  Equal to the activity coefficient of ',        ACT 0280
     &         'aqueous CO2 ?'                                          ACT 0290
      PRINT *, '     1)  Equal to unity ?'                              ACT 0300
      PRINT USING, '          [Current = ', NUFLAG(SAMP), '] '          ACT 0310
                                                                        ACT 0320
      TMPVAL = NUFLAG(SAMP)                                             ACT 0330
      CALL IANSWR (NUFLAG(SAMP))                                        ACT 0340
                                                                        ACT 0350
      IF (NUFLAG(SAMP) .LT. 0 .OR. NUFLAG(SAMP) .GT. 1) THEN            ACT 0360
        PRINT *, 'Answer must be in the range [0-1] '                    ACT 0370
        NUFLAG(SAMP) = TMPVAL                                           ACT 0380
        NL = SCREEN - 6                                                 ACT 0390
        GOTO 10                                                         ACT 0400
      END IF                                                            ACT 0410
                                                                        ACT 0420
   20 CONTINUE                                                          ACT 0430
      PRINT *                                                           ACT 0440
      PRINT *, 'Do you wish to use Pitzer''s equations? (Y/N)'           ACT 0450
      IF      (IPIT(SAMP) .EQ. 0) THEN                                  ACT 0460
        PRINT USING, '     [Current =  N] '                             ACT 0470
      ELSE IF (IPIT(SAMP) .EQ. 1) THEN                                  ACT 0480
        PRINT USING, '     [Current =  Y] '                             ACT 0490
      END IF                                                            ACT 0500
                                                                        ACT 0510
      READ '(A)', ANS                                                   ACT 0520
                                                                        ACT 0530
      IF (ANS .NE. ' ') THEN                                            ACT 0540
```

```
      IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                    ACT 0550
        IPIT(SAMP) = 1                                                 ACT 0560
      ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                    ACT 0570
        IPIT(SAMP) = 0                                                 ACT 0580
      ELSE                                                             ACT 0590
        PRINT *, 'Answer must be in [Y, y, N, n] '                     ACT 0600
        NL = SCREEN - 5                                                ACT 0610
        CALL CLEAR (NL)                                                ACT 0620
        GOTO 20                                                        ACT 0630
      END IF                                                           ACT 0640
    END IF                                                             ACT 0650
                                                                       ACT 0660
    RETURN                                                             ACT 0670
    END                                                                ACT 0680
```

```
      SUBROUTINE ANSWER (DEFALT)                                       ANS 0010
C ======================================================================|ANS 0020
C     Determines if a double precision answer is valid                 |ANS 0030
C ----------------------------------------------------------------------|ANS 0040
                                                                       ANS 0050
      INTEGER ACTLEN                                                   ANS 0060
                                                                       ANS 0070
      CHARACTER * 20 NANS                                              ANS 0080
                                                                       ANS 0090
      DOUBLE PRECISION DEFALT, TMPVAL                                  ANS 0100
                                                                       ANS 0110
      EXTERNAL UPCASE                                                  ANS 0120
                                                                       ANS 0130
C ======================================================================|ANS 0140
                                                                       ANS 0150
      TMPVAL = DEFALT                                                  ANS 0160
   10 CONTINUE                                                         ANS 0170
      NANS = ' '                                                       ANS 0180
      READ '(A20)', NANS                                               ANS 0190
                                                                       ANS 0200
      IF (NANS .NE. ' ') THEN                                          ANS 0210
        ACTLEN = 20                                                    ANS 0220
        CALL UPCASE (NANS, ACTLEN)                                     ANS 0230
        READ (NANS, *, ERR = 100) DEFALT                               ANS 0240
      END IF                                                           ANS 0250
                                                                       ANS 0260
      RETURN                                                           ANS 0270
                                                                       ANS 0280
  100 CONTINUE                                                         ANS 0290
      PRINT *, 'ERROR!  Invalid entry try again.'                      ANS 0300
      DEFALT = TMPVAL                                                  ANS 0310
      GOTO 10                                                          ANS 0320
                                                                       ANS 0330
      END                                                              ANS 0340
```

```
      SUBROUTINE BASIC                                                    BAS 0010
C ================================================================================|BAS 0020
C     Displays basic option menu and directs choice to proper sub          |BAS 0030
C --------------------------------------------------------------------------|BAS 0040
                                                                           BAS 0050
      INTEGER MAX, SCREEN                                                  BAS 0060
      CHARACTER * 10 OPTION                                                BAS 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)               BAS 0080
                                                                           BAS 0090
      INTEGER CHOICE, NL, SAMP                                             BAS 0100
                                                                           BAS 0110
      CHARACTER *  5 UNITS(MAX)                                            BAS 0120
      CHARACTER * 80 FLNAME, TITLE(MAX)                                    BAS 0130
                                                                           BAS 0140
      DOUBLE PRECISION CUNITS(35, MAX), DENS(MAX), EHM(MAX), EHMC(MAX)     BAS 0150
      DOUBLE PRECISION EMFZSC(MAX), HITEMP(MAX), PH(MAX), PRESS(MAX)       BAS 0160
      DOUBLE PRECISION TEMP(MAX), TIC(MAX)                                 BAS 0170
                                                                           BAS 0180
      EXTERNAL CLEAR, IANSWR, LINE01, LINE02, LINE03, LINE09               BAS 0190
      EXTERNAL MAJORS, MINORS                                              BAS 0200
                                                                           BAS 0210
      COMMON           SAMP                                                BAS 0220
      COMMON /COM1  / TITLE, UNITS, FLNAME                                 BAS 0230
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                            BAS 0240
      COMMON /COM3  / PH, EHM, EHMC, EMFZSC                                BAS 0250
      COMMON /COM4  / CUNITS, TIC                                          BAS 0260
                                                                           BAS 0270
C ================================================================================|BAS 0280
                                                                           BAS 0290
      NL = SCREEN                                                          BAS 0300
      CHOICE = 0                                                           BAS 0310
                                                                           BAS 0320
   10 CONTINUE                                                             BAS 0330
      CALL CLEAR (NL)                                                      BAS 0340
                                                                           BAS 0350
      PRINT OPTION, '    BASIC PARAMETERS MENU'                            BAS 0360
      PRINT *                                                              BAS 0370
      PRINT OPTION, '1)  Enter Title and Units'                            BAS 0380
      PRINT *                                                              BAS 0390
      PRINT OPTION, '2)  Enter Temperatures, Density, and Pressure'        BAS 0400
      PRINT *                                                              BAS 0410
      PRINT OPTION, '3)  Enter pH, and Eh'                                 BAS 0420
      PRINT *                                                              BAS 0430
      PRINT OPTION, '4)  Enter Concentrations for Major Species'           BAS 0440
      PRINT *                                                              BAS 0450
      PRINT OPTION, '5)  Enter Concentrations for Minor Species'           BAS 0460
      PRINT *                                                              BAS 0470
      PRINT OPTION, '6)  Enter Concentrations for Organic Species'         BAS 0480
      PRINT *                                                              BAS 0490
      PRINT OPTION, '7)  Return to Options Menu'                           BAS 0500
      PRINT *                                                              BAS 0510
      PRINT *                                                              BAS 0520
      PRINT OPTION, '    Enter Choice (1-7) '                              BAS 0530
                                                                           BAS 0540
```

```
      CALL IANSWR (CHOICE)                                                  BAS 0550
                                                                            BAS 0560
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 7) THEN                            BAS 0570
        PRINT *, 'Answer must be in the range [1-7] '                       BAS 0580
        NL = SCREEN - 20                                                    BAS 0590
        CHOICE = 0                                                          BAS 0600
        GOTO 10                                                             BAS 0610
      END IF                                                                BAS 0620
                                                                            BAS 0630
      IF      (CHOICE .EQ. 1) THEN                                          BAS 0640
        CALL LINE01                                                         BAS 0650
      ELSE IF (CHOICE .EQ. 2) THEN                                          BAS 0660
        CALL LINE02                                                         BAS 0670
      ELSE IF (CHOICE .EQ. 3) THEN                                          BAS 0680
        CALL LINE03                                                         BAS 0690
      ELSE IF (CHOICE .EQ. 4) THEN                                          BAS 0700
        CALL MAJORS                                                         BAS 0710
      ELSE IF (CHOICE .EQ. 5) THEN                                          BAS 0720
        CALL MINORS                                                         BAS 0730
      ELSE IF (CHOICE .EQ. 6) THEN                                          BAS 0740
        CALL LINE09                                                         BAS 0750
      ELSE IF (CHOICE .EQ. 7) THEN                                          BAS 0760
        RETURN                                                              BAS 0770
      END IF                                                                BAS 0780
                                                                            BAS 0790
      NL = SCREEN - 19                                                      BAS 0800
      CHOICE = 0                                                            BAS 0810
      GOTO 10                                                               BAS 0820
                                                                            BAS 0830
      END                                                                   BAS 0840
```

```
      SUBROUTINE BOILIT                                                     BOI 0010
C ====================================================================|BOI 0020
C     Gets input for the boiling option.                              |BOI 0030
C --------------------------------------------------------------------|BOI 0040
                                                                            BOI 0050
      INTEGER MAX, SCREEN                                                   BOI 0060
      CHARACTER * 10 OPTION                                                 BOI 0070
      DOUBLE PRECISION CPUMIN                                               BOI 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10)                                BOI 0090
      PARAMETER (OPTION = '(10X, A)', SCREEN = 24)                          BOI 0100
                                                                            BOI 0110
      INTEGER I, IBMIX(MAX), IDDP(MAX), IDMIX(50,MAX)                       BOI 0120
      INTEGER IDSAT(MAX), INMIX(MAX), IRXDP(10,MAX), ITMIX(MAX)             BOI 0130
      INTEGER ITT(MAX), SAMP                                                BOI 0140
                                                                            BOI 0150
      CHARACTER * 80 MIXFLE(MAX), OUTIN(MAX)                                BOI 0160
                                                                            BOI 0170
      DOUBLE PRECISION AMOL(50,MAX), DFRAC1(MAX), DP(MAX), FBOIL(MAX)       BOI 0180
      DOUBLE PRECISION INC(MAX), RXDP(10,MAX), TMPVAL                       BOI 0190
```

```
                                                                      BOI 0200
      EXTERNAL ANSWER, CLEAR                                          BOI 0210
                                                                      BOI 0220
      INTRINSIC DABS                                                  BOI 0230
                                                                      BOI 0240
      COMMON           SAMP                                           BOI 0250
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,      BOI 0260
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL   BOI 0270
      COMMON /COM20 / MIXFLE, OUTIN                                   BOI 0280
                                                                      BOI 0290
C ======================================================================|BOI 0300
                                                                      BOI 0310
      CALL CLEAR (SCREEN)                                             BOI 0320
                                                                      BOI 0330
C ----------------------------------------------------------------------|BOI 0340
C     Reset other option based on these variables                      |BOI 0350
C ----------------------------------------------------------------------|BOI 0360
                                                                      BOI 0370
      IBMIX(SAMP)  = 3                                                BOI 0380
      ITMIX(SAMP)  = 0                                                BOI 0390
      IDDP(SAMP)   = 0                                                BOI 0400
      IDSAT(SAMP)  = 0                                                BOI 0410
      ITT(SAMP)    = 0                                                BOI 0420
      DP(SAMP)     = 0.0                                              BOI 0430
      INMIX(SAMP)  = 0                                                BOI 0440
      DFRAC1(SAMP) = 0.0                                              BOI 0450
      INC(SAMP)    = 0.0                                              BOI 0460
      MIXFLE(SAMP) = ' '                                              BOI 0470
                                                                      BOI 0480
      DO 60 I = 1, 10                                                 BOI 0490
        RXDP (I,SAMP) = 0.0                                           BOI 0500
        IRXDP(I,SAMP) = 0                                             BOI 0510
   60 CONTINUE                                                        BOI 0520
                                                                      BOI 0530
      DO 70 I = 1, 50                                                 BOI 0540
        IDMIX(I,SAMP) = 0                                             BOI 0550
        AMOL(I,SAMP)  = 0.0                                           BOI 0560
   70 CONTINUE                                                        BOI 0570
                                                                      BOI 0580
   80 CONTINUE                                                        BOI 0590
                                                                      BOI 0600
      PRINT *, 'Fraction of the solution to be boiled-off as steam ?' BOI 0610
      PRINT '(35X, A, E10.4, A)', ' [Current = ', FBOIL(SAMP), '] '   BOI 0620
      TMPVAL = FBOIL(SAMP)                                            BOI 0630
      CALL ANSWER (FBOIL(SAMP))                                       BOI 0640
                                                                      BOI 0650
      IF (FBOIL(SAMP) .GT. 9.9D-1) THEN                               BOI 0660
        PRINT *                                                       BOI 0670
        PRINT *, 'Value must be cannot be greater than 0.99.'         BOI 0680
        PRINT *                                                       BOI 0690
        FBOIL(SAMP) = TMPVAL                                          BOI 0700
        GOTO 80                                                       BOI 0710
      END IF                                                          BOI 0720
                                                                      BOI 0730
```

```
      IF (DABS(FBOIL(SAMP)) .LE. CPUMIN) THEN                          BOI 0740
        IBMIX(SAMP) = 0                                                BOI 0750
      END IF                                                           BOI 0760
                                                                       BOI 0770
      RETURN                                                           BOI 0780
      END                                                              BOI 0790



      SUBROUTINE CATION                                                CAT 0010
C ==========================================================================|CAT 0020
C     Selects complexes for the additional cation                        |CAT 0030
C --------------------------------------------------------------------------|CAT 0040
                                                                       CAT 0050
      INTEGER MAX, SCREEN                                              CAT 0060
      CHARACTER * 10 OPTION                                            CAT 0070
      DOUBLE PRECISION CPUMIN                                          CAT 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, OPTION = '(10X, A)')      CAT 0090
      PARAMETER (SCREEN = 24)                                          CAT 0100
                                                                       CAT 0110
      INTEGER ACTLEN, ACTUAL, ANSR(3,MAX), CHOICE, I, ILQ(11), L       CAT 0120
      INTEGER LENGTH, ND(2,45,MAX), NL, SAMP, Z(3,MAX), ZCOM           CAT 0130
                                                                       CAT 0140
      CHARACTER *  4 HOLD(11)                                          CAT 0150
      CHARACTER *  8 PAGE(45,MAX)                                      CAT 0160
                                                                       CAT 0170
      DOUBLE PRECISION CONC(3,MAX), DA, DENS(MAX), DHA(3,MAX)          CAT 0180
      DOUBLE PRECISION DNA(45,MAX), GFW(3,MAX), HITEMP(MAX)            CAT 0190
      DOUBLE PRECISION PRESS(MAX), TEMP(MAX), XD(2,45,MAX)             CAT 0200
                                                                       CAT 0210
      EXTERNAL ANSWER, CLEAR, IANSWR, LENGTH                           CAT 0220
                                                                       CAT 0230
      INTRINSIC DABS, IABS                                             CAT 0240
                                                                       CAT 0250
      COMMON           SAMP                                            CAT 0260
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                        CAT 0270
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                          CAT 0280
      COMMON /COM16 / PAGE                                             CAT 0290
      COMMON /COM17 / ND, XD, DNA                                      CAT 0300
                                                                       CAT 0310
      DATA HOLD /'Cl', 'SO4', 'HCO3', 'OH', 'PO4', 'F',                CAT 0320
     &          'Ace', 'CO3', 'HS', 'Oxy', 'Suc'/                      CAT 0330
      DATA ILQ  /-1, -2, -1, -1, -3, -1, -1, -2, -1, -2, -2/           CAT 0340
                                                                       CAT 0350
C ==========================================================================|CAT 0360
                                                                       CAT 0370
      NL = SCREEN                                                      CAT 0380
      CHOICE = -1                                                      CAT 0390
                                                                       CAT 0400
   10 CONTINUE                                                         CAT 0410
      CALL CLEAR (NL)                                                  CAT 0420
                                                                       CAT 0430
```

```
      PRINT *, 'Enter the number of the complex or a 0 to return'
      PRINT *
      PRINT OPTION, '1)  Cl-              8)  CO3=    '
      PRINT OPTION, '2)  SO4=             9)  HS-     '
      PRINT OPTION, '3)  HCO3-           10)  C2O4=   '
      PRINT OPTION, '4)  OH-             11)  C4H4O4=-'
      PRINT OPTION, '5)  PO4-3           12)  Anion1  '
      PRINT OPTION, '6)  F-              13)  Anion2  '
      PRINT OPTION, '7)  CH3COO-                      '
      PRINT *

      CALL IANSWR (CHOICE)

      IF (CHOICE .LT. 0 .OR. CHOICE .GT. 13) THEN
        PRINT *, 'Answer must be in the range [0-13] '
        CHOICE = -1
        NL = SCREEN - 12
        GOTO 10
      END IF

      ACTUAL = 31 + CHOICE

      IF (CHOICE .GT. 0 .AND. CHOICE .LT. 14) THEN

        ACTLEN = 8
        L = LENGTH (PAGE(31,SAMP), ACTLEN)

        IF (CHOICE .LE. 11) THEN
          PAGE(ACTUAL,SAMP) = PAGE(31,SAMP)(1:L) // HOLD(CHOICE)
          ZCOM = Z(3,SAMP) + ILQ(CHOICE)
        ELSE IF (CHOICE .EQ. 12) THEN
          PAGE(ACTUAL,SAMP) = PAGE(31,SAMP)(1:L) // PAGE(1,SAMP)
          ZCOM = Z(3,SAMP) + Z(1,SAMP)
        ELSE IF (CHOICE .EQ. 13) THEN
          PAGE(ACTUAL,SAMP) = PAGE(31,SAMP)(1:L) // PAGE(16,SAMP)
          ZCOM = Z(3,SAMP) + Z(2,SAMP)
        END IF

        IF (IABS(ZCOM) .EQ. 0) DA =  0.0
        IF (IABS(ZCOM) .EQ. 1) DA =  4.5
        IF (IABS(ZCOM) .EQ. 2) DA =  5.4
        IF (IABS(ZCOM) .EQ. 3) DA =  9.0
        IF (IABS(ZCOM) .GE. 4) DA = 12.0

        IF (IABS(ZCOM) .GT. 0) THEN
          PRINT *, 'What is the Debye-Huckel A of the complex ?'
          IF (DNA(ACTUAL,SAMP) .LT. CPUMIN) THEN
            PRINT '(10X, A, F6.2, A)', '[Current = ', DA, '] '
          ELSE
            PRINT '(10X, A, F6.2, A)', '[Current = ', DNA(ACTUAL,SAMP),
     &                                 '] '
          END IF

          CALL ANSWER (DNA(ACTUAL,SAMP))
```

```
                                                                      CAT 0980
      IF (DNA(ACTUAL,SAMP) .LT. CPUMIN) DNA(ACTUAL,SAMP) = DA         CAT 0990
    END IF                                                            CAT 1000
                                                                      CAT 1010
    PRINT *                                                           CAT 1020
    PRINT '(1X, A, A, A, F6.2, A)', 'What is the log k of ',          CAT 1030
&          PAGE(ACTUAL,SAMP), ' at ', TEMP(SAMP), ' ?'              CAT 1040
    PRINT '(10X, A, F6.2, A)', '[Current = ', XD(1,ACTUAL,SAMP),      CAT 1050
&                              '] '                                   CAT 1060
    CALL ANSWER (XD(1,ACTUAL,SAMP))                                   CAT 1070
                                                                      CAT 1080
    IF (DABS(XD(1,ACTUAL,SAMP)) .GT. CPUMIN) THEN                     CAT 1090
      ND(1,ACTUAL,SAMP) = CHOICE + 1                                  CAT 1100
    ELSE                                                              CAT 1110
      ND(1,ACTUAL,SAMP) = 0                                           CAT 1120
    END IF                                                            CAT 1130
                                                                      CAT 1140
    IF (HITEMP(SAMP) .GT. CPUMIN) THEN                                CAT 1150
      PRINT '(1X,A,A,A,F6.2,A)', 'What is the log k of ',             CAT 1160
&           PAGE(ACTUAL,SAMP), ' at ', HITEMP(SAMP), ' ?'           CAT 1170
      PRINT '(10X, A, F6.2, A)', '[Current = ', XD(2,ACTUAL,SAMP),    CAT 1180
&                              '] '                                   CAT 1190
      CALL ANSWER (XD(2,ACTUAL,SAMP))                                 CAT 1200
                                                                      CAT 1210
      IF (DABS(XD(2,ACTUAL,SAMP)) .GT. CPUMIN) THEN                   CAT 1220
        ND(2,ACTUAL,SAMP) = CHOICE + 1                                CAT 1230
      ELSE                                                            CAT 1240
        ND(2,ACTUAL,SAMP) = 0                                         CAT 1250
      END IF                                                          CAT 1260
                                                                      CAT 1270
    END IF                                                            CAT 1280
  END IF                                                              CAT 1290
                                                                      CAT 1300
  IF (CHOICE .NE. 0) THEN                                             CAT 1310
    NL = SCREEN - 11                                                  CAT 1320
    GOTO 10                                                           CAT 1330
  END IF                                                              CAT 1340
                                                                      CAT 1350
  ANSR(3,SAMP) = 0                                                    CAT 1360
                                                                      CAT 1370
  DO 20 I = 32, 44                                                    CAT 1380
    IF      (ND(1,I,SAMP) .GT. 0) THEN                                CAT 1390
      ANSR(3,SAMP) = ANSR(3,SAMP) + 1                                 CAT 1400
    ELSE IF (ND(2,I,SAMP) .GT. 0) THEN                                CAT 1410
      ANSR(3,SAMP) = ANSR(3,SAMP) + 1                                 CAT 1420
    END IF                                                            CAT 1430
20 CONTINUE                                                           CAT 1440
                                                                      CAT 1450
  RETURN                                                              CAT 1460
  END                                                                 CAT 1470
```

```
      SUBROUTINE CLEAR (NLINES)                                          CLE 0010
C ================================================================|CLE 0020
C     Print NLINES blank lines to clear the screen                |CLE 0030
C ----------------------------------------------------------------|CLE 0040
                                                                         CLE 0050
      INTEGER I, NLINES                                                  CLE 0060
                                                                         CLE 0070
C ================================================================|CLE 0080
                                                                         CLE 0090
      DO 10  I = 1, NLINES                                               CLE 0100
        PRINT *                                                          CLE 0110
   10 CONTINUE                                                           CLE 0120
                                                                         CLE 0130
      RETURN                                                             CLE 0140
      END                                                                CLE 0150
```

```
      SUBROUTINE COMPLX (NUM)                                            COM 0010
C ================================================================|COM 0020
C     Selects complexes for the additional anions                 |COM 0030
C ----------------------------------------------------------------|COM 0040
                                                                         COM 0050
      INTEGER MAX, SCREEN                                                COM 0060
      CHARACTER * 10 OPTION                                              COM 0070
      DOUBLE PRECISION CPUMIN                                            COM 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, OPTION = '(10X, A)')        COM 0090
      PARAMETER (SCREEN = 24)                                            COM 0100
                                                                         COM 0110
      INTEGER ACTUAL, ANSR(3,MAX), CHOICE, I, ILQ(14)                    COM 0120
      INTEGER ND(2,45,MAX), NL, NUM, SAMP, Z(3,MAX), ZCOM                COM 0130
                                                                         COM 0140
      CHARACTER *  2 HOLD(14)                                            COM 0150
      CHARACTER *  8 PAGE(45,MAX)                                        COM 0160
                                                                         COM 0170
      DOUBLE PRECISION CONC(3,MAX), DA, DENS(MAX), DHA(3,MAX)            COM 0180
      DOUBLE PRECISION DNA(45,MAX), GFW(3,MAX), HITEMP(MAX)              COM 0190
      DOUBLE PRECISION PRESS(MAX), TEMP(MAX), XD(2,45,MAX)               COM 0200
                                                                         COM 0210
      EXTERNAL ANSWER, CLEAR, IANSWR                                     COM 0220
                                                                         COM 0230
      INTRINSIC DABS, IABS                                               COM 0240
                                                                         COM 0250
      COMMON           SAMP                                              COM 0260
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                          COM 0270
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                            COM 0280
      COMMON /COM16 / PAGE                                               COM 0290
      COMMON /COM17 / ND, XD, DNA                                        COM 0300
                                                                         COM 0310
      DATA HOLD /' H', 'H2', 'Al', 'Ba', 'Ca', 'Cu', 'Fe', ' K', 'Mg',   COM 0320
     &          'Mn', 'Na', 'Pb', 'Sr', 'Zn'/                            COM 0330
      DATA ILQ  /1, 2, 3, 2, 2, 1, 2, 1, 2, 2, 1, 2, 2, 2/              COM 0340
```

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C ================================================================|COM 0360
                                                                  COM 0370
      NL = SCREEN                                                 COM 0380
      CHOICE = -1                                                 COM 0390
                                                                  COM 0400
   10 CONTINUE                                                    COM 0410
      CALL CLEAR (NL)                                             COM 0420
                                                                  COM 0430
      PRINT *, 'Enter the number of the complex or a 0 to return' COM 0440
      PRINT *                                                     COM 0450
      PRINT OPTION, '1)   H+              8)   K+ '               COM 0460
      PRINT OPTION, '2)  2H+              9)  Mg++'               COM 0470
      PRINT OPTION, '3)  Al+3            10)  Mn++'               COM 0480
      PRINT OPTION, '4)  Ba++            11)  Na+ '               COM 0490
      PRINT OPTION, '5)  Ca++            12)  Pb++'               COM 0500
      PRINT OPTION, '6)  Cu+             13)  Sr++'               COM 0510
      PRINT OPTION, '7)  Fe++            14)  Zn++'               COM 0520
      PRINT *                                                     COM 0530
                                                                  COM 0540
      CALL IANSWR (CHOICE)                                        COM 0550
                                                                  COM 0560
      IF (CHOICE .LT. 0 .OR. CHOICE .GT. 14) THEN                 COM 0570
        PRINT *                                                   COM 0580
        PRINT *, 'Answer must be in the range [0-14] '             COM 0590
        NL = SCREEN - 12                                          COM 0600
        CHOICE = -1                                               COM 0610
        GOTO 10                                                   COM 0620
      END IF                                                      COM 0630
                                                                  COM 0640
      ACTUAL = NUM + CHOICE                                       COM 0650
                                                                  COM 0660
      IF (CHOICE .GT. 0 .AND. CHOICE .LT. 15) THEN                COM 0670
        PAGE(ACTUAL,SAMP) = HOLD(CHOICE) // PAGE(NUM,SAMP)        COM 0680
                                                                  COM 0690
        IF (NUM .EQ. 1) THEN                                      COM 0700
          ZCOM = Z(1,SAMP) + ILQ(CHOICE)                          COM 0710
        ELSE                                                      COM 0720
          ZCOM = Z(2,SAMP) + ILQ(CHOICE)                          COM 0730
        END IF                                                    COM 0740
                                                                  COM 0750
        IF (IABS(ZCOM) .EQ. 0) DA =  0.0                          COM 0760
        IF (IABS(ZCOM) .EQ. 1) DA =  4.5                          COM 0770
        IF (IABS(ZCOM) .EQ. 2) DA =  5.4                          COM 0780
        IF (IABS(ZCOM) .EQ. 3) DA =  9.0                          COM 0790
        IF (IABS(ZCOM) .GE. 4) DA = 12.0                          COM 0800
                                                                  COM 0810
        IF (IABS(ZCOM) .GT. 0) THEN                               COM 0820
          PRINT *, 'What is the Debye-Huckel A of the complex ?'  COM 0830
          IF (DNA(ACTUAL,SAMP) .LT. CPUMIN) THEN                  COM 0840
            PRINT '(10X, A, F6.2, A)', '[Current = ', DA, '] '    COM 0850
          ELSE                                                    COM 0860
            PRINT '(10X, A, F6.2, A)', '[Current = ', DNA(ACTUAL,SAMP), COM 0870
     &                                 '] '                       COM 0880
```

```
      END IF                                                              COM 0890
                                                                          COM 0900
      CALL ANSWER (DNA(ACTUAL,SAMP))                                      COM 0910
                                                                          COM 0920
      IF (DNA(ACTUAL,SAMP) .LT. CPUMIN) DNA(ACTUAL,SAMP) = DA             COM 0930
    END IF                                                                COM 0940
                                                                          COM 0950
    PRINT *                                                               COM 0960
    PRINT '(1X, A, A, A, F6.2, A)', 'What is the log k of ',              COM 0970
&          PAGE(ACTUAL,SAMP), ' at ', TEMP(SAMP), ' ?'                    COM 0980
    PRINT '(10X, A, F6.2, A)', '[Current = ', XD(1,ACTUAL,SAMP),          COM 0990
&                              '] '                                       COM 1000
                                                                          COM 1010
    CALL ANSWER (XD(1,ACTUAL,SAMP))                                       COM 1020
                                                                          COM 1030
    IF (DABS(XD(1,ACTUAL,SAMP)) .GT. CPUMIN) THEN                         COM 1040
      ND(1,ACTUAL,SAMP) = CHOICE + 1                                      COM 1050
    ELSE                                                                  COM 1060
      ND(1,ACTUAL,SAMP) = 0                                               COM 1070
    END IF                                                                COM 1080
                                                                          COM 1090
    IF (HITEMP(SAMP) .GT. CPUMIN) THEN                                    COM 1100
      PRINT '(1X,A,A,A,F6.2,A)', 'What is the log k of ',                 COM 1110
&            PAGE(ACTUAL,SAMP), ' at ', HITEMP(SAMP), ' ?'                COM 1120
      PRINT '(10X, A, F6.2, A)', '[Current = ', XD(2,ACTUAL,SAMP),        COM 1130
&                              '] '                                       COM 1140
                                                                          COM 1150
      CALL ANSWER (XD(2,ACTUAL,SAMP))                                     COM 1160
                                                                          COM 1170
      IF (DABS(XD(2,ACTUAL,SAMP)) .GT. CPUMIN) THEN                       COM 1180
        ND(2,ACTUAL,SAMP) = CHOICE + 1                                    COM 1190
      ELSE                                                                COM 1200
        ND(2,ACTUAL,SAMP) = 0                                             COM 1210
      END IF                                                              COM 1220
                                                                          COM 1230
    END IF                                                                COM 1240
  END IF                                                                  COM 1250
                                                                          COM 1260
  IF (CHOICE .NE. 0) THEN                                                 COM 1270
    NL = SCREEN - 11                                                      COM 1280
    GOTO 10                                                               COM 1290
  END IF                                                                  COM 1300
                                                                          COM 1310
  ANSR(1,SAMP) = 0                                                        COM 1320
  ANSR(2,SAMP) = 0                                                        COM 1330
                                                                          COM 1340
  DO 20 I = 2, 15                                                         COM 1350
    IF      (ND(1,I,SAMP) .GT. 0) THEN                                    COM 1360
      ANSR(1,SAMP) = ANSR(1,SAMP) + 1                                     COM 1370
    ELSE IF (ND(2,I,SAMP) .GT. 0) THEN                                    COM 1380
      ANSR(1,SAMP) = ANSR(1,SAMP) + 1                                     COM 1390
    END IF                                                                COM 1400
                                                                          COM 1410
    IF      (ND(1,I+15,SAMP) .GT. 0) THEN                                 COM 1420
```

```
          ANSR(2,SAMP) = ANSR(2,SAMP) + 1                                COM 1430
        ELSE IF (ND(2,I+15,SAMP) .GT. 0) THEN                            COM 1440
          ANSR(2,SAMP) = ANSR(2,SAMP) + 1                                COM 1450
        END IF                                                           COM 1460
   20 CONTINUE                                                           COM 1470
                                                                         COM 1480
      RETURN                                                             COM 1490
      END                                                                COM 1500




      SUBROUTINE DSLPPT                                                  DSL 0010
C ================================================================      |DSL 0020
C     Selects values for the dissolution/precipitation option          |DSL 0030
C ----------------------------------------------------------------      |DSL 0040
                                                                         DSL 0050
      INTEGER MAX, SCREEN                                                DSL 0060
      CHARACTER * 15 OPTION, USING                                       DSL 0070
      DOUBLE PRECISION CPUMIN                                            DSL 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, OPTION = '(10X, A, A)')     DSL 0090
      PARAMETER (SCREEN = 24, USING = '(15X, A, I4, A)')                 DSL 0100
                                                                         DSL 0110
      INTEGER CHOICE, I, IBMIX(MAX), IDDP(MAX)                           DSL 0120
      INTEGER IDMIX(50,MAX), IDSAT(MAX), INMIX(MAX)                      DSL 0130
      INTEGER IRXDP(10,MAX), ITMIX(MAX), ITT(MAX), NL, SAMP, TMPVAL      DSL 0140
                                                                         DSL 0150
      CHARACTER * 80 MIXFLE(MAX), OUTIN(MAX)                             DSL 0160
                                                                         DSL 0170
      DOUBLE PRECISION AMOL(50,MAX), DFRAC1(MAX), DP(MAX), FBOIL(MAX)    DSL 0180
      DOUBLE PRECISION INC(MAX), RXDP(10,MAX)                            DSL 0190
                                                                         DSL 0200
      EXTERNAL ANSWER, CLEAR, IANSWR                                     DSL 0210
                                                                         DSL 0220
      COMMON           SAMP                                              DSL 0230
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,         DSL 0240
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL      DSL 0250
      COMMON /COM20 / MIXFLE, OUTIN                                      DSL 0260
                                                                         DSL 0270
C ================================================================      |DSL 0280
                                                                         DSL 0290
      INMIX(SAMP)  = 0                                                   DSL 0300
      DFRAC1(SAMP) = 0.0                                                 DSL 0310
      INC(SAMP)    = 0.0                                                 DSL 0320
      FBOIL(SAMP)  = 0.0                                                 DSL 0330
      MIXFLE(SAMP) = ' '                                                 DSL 0340
      NL = SCREEN                                                        DSL 0350
                                                                         DSL 0360
  100 CONTINUE                                                           DSL 0370
      CALL CLEAR (NL)                                                    DSL 0380
                                                                         DSL 0390
      IF      (ITMIX(SAMP) .LT. 0) THEN                                  DSL 0400
        CHOICE = 2                                                       DSL 0410
```

```
 ELSE IF (ITMIX(SAMP) .GT. 0) THEN                                    DSL 0420
   CHOICE = 5                                                         DSL 0430
 ELSE                                                                 DSL 0440
   IF      (IDSAT(SAMP) .EQ. IDDP(SAMP) .AND.                         DSL 0450
&           IDSAT(SAMP) .NE. 0) THEN                                  DSL 0460
     CHOICE = 1                                                       DSL 0470
   ELSE IF (IDSAT(SAMP) .NE. IDDP(SAMP) .AND.                         DSL 0480
&           IDDP(SAMP)  .NE. 0) THEN                                  DSL 0490
     CHOICE = 3                                                       DSL 0500
   ELSE IF (IDSAT(SAMP) .NE. IDDP(SAMP) .AND.                         DSL 0510
&           IDDP(SAMP)  .EQ. 0) THEN                                  DSL 0520
     CHOICE = 4                                                       DSL 0530
   ELSE                                                               DSL 0540
     IBMIX(SAMP) = 0                                                  DSL 0550
     CHOICE = 6                                                       DSL 0560
   END IF                                                             DSL 0570
 END IF                                                               DSL 0580
                                                                      DSL 0590
 PRINT OPTION, '    DISSOLUTION / PRECIPITATION MENU'                 DSL 0600
 PRINT *                                                              DSL 0610
 PRINT OPTION, '1)  Dissolve/Precipitate a mineral to saturation'     DSL 0620
 PRINT *                                                              DSL 0630
 PRINT OPTION, '2)  Dissolve/Precipitate a specific mineral',         DSL 0640
&              ' amount'                                             DSL 0650
 PRINT *                                                              DSL 0660
 PRINT OPTION, '3)  Equilibrate solution with a mineral from',        DSL 0670
&              ' the dissolution/'                                   DSL 0680
 PRINT OPTION, '    precipitation of another mineral'                 DSL 0690
 PRINT *                                                              DSL 0700
 PRINT OPTION, '4)  Equilibrate solution with a mineral by',          DSL 0710
&              ' titrating'                                          DSL 0720
 PRINT OPTION, '    aqueous species'                                  DSL 0730
 PRINT *                                                              DSL 0740
 PRINT OPTION, '5)  Add/Subtract a specific amount of aqueous',       DSL 0750
&              ' species'                                            DSL 0760
 PRINT *                                                              DSL 0770
 PRINT OPTION, '6)  Return to Mass Transfer Menu'                     DSL 0780
 PRINT *                                                              DSL 0790
 PRINT *                                                              DSL 0800
 PRINT OPTION, '    Enter Choice (1-6) '                              DSL 0810
 PRINT *                                                              DSL 0820
 PRINT '(14X, A, I2, A)', '[Current = ', CHOICE, '] '                 DSL 0830
                                                                      DSL 0840
 CALL IANSWR (CHOICE)                                                 DSL 0850
                                                                      DSL 0860
 IF (CHOICE .LT. 1 .OR. CHOICE .GT. 6) THEN                           DSL 0870
   PRINT *, 'Answer must be in the range [1-6] '                       DSL 0880
   NL = SCREEN - 22                                                   DSL 0890
   GOTO 100                                                           DSL 0900
 END IF                                                               DSL 0910
                                                                      DSL 0920
 IF      (CHOICE .EQ. 1) THEN                                         DSL 0930
   IBMIX(SAMP) = 1                                                    DSL 0940
   ITMIX(SAMP) = 0                                                    DSL 0950
```

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      CALL CLEAR (SCREEN - 3)                                          DSL 0960
      PRINT *, 'ID number of the mineral to be saturated'              DSL 0970
      PRINT USING, '[Current = ', IDSAT(SAMP), '] '                    DSL 0980
      CALL IANSWR (IDSAT(SAMP))                                        DSL 0990
      IDDP(SAMP) = IDSAT(SAMP)                                         DSL 1000
    ELSE IF (CHOICE .EQ. 2) THEN                                       DSL 1010
      IBMIX(SAMP) = 1                                                  DSL 1020
      ITMIX(SAMP) = -1                                                 DSL 1030
      CALL CLEAR (SCREEN - 3)                                          DSL 1040
      PRINT *, 'ID number of the mineral'                              DSL 1050
      PRINT USING, '[Current = ', IDDP(SAMP), '] '                     DSL 1060
      CALL IANSWR (IDDP(SAMP))                                         DSL 1070
      PRINT *                                                          DSL 1080
                                                                       DSL 1090
      PRINT *, 'Moles/Kg of H2O of the mineral species'                DSL 1100
      PRINT '(15X,A,1P,E10.4,A)', '[Current = ', AMOL(1,SAMP), '] '    DSL 1110
      CALL ANSWER (AMOL(1,SAMP))                                       DSL 1120
    ELSE IF (CHOICE .EQ. 3) THEN                                       DSL 1130
      IBMIX(SAMP) = 1                                                  DSL 1140
      ITMIX(SAMP) = 0                                                  DSL 1150
      CALL CLEAR (SCREEN - 3)                                          DSL 1160
      PRINT *, 'ID number of the mineral to be equilibrated'           DSL 1170
      PRINT USING, '[Current = ', IDSAT(SAMP), '] '                    DSL 1180
      CALL IANSWR (IDSAT(SAMP))                                        DSL 1190
      PRINT *                                                          DSL 1200
                                                                       DSL 1210
      PRINT *, 'ID number of the mineral to be dissolved / ',          DSL 1220
     &         'precipitated'                                          DSL 1230
      PRINT USING, '[Current = ', IDDP(SAMP), '] '                     DSL 1240
      CALL IANSWR (IDDP(SAMP))                                         DSL 1250
    ELSE IF (CHOICE .EQ. 4) THEN                                       DSL 1260
      IBMIX(SAMP) = 1                                                  DSL 1270
      ITMIX(SAMP) = 0                                                  DSL 1280
      CALL CLEAR (SCREEN - 3)                                          DSL 1290
      PRINT *, 'ID number of the mineral to be equilibrated'           DSL 1300
      PRINT USING, '[Current = ', IDSAT(SAMP), '] '                    DSL 1310
      CALL IANSWR (IDSAT(SAMP))                                        DSL 1320
      PRINT *                                                          DSL 1330
                                                                       DSL 1340
      IDDP(SAMP) = 0                                                   DSL 1350
                                                                       DSL 1360
10    CONTINUE                                                         DSL 1370
      PRINT *, 'Total number of aqueous species to be added/',         DSL 1380
     &         'subtracted'                                            DSL 1390
      PRINT USING, '[Current = ', ITT(SAMP), '] '                      DSL 1400
                                                                       DSL 1410
      TMPVAL = ITT(SAMP)                                               DSL 1420
      CALL IANSWR (ITT(SAMP))                                          DSL 1430
                                                                       DSL 1440
      IF (ITT(SAMP) .LT. 0 .OR. ITT(SAMP) .GT. 10) THEN                DSL 1450
        PRINT *, 'Answer must be in the range [0-10] '                  DSL 1460
        NL = SCREEN - 4                                                DSL 1470
        ITT(SAMP) = TMPVAL                                             DSL 1480
        CALL CLEAR (NL)                                                DSL 1490
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      GOTO 10                                                          DSL 1500
    END IF                                                             DSL 1510
                                                                       DSL 1520
    PRINT *, 'Enter value for multiplication factor for aqueous',      DSL 1530
&           ' components.'                                             DSL 1540
    PRINT *, '     + x.x ) For dissolution '                           DSL 1550
    PRINT *, '     - x.x ) For precipitation'                          DSL 1560
    PRINT *, '       0.0 ) To have computer decide'                    DSL 1570
    PRINT '(15X, A, E10.4, A)', '[Current = ', DP(SAMP), '] '          DSL 1580
                                                                       DSL 1590
    CALL ANSWER (DP(SAMP))                                             DSL 1600
    PRINT *                                                            DSL 1610
                                                                       DSL 1620
    DO 20 I = 1, ITT(SAMP)                                             DSL 1630
      PRINT '(5X, A, I2)', 'Species #', I                              DSL 1640
      PRINT *                                                          DSL 1650
                                                                       DSL 1660
      PRINT *, 'ID# of the aqueous species to be',                     DSL 1670
&             ' added/subtracted ?'                                    DSL 1680
      PRINT USING, '[Current = ', IRXDP(I,SAMP), '] '                  DSL 1690
      CALL IANSWR (IRXDP(I,SAMP))                                      DSL 1700
      PRINT *                                                          DSL 1710
                                                                       DSL 1720
      PRINT *, 'Stoichiometric coefficient of aqueous species to',     DSL 1730
&             ' be added/subtracted ?'                                 DSL 1740
      PRINT *, ' (Negative coefficient means subtraction)'             DSL 1750
      PRINT '(15X, A, 1P, G10.4, A)', '[Current = ',                   DSL 1760
&                                      RXDP(I,SAMP), '] '              DSL 1770
      CALL ANSWER (RXDP(I,SAMP))                                       DSL 1780
      PRINT *                                                          DSL 1790
20  CONTINUE                                                           DSL 1800
  ELSE IF (CHOICE .EQ. 5) THEN                                         DSL 1810
    IBMIX(SAMP) = 1                                                    DSL 1820
    CALL CLEAR (SCREEN - 3)                                            DSL 1830
    IF (ITMIX(SAMP) .LT. 0) ITMIX(SAMP) = 0                            DSL 1840
                                                                       DSL 1850
25  CONTINUE                                                           DSL 1860
    PRINT *, 'How many aqueous species to add/subtract ?'              DSL 1870
    PRINT USING, '[Current = ', ITMIX(SAMP), '] '                      DSL 1880
                                                                       DSL 1890
    TMPVAL = ITMIX(SAMP)                                               DSL 1900
    CALL IANSWR (ITMIX(SAMP))                                          DSL 1910
                                                                       DSL 1920
    IF (ITMIX(SAMP) .LT. 0 .OR. ITMIX(SAMP) .GT. 50) THEN              DSL 1930
      PRINT *, 'Answer must be in the range [0-50] '                    DSL 1940
      NL = SCREEN - 4                                                  DSL 1950
      ITMIX(SAMP) = TMPVAL                                             DSL 1960
      CALL CLEAR (NL)                                                  DSL 1970
      GOTO 25                                                          DSL 1980
    END IF                                                             DSL 1990
                                                                       DSL 2000
    DO 30 I = 1, ITMIX(SAMP)                                           DSL 2010
      PRINT '(5X, A, I2)', 'Species #', I                              DSL 2020
      PRINT *                                                          DSL 2030
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                                                                      DSL 2040
      PRINT *, 'ID# of the aqueous species to be ',                   DSL 2050
     &         'added/subtracted ?'                                   DSL 2060
      PRINT USING, '[Current = ', IDMIX(I,SAMP), '] '                 DSL 2070
      CALL IANSWR (IDMIX(I,SAMP))                                     DSL 2080
      PRINT *                                                         DSL 2090
                                                                      DSL 2100
      PRINT *, 'Molality (moles/kg of H2O) of the aqueous species ?'  DSL 2110
      PRINT '(15X, A, 1P, E11.4, A)', '[Current = ', AMOL(I,SAMP),    DSL 2120
     &                                '] '                            DSL 2130
      CALL ANSWER (AMOL(I,SAMP))                                      DSL 2140
      PRINT *                                                         DSL 2150
   30 CONTINUE                                                        DSL 2160
    ELSE IF (CHOICE .EQ. 6) THEN                                      DSL 2170
      RETURN                                                          DSL 2180
    END IF                                                            DSL 2190
                                                                      DSL 2200
    NL = SCREEN - 21                                                  DSL 2210
    GOTO 100                                                          DSL 2220
                                                                      DSL 2230
    END                                                               DSL 2240
```

```
      SUBROUTINE FLAG                                                 FLA 0010
C ----------------------------------------------------------------------|FLA 0020
C     Selects which of the program flags to use                       |FLA 0030
C ----------------------------------------------------------------------|FLA 0040
                                                                      FLA 0050
      INTEGER MAX, SCREEN                                             FLA 0060
      CHARACTER * 10 OPTION                                           FLA 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)          FLA 0080
                                                                      FLA 0090
      INTEGER ALK(MAX), CHOICE, FLAGS(6,MAX), GEOTH(MAX)              FLA 0100
      INTEGER INFORM(MAX), IPIT(MAX), IPRIN1(MAX), IPRIN2(MAX)        FLA 0110
      INTEGER ITIC(MAX), NL, NUFLAG(MAX), RATIO(MAX), SAMP            FLA 0120
                                                                      FLA 0130
      CHARACTER * 80 MIXFLE(MAX), OUTIN(MAX)                          FLA 0140
                                                                      FLA 0150
      DOUBLE PRECISION CONV1(MAX), CONV2(MAX)                         FLA 0160
                                                                      FLA 0170
      EXTERNAL ACTIVE, CLEAR, IANSWR, LINE10, LINE23, PRNTOT, REDOX   FLA 0180
                                                                      FLA 0190
      COMMON           SAMP                                           FLA 0200
      COMMON /COM5  / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2           FLA 0210
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2            FLA 0220
      COMMON /COM14 / FLAGS                                           FLA 0230
      COMMON /COM20 / MIXFLE, OUTIN                                   FLA 0240
                                                                      FLA 0250
C ----------------------------------------------------------------------|FLA 0260
                                                                      FLA 0270
      NL = SCREEN                                                     FLA 0280
```

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      CHOICE = 0                                                        FLA 0290
                                                                        FLA 0300
   10 CONTINUE                                                          FLA 0310
      CALL CLEAR (NL)                                                   FLA 0320
                                                                        FLA 0330
      PRINT OPTION, '     FLAGS MENU'                                   FLA 0340
      PRINT *                                                           FLA 0350
      PRINT OPTION, '1)  Enter Carbonate Distribution'                  FLA 0360
      PRINT *                                                           FLA 0370
      PRINT OPTION, '2)  Enter Activity Coefficient Control'            FLA 0380
      PRINT *                                                           FLA 0390
      PRINT OPTION, '3)  Enter Redox Equilibria'                        FLA 0400
      PRINT *                                                           FLA 0410
      PRINT OPTION, '4)  Enter Printout Control'                        FLA 0420
      PRINT *                                                           FLA 0430
      PRINT OPTION, '5)  Enter Tolerance Control'                       FLA 0440
      PRINT *                                                           FLA 0450
      PRINT OPTION, '6)  Return to Options Menu'                        FLA 0460
      PRINT *                                                           FLA 0470
      PRINT *                                                           FLA 0480
      PRINT OPTION, '     Enter Choice (1-6) '                          FLA 0490
                                                                        FLA 0500
      CALL IANSWR (CHOICE)                                              FLA 0510
                                                                        FLA 0520
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 6) THEN                        FLA 0530
        PRINT *, 'Answer must be in the range [1-6] '                    FLA 0540
        CHOICE = -1                                                     FLA 0550
        NL = SCREEN - 18                                                FLA 0560
        GOTO 10                                                         FLA 0570
      END IF                                                            FLA 0580
                                                                        FLA 0590
      IF      (CHOICE .EQ. 1) THEN                                      FLA 0600
        CALL LINE10 (ALK, ITIC)                                         FLA 0610
      ELSE IF (CHOICE .EQ. 2) THEN                                      FLA 0620
        CALL ACTIVE (NUFLAG, IPIT)                                      FLA 0630
      ELSE IF (CHOICE .EQ. 3) THEN                                      FLA 0640
        CALL REDOX                                                      FLA 0650
      ELSE IF (CHOICE .EQ. 4) THEN                                      FLA 0660
        CALL PRNTOT                                                     FLA 0670
      ELSE IF (CHOICE .EQ. 5) THEN                                      FLA 0680
        CALL LINE23 (CONV1, CONV2)                                      FLA 0690
      ELSE IF (CHOICE .EQ. 6) THEN                                      FLA 0700
        RETURN                                                          FLA 0710
      END IF                                                            FLA 0720
                                                                        FLA 0730
      CHOICE = -1                                                       FLA 0740
      NL = SCREEN - 17                                                  FLA 0750
      GOTO 10                                                           FLA 0760
                                                                        FLA 0770
      END                                                               FLA 0780
```

```
      SUBROUTINE GAPHCO                                                  GAP 0010
C ================================================================== |GAP 0020
C     Selects gas, carobonate mineral saturation, or CO2 option      |GAP 0030
C ------------------------------------------------------------------ |GAP 0040
                                                                       GAP 0050
      INTEGER MAX, SCREEN                                              GAP 0060
      CHARACTER * 25 OPTION, USING, USING1                             GAP 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)           GAP 0080
      PARAMETER (USING  = '(8X, A, I2, A)')                            GAP 0090
      PARAMETER (USING1 = '(8X, A, 1P, E10.4, A)')                     GAP 0100
                                                                       GAP 0110
      INTEGER CHOICE, ICCSAT(MAX), IMCO3(MAX), NL, SAMP, TMPVAL        GAP 0120
                                                                       GAP 0130
      DOUBLE PRECISION DCH4(MAX), DCO2(MAX), DH2S(MAX), DNH3(MAX)      GAP 0140
      DOUBLE PRECISION FCCSAT(MAX), FIXIT(MAX)                         GAP 0150
                                                                       GAP 0160
      EXTERNAL ANSWER, CLEAR, IANSWR, LINE11, LINE13                   GAP 0170
                                                                       GAP 0180
      COMMON           SAMP                                            GAP 0190
      COMMON /COM6  / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,    GAP 0200
     &                FCCSAT                                          GAP 0210
                                                                       GAP 0220
C ================================================================== |GAP 0230
                                                                       GAP 0240
      NL = SCREEN                                                      GAP 0250
      CHOICE = -1                                                      GAP 0260
                                                                       GAP 0270
   10 CONTINUE                                                         GAP 0280
      CALL CLEAR (NL)                                                  GAP 0290
      PRINT OPTION, '    pH MENU'                                      GAP 0300
      PRINT *                                                          GAP 0310
      PRINT OPTION, '1)  Gas Addition Option'                          GAP 0320
      PRINT *                                                          GAP 0330
      PRINT OPTION, '2)  Gas-Water-Oil Distribution Option'            GAP 0340
      PRINT *                                                          GAP 0350
      PRINT OPTION, '3)  Mineral Saturation Option'                    GAP 0360
      PRINT *                                                          GAP 0370
      PRINT OPTION, '4)  CO2 Option'                                   GAP 0380
      PRINT *                                                          GAP 0390
      PRINT OPTION, '5)  Tolerance factor for Mineral and CO2 Options' GAP 0400
      PRINT *                                                          GAP 0410
      PRINT OPTION, '6)  Return to Options Menu'                       GAP 0420
      PRINT *                                                          GAP 0430
      PRINT *                                                          GAP 0440
      PRINT OPTION, '    Enter Choice (1-6) '                          GAP 0450
                                                                       GAP 0460
      CALL IANSWR (CHOICE)                                             GAP 0470
                                                                       GAP 0480
      IF (CHOICE .LT. 0 .OR. CHOICE .GT. 6) THEN                       GAP 0490
        PRINT *, 'Answer must be in the range [1-6] '                   GAP 0500
        NL = SCREEN - 18                                               GAP 0510
        CHOICE = -1                                                    GAP 0520
        GOTO 10                                                        GAP 0530
      END IF                                                           GAP 0540
```

```
                                                                      GAP 0550
   IF      (CHOICE .EQ. 1) THEN                                       GAP 0560
     CALL LINE11 (DCH4, DCO2, DH2S, DNH3)                             GAP 0570
   ELSE IF (CHOICE .EQ. 2) THEN                                       GAP 0580
     CALL LINE13                                                      GAP 0590
   ELSE IF (CHOICE .EQ. 3) THEN                                       GAP 0600
     NL = SCREEN - 8                                                  GAP 0610
20   CONTINUE                                                        GAP 0620
     CALL CLEAR (NL)                                                  GAP 0630
                                                                      GAP 0640
     PRINT *, 'Enter switch for the pH option:'                       GAP 0650
     PRINT *                                                          GAP 0660
     PRINT *, '   0)  Do not use option'                              GAP 0670
     PRINT *, '   1)  Equilibrium with calcite'                       GAP 0680
     PRINT *, '   2)  Equilibrium with dolomite'                      GAP 0690
     PRINT *, '   3)  Equilibrium with siderite'                      GAP 0700
     PRINT USING, '[Current = ', ICCSAT(SAMP), '] '                   GAP 0710
                                                                      GAP 0720
     TMPVAL = ICCSAT(SAMP)                                            GAP 0730
     CALL IANSWR (ICCSAT(SAMP))                                       GAP 0740
                                                                      GAP 0750
     IF (ICCSAT(SAMP) .LT. 0 .OR. ICCSAT(SAMP) .GT. 3) THEN           GAP 0760
         PRINT *, 'Answer must be in the range [0-3] '                 GAP 0770
         ICCSAT(SAMP) = TMPVAL                                        GAP 0780
         NL = SCREEN - 9                                              GAP 0790
         GOTO 20                                                      GAP 0800
     END IF                                                           GAP 0810
   ELSE IF (CHOICE .EQ. 4) THEN                                       GAP 0820
     NL = SCREEN - 11                                                 GAP 0830
30   CONTINUE                                                        GAP 0840
     CALL CLEAR (NL)                                                  GAP 0850
     PRINT *, 'Enter switch for the CO2 option:'                      GAP 0860
     PRINT *                                                          GAP 0870
     PRINT *, '   0)  Do not use option'                              GAP 0880
     PRINT *, '   1)  Saturation with calcite'                        GAP 0890
     PRINT *, '   2)  Saturation with dolomite'                       GAP 0900
     PRINT *, '   3)  Saturation with siderite'                       GAP 0910
     PRINT *, '   4)  For fixing molality of H2CO3'                   GAP 0920
     PRINT *, '   5)  For fixing pH'                                  GAP 0930
     PRINT *, '   6)  For fixing PCO2'                                GAP 0940
     PRINT USING, '[Current = ', IMCO3(SAMP), '] '                    GAP 0950
                                                                      GAP 0960
     TMPVAL = IMCO3(SAMP)                                             GAP 0970
     CALL IANSWR (IMCO3(SAMP))                                        GAP 0980
                                                                      GAP 0990
     IF (IMCO3(SAMP) .LT. 0 .OR. IMCO3(SAMP) .GT. 6) THEN             GAP 1000
       PRINT *, 'Answer must be in the range [0-6] '                   GAP 1010
       IMCO3(SAMP) = TMPVAL                                           GAP 1020
       NL = SCREEN - 12                                               GAP 1030
       GOTO 30                                                        GAP 1040
     ELSE IF (IMCO3(SAMP) .LT. 4) THEN                                GAP 1050
       FIXIT(SAMP) = 0.0                                              GAP 1060
     ELSE IF (IMCO3(SAMP) .EQ. 4) THEN                                GAP 1070
       PRINT *                                                        GAP 1080
```

```
          PRINT *, 'Enter the molality of total dissolved CO2'          GAP 1090
          PRINT USING1, '[Current = ', FIXIT(SAMP), '] '                GAP 1100
          CALL ANSWER (FIXIT(SAMP))                                     GAP 1110
        ELSE IF (IMCO3(SAMP) .EQ. 5) THEN                               GAP 1120
          PRINT *                                                       GAP 1130
          PRINT *, 'Enter the final pH'                                 GAP 1140
          PRINT USING1, '[Current = ', FIXIT(SAMP), '] '                GAP 1150
          CALL ANSWER (FIXIT(SAMP))                                     GAP 1160
        ELSE IF (IMCO3(SAMP) .EQ. 6) THEN                               GAP 1170
          PRINT *                                                       GAP 1180
          PRINT *, 'Enter the partial pressure of CO2 in bars'          GAP 1190
          PRINT USING1, '[Current = ', FIXIT(SAMP), '] '                GAP 1200
          CALL ANSWER (FIXIT(SAMP))                                     GAP 1210
        END IF                                                          GAP 1220
      ELSE IF (CHOICE .EQ. 5) THEN                                      GAP 1230
        CALL CLEAR (SCREEN - 3)                                         GAP 1240
        PRINT *, 'Enter tolerance factor for equilibrium criterion'     GAP 1250
        PRINT USING1, '  [Current = ', FCCSAT(SAMP), '] '              GAP 1260
        CALL ANSWER (FCCSAT(SAMP))                                      GAP 1270
      ELSE IF (CHOICE .EQ. 6) THEN                                      GAP 1280
        RETURN                                                          GAP 1290
      END IF                                                            GAP 1300
                                                                        GAP 1310
      NL = SCREEN - 17                                                  GAP 1320
      CHOICE = -1                                                       GAP 1330
      GOTO 10                                                           GAP 1340
                                                                        GAP 1350
      END                                                               GAP 1360
```

```
      SUBROUTINE IANSWR (DEFALT)                                        IAN 0010
C ======================================================================|IAN 0020
C     Determines if an integer answer is valid                          |IAN 0030
C ----------------------------------------------------------------------|IAN 0040
                                                                        IAN 0050
      INTEGER ACTLEN, DEFALT, TMPVAL                                    IAN 0060
                                                                        IAN 0070
      CHARACTER * 20 NANS                                               IAN 0080
                                                                        IAN 0090
      EXTERNAL UPCASE                                                   IAN 0100
                                                                        IAN 0110
C ======================================================================|IAN 0120
                                                                        IAN 0130
      TMPVAL = DEFALT                                                   IAN 0140
   10 CONTINUE                                                          IAN 0150
      NANS = ' '                                                        IAN 0160
      READ '(A20)', NANS                                                IAN 0170
                                                                        IAN 0180
      IF (NANS .NE. ' ') THEN                                           IAN 0190
        ACTLEN = 20                                                     IAN 0200
        CALL UPCASE (NANS, ACTLEN)                                      IAN 0210
```

```
        READ (NANS, *, ERR = 100) DEFALT                                IAN 0220
      END IF                                                            IAN 0230
                                                                        IAN 0240
      RETURN                                                            IAN 0250
                                                                        IAN 0260
  100 CONTINUE                                                          IAN 0270
      PRINT *, 'ERROR!  Invalid entry try again.'                       IAN 0280
      DEFALT = TMPVAL                                                   IAN 0290
      GOTO 10                                                           IAN 0300
                                                                        IAN 0310
      END                                                               IAN 0320




      SUBROUTINE INIT (MAXSAM, WRTFLE)                                  INI 0010
C ======================================================================|INI 0020
C     Clears all variables and sets them to their default values        |INI 0030
C ----------------------------------------------------------------------|INI 0040
                                                                        INI 0050
      INTEGER MAX                                                       INI 0060
      PARAMETER (MAX = 10)                                              INI 0070
                                                                        INI 0080
      INTEGER ALK(MAX), ANSR(3,MAX)                                     INI 0090
      INTEGER FLAGS(6,MAX), GEOTH(MAX), I                               INI 0100
      INTEGER IBMIX(MAX), ICCSAT(MAX), IDDP(MAX), IDMIX(50,MAX)         INI 0110
      INTEGER IDN(10,10,MAX), IDSAT(MAX), IMCO3(MAX)                    INI 0120
      INTEGER INFORM(MAX), INMIX(MAX), INSP(MAX), IPIT(MAX)             INI 0130
      INTEGER IPRIN1(MAX), IPRIN2(MAX), IRXDP(10,MAX), ISCHG(10,MAX)    INI 0140
      INTEGER ISCOMP(10,MAX), ITIC(MAX), ITMIX(MAX), ITT(MAX), J, L     INI 0150
      INTEGER MAXSAM, MININD(10,5,MAX), ND(2,45,MAX), NDUM(12,MAX)      INI 0160
      INTEGER NUFLAG(MAX), RATIO(MAX), SAMP, WRTFLE, Z(3,MAX)           INI 0170
                                                                        INI 0180
      CHARACTER *  1 ADEX(MAX), ODUM(12,MAX)                            INI 0190
      CHARACTER *  2 TNUM                                               INI 0200
      CHARACTER *  5 UNITS(MAX)                                         INI 0210
      CHARACTER *  8 MINAME(5,MAX), PAGE(45,MAX)                        INI 0220
      CHARACTER * 10 SPN(10,MAX)                                        INI 0230
      CHARACTER * 80 FLNAME, MIXFLE(MAX), OUTIN(MAX), TITLE(MAX)        INI 0240
                                                                        INI 0250
      DOUBLE PRECISION AMOL(50,MAX), CEC(MAX), COEF(10,10,MAX)          INI 0260
      DOUBLE PRECISION CONC(3,MAX), CONV1(MAX), CONV2(MAX)              INI 0270
      DOUBLE PRECISION CUNITS(35,MAX), DCH4(MAX), DCO2(MAX)             INI 0280
      DOUBLE PRECISION DENS(MAX), DFRAC1(MAX), DH2S(MAX), DHA(3,MAX)    INI 0290
      DOUBLE PRECISION DNA(45,MAX), DNH3(MAX), DP(MAX), EHM(MAX)        INI 0300
      DOUBLE PRECISION EHMC(MAX), EMFZSC(MAX), FBOIL(MAX), FCCSAT(MAX)  INI 0310
      DOUBLE PRECISION FIXIT(MAX), GFW(3,MAX), HITEMP(MAX), INC(MAX)    INI 0320
      DOUBLE PRECISION KCH4OL(MAX), KCO2OL(MAX), KH2SOL(MAX)            INI 0330
      DOUBLE PRECISION KRXN(10,MAX), MBASE(10,MAX), MINCO(10,5,MAX)     INI 0340
      DOUBLE PRECISION MINLOG(2,5,MAX), PH(MAX), DSEP(MAX), PRESS(MAX)  INI 0350
      DOUBLE PRECISION RXDP(10,MAX), SAREA(MAX), TAREA(MAX), TCH4M(MAX) INI 0360
      DOUBLE PRECISION TCO2M(MAX), TEMP(MAX), TH2SM(MAX), TIC(MAX)      INI 0370
      DOUBLE PRECISION WROIL(MAX), XD(2,45,MAX), XDUM(12,MAX)           INI 0380
```

```
                                                                      INI 0390
      COMMON           SAMP                                           INI 0400
      COMMON /COM1   / TITLE, UNITS, FLNAME                           INI 0410
      COMMON /COM2   / TEMP, HITEMP, DENS, PRESS                      INI 0420
      COMMON /COM3   / PH, EHM, EHMC, EMFZSC                          INI 0430
      COMMON /COM4   / CUNITS, TIC                                    INI 0440
      COMMON /COM5   / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2          INI 0450
      COMMON /COM6   / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,  INI 0460
     &                 FCCSAT                                       INI 0470
      COMMON /COM7   / TCO2M, TCH4M, TH2SM, WROIL,                    INI 0480
     &                 KCO2OL, KCH4OL, KH2SOL, DSEP                 INI 0490
      COMMON /COM8   / ADEX, SPN                                      INI 0500
      COMMON /COM9   / CEC, TAREA, SAREA, INSP, ISCHG, MBASE, KRXN,   INI 0510
     &                 ISCOMP, COEF, IDN                            INI 0520
      COMMON /COM10  / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,     INI 0530
     &                 IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL INI 0540
      COMMON /COM11  / ODUM                                           INI 0550
      COMMON /COM12  / NDUM, XDUM                                     INI 0560
      COMMON /COM13  / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2           INI 0570
      COMMON /COM14  / FLAGS                                          INI 0580
      COMMON /COM15  / ANSR, CONC, DHA, GFW, Z                        INI 0590
      COMMON /COM16  / PAGE                                           INI 0600
      COMMON /COM17  / ND, XD, DNA                                    INI 0610
      COMMON /COM18  / MINAME                                         INI 0620
      COMMON /COM19  / MINCO, MININD, MINLOG                          INI 0630
      COMMON /COM20  / MIXFLE, OUTIN                                  INI 0640
                                                                      INI 0650
C ----------------------------------------------------------------------INI 0660
                                                                      INI 0670
      SAMP   = 1                                                      INI 0680
      MAXSAM = 1                                                      INI 0690
      WRTFLE = 1                                                      INI 0700
      FLNAME = 'SOLMINEQ.IN'                                          INI 0710
                                                                      INI 0720
      DO 140 L = 1, MAX                                               INI 0730
        WRITE (TNUM, '(I2)') L                                        INI 0740
        TITLE(L)  = 'SAMPLE # ' // TNUM                               INI 0750
        UNITS(L)  = 'MG/L'                                            INI 0760
        OUTIN(L)  = ' '                                               INI 0770
        MIXFLE(L) = ' '                                               INI 0780
                                                                      INI 0790
        TEMP(L)   = 25.0                                              INI 0800
        HITEMP(L) =  0.0                                              INI 0810
        DENS(L)   =  0.0                                              INI 0820
        PRESS(L)  =  0.0                                              INI 0830
                                                                      INI 0840
        PH(L)     =  7.0                                              INI 0850
        EHM(L)    =  9.0                                              INI 0860
        EHMC(L)   =  9.0                                              INI 0870
        EMFZSC(L) =  9.0                                              INI 0880
        TIC(L)    =  0.0                                              INI 0890
                                                                      INI 0900
        DO 10 I = 1, 35                                               INI 0910
          CUNITS(I, L) = 0.0                                          INI 0920
```

```
10    CONTINUE                                                    INI 0930
                                                                  INI 0940
      ALK(L)     = 0                                            INI 0950
      ITIC(L)    = 0                                            INI 0960
      NUFLAG(L)  = 0                                            INI 0970
                                                                  INI 0980
      DO 20 I = 1, 6                                            INI 0990
        FLAGS(I,L)  = 0                                         INI 1000
20    CONTINUE                                                  INI 1010
                                                                  INI 1020
      IPIT(L)    = 0                                            INI 1030
      INFORM(L)  = 0                                            INI 1040
      RATIO(L)   = 0                                            INI 1050
      GEOTH(L)   = 0                                            INI 1060
      IPRIN1(L)  = 0                                            INI 1070
      IPRIN2(L)  = 0                                            INI 1080
                                                                  INI 1090
      CONV1(L)   = 0.00005                                      INI 1100
      CONV2(L)   = 0.00005                                      INI 1110
                                                                  INI 1120
      DCH4(L)    = 0.0                                          INI 1130
      DCO2(L)    = 0.0                                          INI 1140
      DH2S(L)    = 0.0                                          INI 1150
      DNH3(L)    = 0.0                                          INI 1160
      ICCSAT(L)  = 0                                            INI 1170
      IMCO3(L)   = 0                                            INI 1180
      FIXIT(L)   = 0.0                                          INI 1190
      FCCSAT(L)  = 0.05                                         INI 1200
                                                                  INI 1210
      TCO2M(L)   = 0.0                                          INI 1220
      TCH4M(L)   = 0.0                                          INI 1230
      TH2SM(L)   = 0.0                                          INI 1240
      WROIL(L)   = 0.0                                          INI 1250
      KCO2OL(L)  = 0.0                                          INI 1260
      KCH4OL(L)  = 0.0                                          INI 1270
      KH2SOL(L)  = 0.0                                          INI 1280
      DSEP(L)    = 0.0                                          INI 1290
                                                                  INI 1300
      ADEX(L)    = ' '                                          INI 1310
      CEC(L)     = 0.00001                                      INI 1320
      TAREA(L)   = 0.0                                          INI 1330
      SAREA(L)   = 0.0                                          INI 1340
      INSP(L)    = 0                                            INI 1350
                                                                  INI 1360
      DO 40 I = 1, 10                                           INI 1370
        ISCHG(I,L)  = 0                                         INI 1380
        ISCOMP(I,L) = 0                                         INI 1390
        WRITE (TNUM, '(I2)') I                                  INI 1400
        SPN(I,L)    = 'Species ' // TNUM                        INI 1410
        MBASE(I,L)  = 0.0                                       INI 1420
        KRXN(I,L)   = 1.0                                       INI 1430
        DO 30 J = 1, 10                                         INI 1440
          IDN(I,J,L)  = 0                                       INI 1450
          COEF(I,J,L) = 0.0                                     INI 1460
```

```
30      CONTINUE                                                    INI 1470
40    CONTINUE                                                      INI 1480
                                                                    INI 1490
      IBMIX(L)  =  0                                                INI 1500
      ITMIX(L)  =  0                                                INI 1510
      IDSAT(L)  =  0                                                INI 1520
      IDDP(L)   =  0                                                INI 1530
      ITT(L)    =  0                                                INI 1540
      DP(L)     =  0.0                                              INI 1550
      INMIX(L)  =  0                                                INI 1560
                                                                    INI 1570
      DFRAC1(L) = 0.0                                               INI 1580
      INC(L)    = 0.0                                               INI 1590
      FBOIL(L)  = 0.0                                               INI 1600
                                                                    INI 1610
      DO 50 I = 1, 10                                               INI 1620
        IRXDP(I,L) = 0                                              INI 1630
        RXDP(I,L)  = 0.0                                            INI 1640
50    CONTINUE                                                      INI 1650
                                                                    INI 1660
      DO 60 I = 1, 50                                               INI 1670
        IDMIX(I,L) = 0                                              INI 1680
        AMOL(I,L)  = 0.0                                            INI 1690
60    CONTINUE                                                      INI 1700
                                                                    INI 1710
      DO 70 I = 1, 12                                               INI 1720
        ODUM(I,L) = ' '                                             INI 1730
        NDUM(I,L) = 0                                               INI 1740
        XDUM(I,L) = 0.0                                             INI 1750
70    CONTINUE                                                      INI 1760
                                                                    INI 1770
      DO 80 I = 1, 3                                                INI 1780
        ANSR(I,L) = 0                                               INI 1790
        CONC(I,L) = 0.0                                             INI 1800
        DHA(I,L)  = 0.0                                             INI 1810
        GFW(I,L)  = 0.0                                             INI 1820
        Z(I,L)    = 0                                               INI 1830
80    CONTINUE                                                      INI 1840
                                                                    INI 1850
      DO 90 I = 1, 30                                               INI 1860
        PAGE(I,L) = ' '                                             INI 1870
        DNA(I,L)  = 0.0                                             INI 1880
        ND(1,I,L) = 0                                               INI 1890
        ND(2,I,L) = 0                                               INI 1900
        XD(1,I,L) = 0.0                                             INI 1910
        XD(2,I,L) = 0.0                                             INI 1920
90    CONTINUE                                                      INI 1930
                                                                    INI 1940
      PAGE( 1,L) = 'ANION1'                                         INI 1950
      PAGE(16,L) = 'ANION2'                                         INI 1960
      PAGE(31,L) = 'CATION'                                         INI 1970
                                                                    INI 1980
      DO 130 I = 1, 5                                               INI 1990
        WRITE (TNUM, '(I2)') I                                      INI 2000
```

```
          MINAME(I,L) = 'Min #' // TNUM                                  INI 2010
          DO 100 J = 1, 10                                               INI 2020
            MININD(J,I,L) = 0                                            INI 2030
            MINCO(J,I,L)  = 0.0                                          INI 2040
  100     CONTINUE                                                       INI 2050
          DO 110 J = 1, 2                                                INI 2060
            MINLOG(J,I,L) = 0.0                                          INI 2070
  110     CONTINUE                                                       INI 2080
  130   CONTINUE                                                         INI 2090
                                                                         INI 2100
  140 CONTINUE                                                           INI 2110
                                                                         INI 2120
      RETURN                                                             INI 2130
      END                                                                INI 2140
```

```
      SUBROUTINE ION (NUM)                                               ION 0010
C ================================================================      |ION 0020
C     Determines the basic properties for the additional ions          |ION 0030
C ----------------------------------------------------------------      |ION 0040
                                                                         ION 0050
      INTEGER MAX, SCREEN                                                ION 0060
      PARAMETER (MAX = 10, SCREEN = 24)                                  ION 0070
                                                                         ION 0080
      INTEGER ANSR(3,MAX), NUM, SAMP, Z(3,MAX)                           ION 0090
                                                                         ION 0100
      CHARACTER *  8 ANSWR, PAGE(45,MAX)                                 ION 0110
                                                                         ION 0120
      DOUBLE PRECISION CONC(3,MAX), DHA(3,MAX), GFW(3,MAX)               ION 0130
                                                                         ION 0140
      EXTERNAL ANSWER, CLEAR, IANSWR                                     ION 0150
                                                                         ION 0160
      COMMON           SAMP                                              ION 0170
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                            ION 0180
      COMMON /COM16 / PAGE                                               ION 0190
                                                                         ION 0200
C ================================================================      |ION 0210
                                                                         ION 0220
      CALL CLEAR (SCREEN)                                                ION 0230
      PRINT *, 'What is the name of the species ?'                       ION 0240
      PRINT '(1X, A8)', PAGE(NUM,SAMP)                                   ION 0250
      PRINT *                                                            ION 0260
                                                                         ION 0270
      READ '(A8)', ANSWR                                                 ION 0280
                                                                         ION 0290
      IF (ANSWR .NE. ' ') THEN                                           ION 0300
        PAGE(NUM,SAMP) = ANSWR                                           ION 0310
      END IF                                                             ION 0320
                                                                         ION 0330
      IF (NUM .EQ. 16) NUM = 2                                           ION 0340
      IF (NUM .EQ. 31) NUM = 3                                           ION 0350
```

```
                                                                      ION 0360
      PRINT *                                                         ION 0370
      PRINT *, 'What is the charge on the species ?'                  ION 0380
      PRINT '(1X, A, I2, A)', '[Current = ', Z(NUM,SAMP), '] '        ION 0390
                                                                      ION 0400
      CALL IANSWR (Z(NUM,SAMP))                                       ION 0410
                                                                      ION 0420
      PRINT *                                                         ION 0430
      PRINT *, 'What is the hydrated radius of the species ?'         ION 0440
      PRINT '(1X, A, F4.1, A)', '[Current = ', DHA(NUM,SAMP), '] '    ION 0450
                                                                      ION 0460
      CALL ANSWER (DHA(NUM,SAMP))                                     ION 0470
                                                                      ION 0480
      PRINT *                                                         ION 0490
      PRINT *, 'What is the gram formula weight of the species ?'     ION 0500
      PRINT '(1X, A, F9.3, A)', '[Current = ', GFW(NUM,SAMP), '] '    ION 0510
                                                                      ION 0520
      CALL ANSWER (GFW(NUM,SAMP))                                     ION 0530
                                                                      ION 0540
      PRINT *                                                         ION 0550
      PRINT *, 'What is the concentration of the species ?'           ION 0560
      PRINT '(1X, A, F9.3, A)', '[Current = ', CONC(NUM,SAMP), '] '   ION 0570
                                                                      ION 0580
      CALL ANSWER (CONC(NUM,SAMP))                                    ION 0590
                                                                      ION 0600
      RETURN                                                          ION 0610
      END                                                             ION 0620
```

```
      INTEGER FUNCTION LENGTH (STRING, L)                             LEN 0010
C ==========================================================================|LEN 0020
C     Calculates the non-blank length of a string variable given the    |LEN 0030
C     string and its actual length.                                     |LEN 0040
C ---------------------------------------------------------------------|LEN 0050
                                                                        LEN 0060
      INTEGER L                                                       LEN 0070
                                                                      LEN 0080
      CHARACTER STRING*(*)                                            LEN 0090
                                                                      LEN 0100
C ==========================================================================|LEN 0110
                                                                      LEN 0120
   10 CONTINUE                                                        LEN 0130
      IF (L .GT. 1  .AND.  STRING(L:L) .EQ. ' ') THEN                 LEN 0140
        L = L - 1                                                     LEN 0150
        GOTO 10                                                       LEN 0160
      END IF                                                          LEN 0170
                                                                      LEN 0180
      IF (STRING(L:L) .NE. ' ') THEN                                  LEN 0190
        LENGTH = L                                                    LEN 0200
      ELSE                                                            LEN 0210
        LENGTH = 1                                                    LEN 0220
```

```
      END IF                                                            LEN 0230
                                                                        LEN 0240
      RETURN                                                            LEN 0250
                                                                        LEN 0260
      END                                                               LEN 0270



      SUBROUTINE LINE01                                                 L01 0010
C ======================================================================|L01 0020
C     This routine gets the values for the title and the units used     |L01 0030
C ----------------------------------------------------------------------|L01 0040
                                                                        L01 0050
      INTEGER MAX, SCREEN                                               L01 0060
      PARAMETER (MAX = 10, SCREEN = 24)                                 L01 0070
                                                                        L01 0080
      INTEGER ACTLEN, LEN, LENGTH, NL, SAMP, TMPVAL                     L01 0090
                                                                        L01 0100
      CHARACTER *  5 ANS, UNITS(MAX)                                    L01 0110
      CHARACTER * 80 ANSWR, FLNAME, TITLE(MAX)                          L01 0120
                                                                        L01 0130
      EXTERNAL CLEAR, LENGTH, UPCASE                                    L01 0140
                                                                        L01 0150
      INTRINSIC CHAR, ICHAR                                             L01 0160
                                                                        L01 0170
      COMMON           SAMP                                             L01 0180
      COMMON /COM1  / TITLE, UNITS, FLNAME                              L01 0190
                                                                        L01 0200
C ======================================================================|L01 0210
                                                                        L01 0220
      CALL CLEAR (SCREEN)                                               L01 0230
                                                                        L01 0240
      PRINT *, 'Enter the title of this sample'                         L01 0250
      ACTLEN = 80                                                       L01 0260
      LEN = LENGTH (TITLE(SAMP), ACTLEN)                                L01 0270
      PRINT '(1X, A1, A, A1)', '[',TITLE(SAMP)(1:LEN),'] '              L01 0280
      PRINT *                                                           L01 0290
                                                                        L01 0300
      READ '(A80)', ANSWR                                               L01 0310
                                                                        L01 0320
      IF (ANSWR .NE. ' ') THEN                                          L01 0330
        TITLE(SAMP) = ANSWR                                             L01 0340
      END IF                                                            L01 0350
                                                                        L01 0360
      NL = 2                                                            L01 0370
                                                                        L01 0380
   10 CONTINUE                                                          L01 0390
      CALL CLEAR (NL)                                                   L01 0400
      PRINT *, 'Enter Concentration Units (Mg/l, PPM, Mol/l, ',         L01 0410
     &         'Mol/K, Meq/l)'                                          L01 0420
      PRINT '(1X, A1, A5, A1)', '[',UNITS(SAMP),'] '                    L01 0430
      PRINT *                                                           L01 0440
```

```
                                                                      L01 0450
      READ '(A5)', ANS                                                L01 0460
                                                                      L01 0470
      IF (ANS .NE. ' ') THEN                                          L01 0480
        UNITS(SAMP) = ANS                                             L01 0490
        ACTLEN = 5                                                    L01 0500
        CALL UPCASE (UNITS(SAMP), ACTLEN)                             L01 0510
      END IF                                                          L01 0520
                                                                      L01 0530
      IF      (UNITS(SAMP) .EQ. 'MG/L ') THEN                         L01 0540
        TMPVAL = 1                                                    L01 0550
      ELSE IF (UNITS(SAMP) .EQ. 'PPM  ') THEN                         L01 0560
        TMPVAL = 1                                                    L01 0570
      ELSE IF (UNITS(SAMP) .EQ. 'MOL/L') THEN                         L01 0580
        TMPVAL = 1                                                    L01 0590
      ELSE IF (UNITS(SAMP) .EQ. 'MOL/K') THEN                         L01 0600
        TMPVAL = 1                                                    L01 0610
      ELSE IF (UNITS(SAMP) .EQ. 'MEQ/L') THEN                         L01 0620
        TMPVAL = 1                                                    L01 0630
      ELSE                                                            L01 0640
        TMPVAL = 0                                                    L01 0650
      END IF                                                          L01 0660
                                                                      L01 0670
      IF (TMPVAL .NE. 1) THEN                                         L01 0680
        PRINT *, 'Those units are not supported !  Try Again.'        L01 0690
        NL = SCREEN - 5                                               L01 0700
        GOTO 10                                                       L01 0710
      END IF                                                          L01 0720
                                                                      L01 0730
      RETURN                                                          L01 0740
      END                                                             L01 0750
```

```
      SUBROUTINE LINE02                                               L02 0010
C ------------------------------------------------------------------|L02 0020
C     Gets the values for line 2 of the input file.  See table 1      |L02 0030
C ------------------------------------------------------------------|L02 0040
                                                                      L02 0050
      INTEGER MAX, SCREEN                                             L02 0060
      PARAMETER (MAX = 10, SCREEN = 24)                               L02 0070
                                                                      L02 0080
      INTEGER SAMP                                                    L02 0090
                                                                      L02 0100
      DOUBLE PRECISION DENS(MAX), HITEMP(MAX), PRESS(MAX), TEMP(MAX)  L02 0110
                                                                      L02 0120
      EXTERNAL ANSWER, CLEAR                                          L02 0130
                                                                      L02 0140
      COMMON           SAMP                                           L02 0150
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                       L02 0160
                                                                      L02 0170
C ------------------------------------------------------------------|L02 0180
```

```
                                                                      L02 0190
      CALL CLEAR (SCREEN)                                             L02 0200
                                                                      L02 0210
      PRINT *, 'Enter Sampling Temperature'                           L02 0220
      PRINT '(15X, A, F6.2, A)', '[Current = ', TEMP(SAMP), '] '      L02 0230
      CALL ANSWER (TEMP(SAMP))                                        L02 0240
      PRINT *                                                         L02 0250
                                                                      L02 0260
      PRINT *, 'Enter Modeling Temperature'                           L02 0270
      PRINT '(15X, A, F6.2, A)', '[Current = ', HITEMP(SAMP), '] '    L02 0280
      CALL ANSWER (HITEMP(SAMP))                                      L02 0290
      PRINT *                                                         L02 0300
                                                                      L02 0310
      PRINT *, 'Enter Density'                                        L02 0320
      PRINT '(15X, A, F7.4, A)', '[Current = ', DENS(SAMP), '] '      L02 0330
      CALL ANSWER (DENS(SAMP))                                        L02 0340
      PRINT *                                                         L02 0350
                                                                      L02 0360
      PRINT *,  'Enter in Situ Pressure in Bars'                      L02 0370
      PRINT '(15X, A, F8.2, A)', '[Current = ', PRESS(SAMP), '] '     L02 0380
      CALL ANSWER (PRESS(SAMP))                                       L02 0390
      PRINT *                                                         L02 0400
                                                                      L02 0410
      RETURN                                                          L02 0420
      END                                                             L02 0430
```

```
      SUBROUTINE LINE03                                               L03 0010
C ==========================================================================|L03 0020
C     Gets the values for line 3 of the input file. (Except for units   |L03 0030
C     which is grouped with the title.  See table 1                     |L03 0040
C ---------------------------------------------------------------------- |L03 0050
                                                                      L03 0060
      INTEGER MAX, SCREEN                                             L03 0070
      PARAMETER (MAX = 10, SCREEN = 24)                               L03 0080
                                                                      L03 0090
      INTEGER SAMP                                                    L03 0100
                                                                      L03 0110
      DOUBLE PRECISION EHM(MAX), EHMC(MAX), EMFZSC(MAX), PH(MAX)      L03 0120
                                                                      L03 0130
      EXTERNAL ANSWER, CLEAR                                          L03 0140
                                                                      L03 0150
      INTRINSIC DABS                                                  L03 0160
                                                                      L03 0170
      COMMON           SAMP                                           L03 0180
      COMMON /COM3   / PH, EHM, EHMC, EMFZSC                          L03 0190
                                                                      L03 0200
C ==========================================================================|L03 0210
                                                                      L03 0220
      CALL CLEAR (SCREEN)                                             L03 0230
                                                                      L03 0240
```

```
      PRINT '(1X,A,33X,A,F7.4,A)', 'Enter the pH', '[Current = ',       L03 0250
     &                             PH(SAMP), '] '                      L03 0260
      CALL ANSWER (PH(SAMP))                                           L03 0270
      PRINT *                                                          L03 0280
                                                                       L03 0290
      IF (DABS(EHMC(SAMP)) .GE. 9.0 .AND. DABS(EMFZSC(SAMP)) .GE. 9.0) L03 0300
     &  THEN                                                           L03 0310
        PRINT '(1X,A,28X,A,F7.4,A)', 'Enter Eh in Volts', '[Current = ',L03 0320
     &                               EHM(SAMP), '] '                   L03 0330
        CALL ANSWER (EHM(SAMP))                                        L03 0340
        PRINT *                                                        L03 0350
      END IF                                                           L03 0360
                                                                       L03 0370
      IF (DABS(EHM(SAMP)) .GE. 9.0 .AND. DABS(EMFZSC(SAMP)) .GE. 9.0)  L03 0380
     &  THEN                                                           L03 0390
        PRINT '(1X,2A,F7.4,A)', 'Enter Eh with Calomel Reference in ', L03 0400
     &        'Volts     [Current = ', EHMC(SAMP), '] '               L03 0410
        CALL ANSWER (EHMC(SAMP))                                       L03 0420
        PRINT *                                                        L03 0430
      END IF                                                           L03 0440
                                                                       L03 0450
      IF (DABS(EHM(SAMP)) .GE. 9.0 .AND. DABS(EHMC(SAMP)) .GE. 9.0)    L03 0460
     &  THEN                                                           L03 0470
        PRINT '(1X,2A,F7.4,A)', 'Enter Eh with Zobell Reference Cell', L03 0480
     &         ' in Volts [Current = ', EMFZSC(SAMP), '] '             L03 0490
        CALL ANSWER (EMFZSC(SAMP))                                     L03 0500
        PRINT *                                                        L03 0510
      END IF                                                           L03 0520
                                                                       L03 0530
      RETURN                                                           L03 0540
      END                                                              L03 0550
```

```
      SUBROUTINE LINE04                                                L04 0010
C ==========================================================================|L04 0020
C     Gets the values for line 4 of the input file.  See table 1           |L04 0030
C --------------------------------------------------------------------------|L04 0040
                                                                       L04 0050
      INTEGER MAX, SCREEN                                              L04 0060
      CHARACTER * 30 USING                                             L04 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                L04 0080
      PARAMETER (USING = '(1X, A, A, A, 1P, E10.4, A)')                L04 0090
                                                                       L04 0100
      INTEGER I, SAMP                                                  L04 0110
                                                                       L04 0120
      CHARACTER * 2 HOLD(7)                                            L04 0130
                                                                       L04 0140
      DOUBLE PRECISION CUNITS(35, MAX), TIC(MAX)                       L04 0150
                                                                       L04 0160
      EXTERNAL ANSWER, CLEAR                                           L04 0170
                                                                       L04 0180
```

```
      COMMON           SAMP                                                  L04 0190
      COMMON /COM4   / CUNITS, TIC                                           L04 0200
                                                                             L04 0210
      DATA HOLD /'Na', 'K ', 'Li', 'Ca', 'Mg', 'Fe', 'Al'/                   L04 0220
                                                                             L04 0230
C ============================================================================L04 0240
                                                                             L04 0250
      CALL CLEAR (SCREEN)                                                    L04 0260
                                                                             L04 0270
      DO 10 I = 1, 7                                                         L04 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I),' [Current = ',      L04 0290
     &               CUNITS(I,SAMP), '] '                                    L04 0300
        CALL ANSWER (CUNITS(I,SAMP))                                         L04 0310
        PRINT *                                                              L04 0320
   10 CONTINUE                                                               L04 0330
                                                                             L04 0340
      RETURN                                                                 L04 0350
      END                                                                    L04 0360
```

```
      SUBROUTINE LINE05                                                      L05 0010
C ============================================================================L05 0020
C     Gets the values for line 5 of the input file.  See table 1             L05 0030
C ----------------------------------------------------------------------------L05 0040
                                                                             L05 0050
      INTEGER MAX, SCREEN                                                    L05 0060
      CHARACTER * 30 USING, USING1                                           L05 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                      L05 0080
      PARAMETER (USING  = '(1X, A, A, A, 1P, E10.4, A)')                     L05 0090
      PARAMETER (USING1 = '(1X, A, 1P, E10.4, A)')                           L05 0100
                                                                             L05 0110
      INTEGER I, SAMP                                                        L05 0120
                                                                             L05 0130
      CHARACTER * 4 HOLD(6)                                                  L05 0140
                                                                             L05 0150
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                              L05 0160
                                                                             L05 0170
      EXTERNAL ANSWER, CLEAR                                                 L05 0180
                                                                             L05 0190
      COMMON           SAMP                                                  L05 0200
      COMMON /COM4   / CUNITS, TIC                                           L05 0210
                                                                             L05 0220
      DATA HOLD /'SiO2', 'Cl  ', 'SO4 ', 'H2S ', 'HCO3', 'CO3 '/             L05 0230
                                                                             L05 0240
C ============================================================================L05 0250
                                                                             L05 0260
      CALL CLEAR (SCREEN)                                                    L05 0270
                                                                             L05 0280
      DO 10 I = 8, 13                                                        L05 0290
        PRINT USING, 'Enter Concentration of ', HOLD(I-7),                   L05 0300
     &               ' [Current = ', CUNITS(I,SAMP), '] '                    L05 0310
```

```
      CALL ANSWER (CUNITS(I,SAMP))                                      L05 0320
      PRINT *                                                           L05 0330
   10 CONTINUE                                                          L05 0340
                                                                        L05 0350
      PRINT USING1, 'Enter TIC                    [Current = ',         L05 0360
     &              TIC(SAMP), '] '                                    L05 0370
      CALL ANSWER (TIC(SAMP))                                           L05 0380
                                                                        L05 0390
      RETURN                                                            L05 0400
      END                                                               L05 0410
```

```
      SUBROUTINE LINE06                                                 L06 0010
C ================================================================     |L06 0020
C     Gets the values for line 6 of the input file.  See table 1      |L06 0030
C ----------------------------------------------------------------     |L06 0040
                                                                        L06 0050
      INTEGER MAX, SCREEN                                               L06 0060
      CHARACTER * 30 USING                                              L06 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                 L06 0080
      PARAMETER (USING  = '(1X, A, A, A, 1P, E10.4, A)')                L06 0090
                                                                        L06 0100
      INTEGER I, SAMP                                                   L06 0110
                                                                        L06 0120
      CHARACTER * 3 HOLD(7)                                             L06 0130
                                                                        L06 0140
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                         L06 0150
                                                                        L06 0160
      EXTERNAL ANSWER, CLEAR                                            L06 0170
                                                                        L06 0180
      COMMON           SAMP                                             L06 0190
      COMMON /COM4   / CUNITS, TIC                                      L06 0200
                                                                        L06 0210
      DATA HOLD /'F  ', 'PO4', 'NO3', 'NH3', 'B  ', 'Sr ', 'Ba '/       L06 0220
                                                                        L06 0230
C ================================================================     |L06 0240
                                                                        L06 0250
      CALL CLEAR (SCREEN)                                               L06 0260
                                                                        L06 0270
      DO 10 I = 14, 20                                                  L06 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-13),             L06 0290
     &               ' [Current = ', CUNITS(I,SAMP), '] '               L06 0300
        CALL ANSWER (CUNITS(I,SAMP))                                    L06 0310
        PRINT *                                                         L06 0320
   10 CONTINUE                                                          L06 0330
                                                                        L06 0340
      RETURN                                                            L06 0350
      END                                                               L06 0360
```

```
      SUBROUTINE LINE07                                                 L07 0010
C ==========================================================================|L07 0020
C     Gets the values for line 7 of the input file.  See table 1          |L07 0030
C --------------------------------------------------------------------------|L07 0040
                                                                          L07 0050
      INTEGER MAX, SCREEN                                                 L07 0060
      CHARACTER * 30 USING                                                L07 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                   L07 0080
      PARAMETER (USING  = '(1X, A, A, A, 1P, E10.4, A)')                  L07 0090
                                                                          L07 0100
      INTEGER I, SAMP                                                     L07 0110
                                                                          L07 0120
      CHARACTER * 2 HOLD(6)                                               L07 0130
                                                                          L07 0140
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                           L07 0150
                                                                          L07 0160
      EXTERNAL ANSWER, CLEAR                                              L07 0170
                                                                          L07 0180
      COMMON           SAMP                                               L07 0190
      COMMON /COM4   / CUNITS, TIC                                        L07 0200
                                                                          L07 0210
      DATA HOLD /'Pb', 'Zn', 'Cu', 'Mn', 'Hg', 'Ag'/                      L07 0220
                                                                          L07 0230
C ==========================================================================|L07 0240
                                                                          L07 0250
      CALL CLEAR (SCREEN)                                                 L07 0260
                                                                          L07 0270
      DO 10 I = 21, 26                                                    L07 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-20),               L07 0290
     &               ' [Current = ', CUNITS(I,SAMP), '] '                 L07 0300
        CALL ANSWER (CUNITS(I,SAMP))                                      L07 0310
        PRINT *                                                           L07 0320
   10 CONTINUE                                                            L07 0330
                                                                          L07 0340
      RETURN                                                              L07 0350
      END                                                                 L07 0360
```

```
      SUBROUTINE LINE08                                                 L08 0010
C ==========================================================================|L08 0020
C     Gets the values for line 8 of the input file.  See table 1          |L08 0030
C --------------------------------------------------------------------------|L08 0040
                                                                          L08 0050
      INTEGER MAX, SCREEN                                                 L08 0060
      CHARACTER * 30 USING                                                L08 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                   L08 0080
      PARAMETER (USING  = '(1X, A, A, A, 1P, E10.4, A)')                  L08 0090
                                                                          L08 0100
      INTEGER I, SAMP                                                     L08 0110
                                                                          L08 0120
      CHARACTER * 2 HOLD(3)                                               L08 0130
```

```
                                                                      L08 0140
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                       L08 0150
                                                                      L08 0160
      EXTERNAL ANSWER, CLEAR                                          L08 0170
                                                                      L08 0180
      COMMON           SAMP                                           L08 0190
      COMMON /COM4  / CUNITS, TIC                                     L08 0200
                                                                      L08 0210
      DATA HOLD /'As', 'U ', 'V '/                                    L08 0220
                                                                      L08 0230
C ====================================================================|L08 0240
                                                                      L08 0250
      CALL CLEAR (SCREEN)                                             L08 0260
                                                                      L08 0270
      DO 10 I = 27, 29                                                L08 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-26),           L08 0290
     &               ' [Current = ', CUNITS(I,SAMP), '] '             L08 0300
        CALL ANSWER (CUNITS(I,SAMP))                                  L08 0310
        PRINT *                                                       L08 0320
   10 CONTINUE                                                        L08 0330
                                                                      L08 0340
      RETURN                                                          L08 0350
      END                                                             L08 0360
```

```
      SUBROUTINE LINE09                                               L09 0010
C ====================================================================|L09 0020
C     Gets the values for line 9 of the input file.  See table 1      |L09 0030
C --------------------------------------------------------------------|L09 0040
                                                                      L09 0050
      INTEGER MAX, SCREEN                                             L09 0060
      CHARACTER * 30 USING                                            L09 0070
      PARAMETER (MAX = 10, SCREEN = 24)                               L09 0080
      PARAMETER (USING  = '(1X, A, A, A, 1P, E10.4, A)')              L09 0090
                                                                      L09 0100
      INTEGER I, SAMP                                                 L09 0110
                                                                      L09 0120
      CHARACTER * 9 HOLD(4)                                           L09 0130
                                                                      L09 0140
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                       L09 0150
                                                                      L09 0160
      EXTERNAL ANSWER, CLEAR                                          L09 0170
                                                                      L09 0180
      COMMON           SAMP                                           L09 0190
      COMMON /COM4  / CUNITS, TIC                                     L09 0200
                                                                      L09 0210
      DATA HOLD /'Acetate  ', 'Oxalate  ', 'Succinate', 'Methane  '/  L09 0220
                                                                      L09 0230
C ====================================================================|L09 0240
                                                                      L09 0250
      CALL CLEAR (SCREEN)                                             L09 0260
```

```
                                                                      L09 0270
      DO 10 I = 30, 33                                                L09 0280
        PRINT USING, 'Enter Concentration of ', HOLD(I-29),           L09 0290
     &               ' [Current = ', CUNITS(I,SAMP), '] '             L09 0300
        CALL ANSWER (CUNITS(I,SAMP))                                  L09 0310
        PRINT *                                                       L09 0320
   10 CONTINUE                                                        L09 0330
                                                                      L09 0340
      RETURN                                                          L09 0350
      END                                                             L09 0360
```

```
      SUBROUTINE LINE10 (ALK, ITIC)                                   L10 0010
C ====================================================================|L10 0020
C     Gets the values for line 10 of the input file.  See table 1     |L10 0030
C --------------------------------------------------------------------|L10 0040
                                                                      L10 0050
      INTEGER MAX, SCREEN                                             L10 0060
      CHARACTER * 15 USING                                            L10 0070
      PARAMETER (MAX = 10, SCREEN = 24, USING = '(1X, A, I2, A)')     L10 0080
                                                                      L10 0090
      INTEGER ALK(MAX), ITIC(MAX), NL, SAMP, TMPVAL                   L10 0100
                                                                      L10 0110
      CHARACTER * 1 ANS                                               L10 0120
                                                                      L10 0130
      EXTERNAL CLEAR, IANSWR                                          L10 0140
                                                                      L10 0150
      COMMON          SAMP                                            L10 0160
                                                                      L10 0170
C ====================================================================|L10 0180
                                                                      L10 0190
      NL = SCREEN                                                     L10 0200
                                                                      L10 0210
   10 CONTINUE                                                        L10 0220
      CALL CLEAR (NL)                                                 L10 0230
      PRINT *, 'What does the concentration of bicarbonate/carbonate' L10 0240
      PRINT *, 'refer to:'                                            L10 0250
      PRINT *, '     0 = Total Alkalinity as HCO3/CO3?'               L10 0260
      PRINT *, '     1 = Carbonate Alkalinity as HCO3/CO3?'           L10 0270
      PRINT *, '     2 = Total Inorganic Carbon (TIC)?'               L10 0280
      PRINT USING, '          [Current = ', ALK(SAMP), '] '           L10 0290
                                                                      L10 0300
      TMPVAL = ALK(SAMP)                                              L10 0310
      CALL IANSWR (ALK(SAMP))                                         L10 0320
                                                                      L10 0330
      IF (ALK(SAMP) .LT. 0 .OR. ALK(SAMP) .GT. 2) THEN                L10 0340
        PRINT *, 'Answer must be in the range [0-2].'                  L10 0350
        ALK(SAMP) = TMPVAL                                            L10 0360
        NL = SCREEN - 8                                               L10 0370
        GOTO 10                                                       L10 0380
      END IF                                                          L10 0390
```

```
                                                                      L10 0400
      NL = 2                                                          L10 0410
                                                                      L10 0420
   20 CONTINUE                                                        L10 0430
      CALL CLEAR (NL)                                                 L10 0440
      PRINT *, 'Do you wish to use TIC for the distribution of'       L10 0450
      PRINT *, 'carbonate species at high temperature? (Y/N)'         L10 0460
      IF      (ITIC(SAMP) .EQ. 0) THEN                                L10 0470
        PRINT USING, '     [Current =  N] '                           L10 0480
      ELSE IF (ITIC(SAMP) .EQ. 1) THEN                                L10 0490
        PRINT USING, '     [Current =  Y] '                           L10 0500
      END IF                                                          L10 0510
                                                                      L10 0520
      READ '(A)', ANS                                                 L10 0530
                                                                      L10 0540
      IF (ANS .NE. ' ') THEN                                          L10 0550
        IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                      L10 0560
          ITIC(SAMP) = 1                                              L10 0570
        ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                 L10 0580
          ITIC(SAMP) = 0                                              L10 0590
        ELSE                                                          L10 0600
          PRINT *, 'Answer must be in [Y, y, N, n] '                  L10 0610
          NL = SCREEN - 5                                             L10 0620
          GOTO 20                                                     L10 0630
        END IF                                                        L10 0640
      END IF                                                          L10 0650
                                                                      L10 0660
      RETURN                                                          L10 0670
      END                                                             L10 0680
```

```
      SUBROUTINE LINE11 (DCH4, DCO2, DH2S, DNH3)                      L11 0010
C ----------------------------------------------------------------------|L11 0020
C     Gets the values for line 11 of the input file.  See table 1       |L11 0030
C ----------------------------------------------------------------------|L11 0040
                                                                        L11 0050
      INTEGER MAX, SCREEN                                               L11 0060
      CHARACTER * 25 USING                                              L11 0070
      PARAMETER (MAX = 10, SCREEN = 24)                                 L11 0080
      PARAMETER (USING = '(1X, A, 1P, E10.4, A)')                       L11 0090
                                                                        L11 0100
      INTEGER SAMP                                                      L11 0110
                                                                        L11 0120
      DOUBLE PRECISION DCH4(MAX), DCO2(MAX), DH2S(MAX), DNH3(MAX)       L11 0130
                                                                        L11 0140
      EXTERNAL ANSWER, CLEAR                                            L11 0150
                                                                        L11 0160
      COMMON           SAMP                                             L11 0170
                                                                        L11 0180
C ----------------------------------------------------------------------|L11 0190
                                                                        L11 0200
```

```
      CALL CLEAR (SCREEN)                                                L11 0210
                                                                         L11 0220
      PRINT *, 'Enter amount of CH4 lost prior to pH measurment in ',    L11 0230
     &         'moles/kg'                                                L11 0240
      PRINT USING, '      [Current = ', DCH4(SAMP), '] '                 L11 0250
      CALL ANSWER (DCH4(SAMP))                                           L11 0260
      PRINT *                                                            L11 0270
                                                                         L11 0280
      PRINT *, 'Enter amount of CO2 lost prior to pH measurment in ',    L11 0290
     &         'moles/kg'                                                L11 0300
      PRINT USING, '      [Current = ', DCO2(SAMP), '] '                 L11 0310
      CALL ANSWER (DCO2(SAMP))                                           L11 0320
      PRINT *                                                            L11 0330
                                                                         L11 0340
      PRINT *, 'Enter amount of H2S lost prior to pH measurment in ',    L11 0350
     &         'moles/kg'                                                L11 0360
      PRINT USING, '      [Current = ', DH2S(SAMP), '] '                 L11 0370
      CALL ANSWER (DH2S(SAMP))                                           L11 0380
      PRINT *                                                            L11 0390
                                                                         L11 0400
      PRINT *, 'Enter amount of NH3 lost prior to pH measurment in ',    L11 0410
     &         'moles/kg'                                                L11 0420
      PRINT USING, '      [Current = ', DNH3(SAMP), '] '                 L11 0430
      CALL ANSWER (DNH3(SAMP))                                           L11 0440
                                                                         L11 0450
      RETURN                                                             L11 0460
      END                                                                L11 0470
```

```
      SUBROUTINE LINE13                                                  L13 0010
C ================================================================      |L13 0020
C     Gets the values for line 13 of the input file.  See table 1      |L13 0030
C ----------------------------------------------------------------      |L13 0040
                                                                         L13 0050
      INTEGER MAX, SCREEN                                                L13 0060
      PARAMETER (MAX = 10, SCREEN = 24)                                  L13 0070
                                                                         L13 0080
      INTEGER SAMP                                                       L13 0090
                                                                         L13 0100
      DOUBLE PRECISION TCO2M(MAX), TCH4M(MAX), TH2SM(MAX), WROIL(MAX)    L13 0110
      DOUBLE PRECISION KCO2OL(MAX), KCH4OL(MAX), KH2SOL(MAX), DSEP(MAX)  L13 0120
                                                                         L13 0130
      EXTERNAL ANSWER, CLEAR                                             L13 0140
                                                                         L13 0150
      COMMON           SAMP                                              L13 0160
      COMMON /COM7   / TCO2M, TCH4M, TH2SM, WROIL,                       L13 0170
     &                 KCO2OL, KCH4OL, KH2SOL, DSEP                     L13 0180
                                                                         L13 0190
C ================================================================      |L13 0200
                                                                         L13 0210
      CALL CLEAR (SCREEN)                                                L13 0220
```

```
                                                                      L13 0230
   PRINT 10, 'Enter moles of CO2 (per kg of water) to be',            L13 0240
  &          ' distributed between'                                   L13 0250
   PRINT 20, ' oil, water, and vapor.           ',                    L13 0260
  &          ' [Current = ', TCO2M(SAMP), '] '                        L13 0270
   CALL ANSWER (TCO2M(SAMP))                                          L13 0280
                                                                      L13 0290
   PRINT 10, 'Enter moles of CH4 (per kg of water) to be',            L13 0300
  &          ' distributed between'                                   L13 0310
   PRINT 20, ' oil, water, and vapor.           ',                    L13 0320
  &          ' [Current = ', TCH4M(SAMP), '] '                        L13 0330
   CALL ANSWER (TCH4M(SAMP))                                          L13 0340
                                                                      L13 0350
   PRINT 10, 'Enter moles of H2S (per kg of water) to be',            L13 0360
  &          ' distributed between'                                   L13 0370
   PRINT 20, ' oil, water, and vapor.           ',                    L13 0380
  &          ' [Current = ', TH2SM(SAMP), '] '                        L13 0390
   CALL ANSWER (TH2SM(SAMP))                                          L13 0400
                                                                      L13 0410
   PRINT 20, 'Oil to water weight ratio         ', '[Current = ',     L13 0420
  &          WROIL(SAMP), '] '                                        L13 0430
   CALL ANSWER (WROIL(SAMP))                                          L13 0440
                                                                      L13 0450
   PRINT 10, 'Henry''s law coefficient for the solubility',           L13 0460
  &          ' of CO2 in oil'                                         L13 0470
   PRINT 30, '[Current = ', KCO2OL(SAMP), '] '                        L13 0480
   CALL ANSWER (KCO2OL(SAMP))                                         L13 0490
                                                                      L13 0500
   PRINT 10, 'Henry''s law coefficient for the solubility',           L13 0510
  &          ' of CH4 in oil'                                         L13 0520
   PRINT 30, '[Current = ', KCH4OL(SAMP), '] '                        L13 0530
   CALL ANSWER (KCH4OL(SAMP))                                         L13 0540
                                                                      L13 0550
   PRINT 10, 'Henry''s law coefficient for the solubility',           L13 0560
  &          ' of H2S in oil'                                         L13 0570
   PRINT 30, '[Current = ', KH2SOL(SAMP), '] '                        L13 0580
   CALL ANSWER (KH2SOL(SAMP))                                         L13 0590
                                                                      L13 0600
   PRINT 40, 'Density of oil @ 15 Deg C          [Current = ',        L13 0610
  &          DSEP(SAMP), '] '                                         L13 0620
   CALL ANSWER (DSEP(SAMP))                                           L13 0630
                                                                      L13 0640
10 FORMAT (1X, A, A)                                                  L13 0650
20 FORMAT (1X, A, A, 1P, E10.4, A)                                    L13 0660
30 FORMAT (36X, A, 1P, E10.4, A)                                      L13 0670
40 FORMAT (1X, A, 1P, E10.4, A)                                       L13 0680
                                                                      L13 0690
   RETURN                                                             L13 0700
   END                                                                L13 0710
```

```
      SUBROUTINE LINE14                                                  L14 0010
C ================================================================|L14 0020
C     Gets the values for line 14 of the input file.  See table 1  |L14 0030
C ----------------------------------------------------------------|L14 0040
                                                                       L14 0050
      INTEGER MAX, SCREEN                                              L14 0060
      CHARACTER * 15 OPTION                                            L14 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)           L14 0080
                                                                       L14 0090
      INTEGER CHOICE, I, IDN(10,10,MAX), INSP(MAX), ISCHG(10,MAX)      L14 0100
      INTEGER ISCOMP(10,MAX), J, NL, SAMP, TMPVAL                      L14 0110
                                                                       L14 0120
      CHARACTER *  1 ADEX(MAX)                                         L14 0130
      CHARACTER *  2 TNUM                                              L14 0140
      CHARACTER * 10 ANSWR, SPN(10,MAX)                                L14 0150
                                                                       L14 0160
      DOUBLE PRECISION CEC(MAX), COEF(10,10,MAX), KRXN(10,MAX)         L14 0170
      DOUBLE PRECISION MBASE(10,MAX), SAREA(MAX), TAREA(MAX)           L14 0180
                                                                       L14 0190
      EXTERNAL ANSWER, CLEAR, IANSWR                                   L14 0200
                                                                       L14 0210
      COMMON           SAMP                                            L14 0220
      COMMON /COM8   / ADEX, SPN                                       L14 0230
      COMMON /COM9   / CEC, TAREA, SAREA, INSP, ISCHG, MBASE, KRXN,    L14 0240
     &                 ISCOMP, COEF, IDN                             L14 0250
                                                                       L14 0260
C ================================================================|L14 0270
                                                                       L14 0280
      NL = SCREEN                                                      L14 0290
                                                                       L14 0300
   10 CONTINUE                                                         L14 0310
      CALL CLEAR (NL)                                                  L14 0320
      PRINT OPTION, '1)  Adsorption'                                   L14 0330
      PRINT *                                                          L14 0340
      PRINT OPTION, '2)  Ion Exchange'                                 L14 0350
      PRINT *                                                          L14 0360
      PRINT OPTION, '3)  Clear Option'                                 L14 0370
      PRINT *                                                          L14 0380
      PRINT *                                                          L14 0390
      PRINT OPTION, '    Enter Choice (1-3)'                           L14 0400
      PRINT *                                                          L14 0410
                                                                       L14 0420
      IF      (ADEX(SAMP) .EQ. 'A' .OR. ADEX(SAMP) .EQ. 'a') THEN      L14 0430
        CHOICE = 1                                                     L14 0440
      ELSE IF (ADEX(SAMP) .EQ. 'E' .OR. ADEX(SAMP) .EQ. 'e') THEN      L14 0450
        CHOICE = 2                                                     L14 0460
      ELSE                                                             L14 0470
        CHOICE = 3                                                     L14 0480
      END IF                                                           L14 0490
                                                                       L14 0500
      PRINT '(14X, A, I2, A)', '[Current = ', CHOICE, '] '             L14 0510
                                                                       L14 0520
      CALL IANSWR (CHOICE)                                             L14 0530
                                                                       L14 0540
```

```
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 4) THEN                        L14 0550
        PRINT *, 'Answer must be in the range [1-3] '                    L14 0560
        NL = SCREEN - 12                                                L14 0570
        GOTO 10                                                         L14 0580
      END IF                                                            L14 0590
                                                                        L14 0600
      IF      (CHOICE .EQ. 1) THEN                                      L14 0610
        ADEX(SAMP) = 'A'                                                L14 0620
      ELSE IF (CHOICE .EQ. 2) THEN                                      L14 0630
        ADEX(SAMP) = 'E'                                                L14 0640
      ELSE IF (CHOICE .EQ. 3) THEN                                      L14 0650
        ADEX(SAMP)   = ' '                                              L14 0660
        CEC(SAMP)    = 0.00001                                          L14 0670
        TAREA(SAMP)  = 0.0                                              L14 0680
        SAREA(SAMP)  = 0.0                                              L14 0690
        INSP(SAMP)   = 0                                                L14 0700
                                                                        L14 0710
        DO 30 I = 1, 10                                                 L14 0720
          ISCHG(I,SAMP)  = 0                                            L14 0730
          ISCOMP(I,SAMP) = 0                                            L14 0740
          WRITE (TNUM, '(I2)') I                                        L14 0750
          SPN(I,SAMP)    = 'Species ' // TNUM                           L14 0760
          MBASE(I,SAMP)  = 0.0                                          L14 0770
          KRXN(I,SAMP)   = 1.0                                          L14 0780
          DO 20 J = 1, 10                                               L14 0790
            IDN(I,J,SAMP)  = 0                                          L14 0800
            COEF(I,J,SAMP) = 0.0                                        L14 0810
20        CONTINUE                                                      L14 0820
30      CONTINUE                                                        L14 0830
        RETURN                                                          L14 0840
      END IF                                                            L14 0850
                                                                        L14 0860
      PRINT *                                                           L14 0870
      PRINT *, 'What is the cation exchange capacity in',               L14 0880
     &         ' milliequivalents/kg of water ?'                        L14 0890
      PRINT 910, '     [Current = ', CEC(SAMP), '] '                    L14 0900
                                                                        L14 0910
      CALL ANSWER (CEC(SAMP))                                           L14 0920
                                                                        L14 0930
      PRINT *                                                           L14 0940
      PRINT *, 'What is the site density per unit are in sites/sq.',    L14 0950
     &         ' cm. ?'                                                 L14 0960
      PRINT 910, '     [Current = ', TAREA(SAMP), '] '                  L14 0970
                                                                        L14 0980
      CALL ANSWER (TAREA(SAMP))                                         L14 0990
                                                                        L14 1000
      PRINT *                                                           L14 1010
      PRINT *, 'What is the total surface area per kilogram of',        L14 1020
     &         ' solvent in sq. cm. ?'                                  L14 1030
      PRINT 910, '     [Current = ', SAREA(SAMP), '] '                  L14 1040
                                                                        L14 1050
      CALL ANSWER (SAREA(SAMP))                                         L14 1060
                                                                        L14 1070
40    CONTINUE                                                          L14 1080
```

```
      PRINT *                                                           L14 1090
      PRINT *, 'How many surface species are there ?'                   L14 1100
      PRINT 920, '     [Current = ', INSP(SAMP), '] '                   L14 1110
                                                                        L14 1120
      TMPVAL = INSP(SAMP)                                               L14 1130
      CALL IANSWR (INSP(SAMP))                                          L14 1140
                                                                        L14 1150
      IF (INSP(SAMP) .LT. 0 .OR. INSP(SAMP) .GT. 10) THEN               L14 1160
        PRINT *, 'Answer must be in the range [0-10] '                   L14 1170
        INSP(SAMP) = TMPVAL                                             L14 1180
        CALL CLEAR(SCREEN - 5)                                          L14 1190
        GOTO 40                                                         L14 1200
      END IF                                                            L14 1210
                                                                        L14 1220
      DO 80 I = 1, INSP(SAMP)                                           L14 1230
        PRINT '(1X, A, I2)', 'What is the name of species ', I          L14 1240
        PRINT 900, '     [Current = "', SPN(I,SAMP), '"] '              L14 1250
                                                                        L14 1260
        READ '(A10)', ANSWR                                             L14 1270
                                                                        L14 1280
        IF (ANSWR .NE. ' ') THEN                                        L14 1290
          SPN(I,SAMP) = ANSWR                                           L14 1300
        END IF                                                          L14 1310
                                                                        L14 1320
        PRINT *, 'What is the mole fraction of ', SPN(I,SAMP), ' ?'     L14 1330
        PRINT 910, '     [Current = ', MBASE(I,SAMP), '] '              L14 1340
                                                                        L14 1350
        CALL ANSWER (MBASE(I,SAMP))                                     L14 1360
                                                                        L14 1370
        PRINT *, 'What is the charge of ', SPN(I,SAMP), ' ?'            L14 1380
        PRINT 920, '     [Current = ', ISCHG(I,SAMP), '] '              L14 1390
                                                                        L14 1400
        CALL IANSWR (ISCHG(I,SAMP))                                     L14 1410
                                                                        L14 1420
        PRINT *, 'What is the dissociation constant for the reaction',  L14 1430
     &           ' of ', SPN(I,SAMP), ' ?'                              L14 1440
        PRINT 910, '     [Current = ', KRXN(I,SAMP), '] '               L14 1450
                                                                        L14 1460
        CALL ANSWER (KRXN(I,SAMP))                                      L14 1470
                                                                        L14 1480
50    CONTINUE                                                          L14 1490
        PRINT *                                                         L14 1500
        PRINT *, 'How many components are in the dissociation',         L14 1510
     &           ' reaction of ', SPN(I,SAMP), ' ?'                     L14 1520
        PRINT 920, '     [Current = ', ISCOMP(I,SAMP), '] '             L14 1530
                                                                        L14 1540
        TMPVAL = ISCOMP(I,SAMP)                                         L14 1550
        CALL IANSWR (ISCOMP(I,SAMP))                                    L14 1560
                                                                        L14 1570
        IF (ISCOMP(I,SAMP) .LT. 0 .OR. ISCOMP(I,SAMP) .GT. 10) THEN     L14 1580
          PRINT *, 'Answer must be in the range [0-10] '                 L14 1590
          ISCOMP(I,SAMP) = TMPVAL                                       L14 1600
          CALL CLEAR (SCREEN - 5)                                       L14 1610
          GOTO 50                                                       L14 1620
```

```
      END IF                                                            L14 1630
                                                                        L14 1640
      DO 70 J = 1, ISCOMP(I,SAMP)                                       L14 1650
 60     CONTINUE                                                        L14 1660
        PRINT *                                                         L14 1670
        PRINT '(1X, A, A, I2)', 'What is the index number of',          L14 1680
     &                          ' species #', J                        L14 1690
        PRINT '(15X, A, I3, A)', '[Current = ', IDN(I,J,SAMP), ' ] '    L14 1700
                                                                        L14 1710
        TMPVAL = IDN(I,J,SAMP)                                          L14 1720
        CALL IANSWR (IDN(I,J,SAMP))                                     L14 1730
                                                                        L14 1740
        IF (IDN(I,J,SAMP) .LT. 0) THEN                                  L14 1750
          PRINT *, 'Answer must be >= 0'                                L14 1760
          IDN(I,J,SAMP) = TMPVAL                                        L14 1770
          CALL CLEAR (SCREEN - 5)                                       L14 1780
          GOTO 60                                                       L14 1790
        END IF                                                          L14 1800
                                                                        L14 1810
        PRINT '(1X, A, A, I2)', 'What is the reaction coefficient',     L14 1820
     &                          ' of species #', J                     L14 1830
        PRINT '(15X, A, I3, A)', '[Current = ', COEF(I,J,SAMP), ' ] '   L14 1840
                                                                        L14 1850
        CALL ANSWER (COEF(I,J,SAMP))                                    L14 1860
 70   CONTINUE                                                          L14 1870
 80 CONTINUE                                                            L14 1880
                                                                        L14 1890
      RETURN                                                            L14 1900
                                                                        L14 1910
900 FORMAT (1X, A, A, A)                                                L14 1920
910 FORMAT (1X, A, 1P, E10.4, A)                                        L14 1930
920 FORMAT (1X, A, I4, A)                                               L14 1940
                                                                        L14 1950
      END                                                               L14 1960
```

```
      SUBROUTINE LINE16                                                 L16 0010
C ======================================================================|L16 0020
C     Gets the values for line 16 of the input file.  See table 1       |L16 0030
C ----------------------------------------------------------------------|L16 0040
                                                                        L16 0050
      INTEGER MAX, SCREEN                                               L16 0060
      CHARACTER * 20 OPTION, USING                                      L16 0070
      DOUBLE PRECISION CPUMIN                                           L16 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, SCREEN = 24)               L16 0090
      PARAMETER (OPTION =  '(1X, A, F6.2, A)')                          L16 0100
      PARAMETER (USING = '(15X, A, E10.4, A)')                          L16 0110
                                                                        L16 0120
      INTEGER I, NDUM(12,MAX), NL, SAMP                                 L16 0130
                                                                        L16 0140
      CHARACTER *  1 ANS, ODUM(12,MAX)                                  L16 0150
```

```
                                                                        L16 0160
      DOUBLE PRECISION DENS(MAX), HITEMP(MAX), PRESS(MAX), TEMP(MAX)    L16 0170
      DOUBLE PRECISION XDUM(12,MAX)                                     L16 0180
                                                                        L16 0190
      EXTERNAL ANSWER, CLEAR, IANSWR, UPCASE                            L16 0200
                                                                        L16 0210
      COMMON           SAMP                                             L16 0220
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                         L16 0230
      COMMON /COM11 / ODUM                                              L16 0240
      COMMON /COM12 / NDUM, XDUM                                        L16 0250
                                                                        L16 0260
C ======================================================================L16 0270
                                                                        L16 0280
      CALL CLEAR (SCREEN)                                               L16 0290
                                                                        L16 0300
      PRINT OPTION, 'Do you wish to enter new Log K values for ',       L16 0310
     &              TEMP(SAMP), ' degrees ? '                          L16 0320
      READ '(A1)', ANS                                                  L16 0330
                                                                        L16 0340
      I = 1                                                             L16 0350
                                                                        L16 0360
      NL = 2                                                            L16 0370
                                                                        L16 0380
      IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                          L16 0390
   10   CONTINUE                                                       L16 0400
        CALL CLEAR (NL)                                                 L16 0410
        PRINT *, 'Enter an (A)queous complex, a (M)ineral ',            L16 0420
     &           'dissociation or (Q)uit ?'                            L16 0430
        PRINT '(15X, A, A, A)', '[Current = ', ODUM(I,SAMP), ' ] '      L16 0440
                                                                        L16 0450
        READ '(A1)', ANS                                                L16 0460
                                                                        L16 0470
        CALL UPCASE (ANS, 1)                                            L16 0480
                                                                        L16 0490
        IF (ANS .NE. 'A' .AND. ANS .NE. 'M' .AND.                       L16 0500
     &      ANS .NE. 'Q' .AND. ANS .NE. ' ') THEN                       L16 0510
          PRINT *, 'Answer must be in the range [A, a, M, m, Q, q] '     L16 0520
          NL = SCREEN - 4                                               L16 0530
          ANS = ODUM(I,SAMP)                                            L16 0540
          GOTO 10                                                       L16 0550
        END IF                                                          L16 0560
                                                                        L16 0570
        IF (ANS .EQ. 'A' .OR. ANS .EQ. 'M') ODUM(I,SAMP) = ANS          L16 0580
                                                                        L16 0590
        IF (ANS .NE. 'Q') THEN                                          L16 0600
          PRINT *, 'Enter the ID # of the Log K to change'              L16 0610
          PRINT '(15X, A, I4, A)', '[Current = ', NDUM(I,SAMP), '] '    L16 0620
          CALL IANSWR (NDUM(I,SAMP))                                    L16 0630
                                                                        L16 0640
          IF (ANS .EQ. 'A') THEN                                        L16 0650
            PRINT *, 'What is the Log K for the dissociation ',         L16 0660
     &               'reaction ? '                                      L16 0670
            PRINT USING, '[Current = ', XDUM(I,SAMP), '] '              L16 0680
            CALL ANSWER (XDUM(I,SAMP))                                  L16 0690
```

```
      ELSE                                                              L16 0700
        PRINT *, 'What is the Log K for the dissolution reaction ? 'L16 0710
        PRINT USING, '[Current = ', XDUM(I,SAMP), '] '                  L16 0720
        CALL ANSWER (XDUM(I,SAMP))                                      L16 0730
      END IF                                                            L16 0740
    END IF                                                              L16 0750
                                                                        L16 0760
    IF (ANS .NE. 'Q' .AND. I .LT. 6) THEN                               L16 0770
      I = I + 1                                                         L16 0780
      NL = 2                                                            L16 0790
      GOTO 10                                                           L16 0800
    END IF                                                              L16 0810
  END IF                                                                L16 0820
                                                                        L16 0830
  CALL CLEAR (SCREEN)                                                   L16 0840
                                                                        L16 0850
  IF (HITEMP(SAMP) .LE. CPUMIN) GOTO 30                                 L16 0860
                                                                        L16 0870
  PRINT OPTION, 'Do you wish to enter new Log K values for',            L16 0880
 &              HITEMP(SAMP), ' degrees ? '                            L16 0890
  READ '(A1)', ANS                                                      L16 0900
                                                                        L16 0910
  I = 7                                                                 L16 0920
  NL = 2                                                                L16 0930
                                                                        L16 0940
  IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                              L16 0950
20  CONTINUE                                                          L16 0960
    CALL CLEAR (NL)                                                     L16 0970
    PRINT *, 'Enter an (A)queous complex, a (M)ineral ',                L16 0980
 &           'dissociation or (Q)uit ?'                                 L16 0990
    PRINT '(15X, A, A, A)', '[Current = ', ODUM(I,SAMP), ' ] '          L16 1000
                                                                        L16 1010
    READ '(A1)', ANS                                                    L16 1020
                                                                        L16 1030
    CALL UPCASE (ANS, 1)                                                L16 1040
                                                                        L16 1050
    IF (ANS .NE. 'A' .AND. ANS .NE. 'M' .AND.                           L16 1060
 &      ANS .NE. 'Q' .AND. ANS .NE. ' ') THEN                          L16 1070
      PRINT *, 'Answer must be in the range [A, a, M, m, Q, q] '        L16 1080
      NL = SCREEN - 4                                                   L16 1090
      GOTO 20                                                           L16 1100
    END IF                                                              L16 1110
                                                                        L16 1120
    IF (ANS .EQ. 'A' .OR. ANS .EQ. 'M') ODUM(I,SAMP) = ANS              L16 1130
                                                                        L16 1140
    IF (ANS .NE. 'Q') THEN                                              L16 1150
      PRINT *, 'Enter the ID # of the Log K to change'                   L16 1160
      PRINT '(15X, A, I4, A)', '[Current = ', NDUM(I,SAMP), '] '        L16 1170
      CALL IANSWR (NDUM(I,SAMP))                                        L16 1180
                                                                        L16 1190
      PRINT *, 'What is the Log K for the dissociation reaction ?'      L16 1200
      PRINT '(15X, A, E10.4, A)', '[Current = ', XDUM(I,SAMP), '] '     L16 1210
      CALL ANSWER (XDUM(I,SAMP))                                        L16 1220
    END IF                                                              L16 1230
```

```
                                                                      L18 0940
      END                                                             L18 0950



      SUBROUTINE LINE20 (CHOICE)                                      L20 0010
C ==========================================================================|L20 0020
C     Gets the values for line 20 of the input file.  See table 1         |L20 0030
C --------------------------------------------------------------------------|L20 0040
                                                                      L20 0050
      INTEGER MAX, SCREEN                                             L20 0060
      CHARACTER * 15 OPTION, USING                                    L20 0070
      DOUBLE PRECISION CPUMIN                                         L20 0080
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, OPTION = '(10X, A)')     L20 0090
      PARAMETER (SCREEN = 24, USING = '(1X, A, I2)')                  L20 0100
                                                                      L20 0110
      INTEGER CHOICE, I, MININD(10,5,MAX), SAMP                       L20 0120
                                                                      L20 0130
      CHARACTER *  8 ANSWR, MINAME(5,MAX)                             L20 0140
                                                                      L20 0150
      DOUBLE PRECISION DENS(MAX), HITEMP(MAX), MINCO(10,5,MAX)        L20 0160
      DOUBLE PRECISION MINLOG(2,5,MAX), PRESS(MAX), TEMP(MAX)         L20 0170
                                                                      L20 0180
      EXTERNAL ANSWER, CLEAR, IANSWR                                  L20 0190
                                                                      L20 0200
      COMMON           SAMP                                           L20 0210
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                       L20 0220
      COMMON /COM18 / MINAME                                          L20 0230
      COMMON /COM19 / MINCO, MININD, MINLOG                           L20 0240
                                                                      L20 0250
C ==========================================================================|L20 0260
                                                                      L20 0270
      CALL CLEAR (SCREEN)                                             L20 0280
                                                                      L20 0290
      PRINT *, 'What is the name of the mineral ? '                   L20 0300
      PRINT '(1X, A8)', MINAME(CHOICE,SAMP)                           L20 0310
      PRINT *                                                         L20 0320
                                                                      L20 0330
      ANSWR = ' '                                                     L20 0340
      READ '(A8)', ANSWR                                              L20 0350
                                                                      L20 0360
      IF (ANSWR .NE. ' ') THEN                                        L20 0370
        MINAME(CHOICE,SAMP) = ANSWR                                   L20 0380
      END IF                                                          L20 0390
                                                                      L20 0400
      DO 10 I = 1, 9                                                  L20 0410
        PRINT *                                                       L20 0420
        PRINT USING, 'What is the index number of species #', I       L20 0430
        PRINT '(15X, A, I3, A)', '[Current = ', MININD(I,CHOICE,SAMP),L20 0440
     &                           '] '                                 L20 0450
        CALL IANSWR (MININD(I,CHOICE,SAMP))                           L20 0460
        IF (MININD(I,CHOICE,SAMP) .EQ. 0) GOTO 20                     L20 0470
```

```
                                                                      L20 0480
      PRINT *                                                         L20 0490
      PRINT USING, 'What is the reaction coefficient of species #', I L20 0500
      PRINT '(15X, A, F5.2, A)', '[Current = ', MINCO(I,CHOICE,SAMP), L20 0510
     &                           '] '                                 L20 0520
      CALL ANSWER (MINCO(I,CHOICE,SAMP))                              L20 0530
   10 CONTINUE                                                        L20 0540
                                                                      L20 0550
   20 CONTINUE                                                        L20 0560
      PRINT *, 'Enter any additional activity parameter the reaction', L20 0570
     &         ' should include.'                                     L20 0580
      PRINT '(15X, A, F5.2, A)', '[Current = ', MINCO(10,CHOICE,SAMP), L20 0590
     &                           '] '                                 L20 0600
      CALL ANSWER (MINCO(10,CHOICE,SAMP))                             L20 0610
                                                                      L20 0620
      PRINT '(1X, A, F5.2)', 'What is the log K of the mineral at ',  L20 0630
     &                    TEMP(SAMP)                                 L20 0640
      PRINT '(15X, A, F5.2, A)', '[Current = ', MINLOG(1,CHOICE,SAMP), L20 0650
     &                           '] '                                 L20 0660
      CALL ANSWER (MINLOG(1,CHOICE,SAMP))                             L20 0670
                                                                      L20 0680
      IF (HITEMP(SAMP) .GT. CPUMIN) THEN                              L20 0690
        PRINT '(1X, A, F5.2)', 'What is the log K of the mineral at ', L20 0700
     &                      HITEMP(SAMP)                            L20 0710
        PRINT '(15X, A, F5.2, A)', '[Current = ', MINLOG(2,CHOICE,SAMP),L20 0720
     &                           '] '                                 L20 0730
        CALL ANSWER (MINLOG(2,CHOICE,SAMP))                           L20 0740
      END IF                                                          L20 0750
                                                                      L20 0760
      RETURN                                                          L20 0770
      END                                                             L20 0780
```

```
      SUBROUTINE LINE23 (CONV1, CONV2)                                L23 0010
C ==========================================================================|L23 0020
C     Gets the values for line 23 of the input file.  See table 1       |L23 0030
C --------------------------------------------------------------------------|L23 0040
                                                                      L23 0050
      INTEGER MAX, SCREEN                                             L23 0060
      CHARACTER * 25 USING                                            L23 0070
      PARAMETER (MAX = 10, SCREEN = 24, USING = '(1X, A, 1P, E10.4, A)')L23 0080
                                                                      L23 0090
      INTEGER SAMP                                                    L23 0100
                                                                      L23 0110
      DOUBLE PRECISION CONV1(MAX), CONV2(MAX)                         L23 0120
                                                                      L23 0130
      EXTERNAL ANSWER, CLEAR                                          L23 0140
                                                                      L23 0150
      COMMON           SAMP                                           L23 0160
                                                                      L23 0170
C ==========================================================================|L23 0180
```

```
                                                                      L16 1240
        IF (ANS .NE. 'Q' .AND. I .LT. 12) THEN                        L16 1250
          I = I + 1                                                   L16 1260
          GOTO 20                                                     L16 1270
        END IF                                                        L16 1280
      END IF                                                          L16 1290
                                                                      L16 1300
   30 CONTINUE                                                        L16 1310
      RETURN                                                          L16 1320
      END                                                             L16 1330




      SUBROUTINE LINE18                                               L18 0010
C ==========================================================================|L18 0020
C     Gets the values for line 18 of the input file.  See table 1           |L18 0030
C --------------------------------------------------------------------------|L18 0040
                                                                      L18 0050
      INTEGER MAX, SCREEN                                             L18 0060
      CHARACTER * 10 OPTION                                           L18 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)          L18 0080
                                                                      L18 0090
      INTEGER ANSR(3,MAX), CHOICE, MININD(10,5,MAX), ND(2,45,MAX)     L18 0100
      INTEGER NL, NUM, SAMP, Z(3,MAX)                                 L18 0110
                                                                      L18 0120
      CHARACTER *  8 MINAME(5,MAX), PAGE(45,MAX)                      L18 0130
                                                                      L18 0140
      DOUBLE PRECISION CONC(3,MAX), DENS(MAX), DHA(3,MAX), DNA(45,MAX) L18 0150
      DOUBLE PRECISION GFW(3,MAX), HITEMP(MAX), MINCO(10,5,MAX)       L18 0160
      DOUBLE PRECISION MINLOG(2,5,MAX), PRESS(MAX), TEMP(MAX)         L18 0170
      DOUBLE PRECISION XD(2,45,MAX)                                   L18 0180
                                                                      L18 0190
      EXTERNAL CATION, CLEAR, COMPLX, IANSWR, ION, MINERL             L18 0200
                                                                      L18 0210
      COMMON           SAMP                                           L18 0220
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                       L18 0230
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                         L18 0240
      COMMON /COM16 / PAGE                                            L18 0250
      COMMON /COM17 / ND, XD, DNA                                     L18 0260
      COMMON /COM18 / MINAME                                          L18 0270
      COMMON /COM19 / MINCO, MININD, MINLOG                           L18 0280
                                                                      L18 0290
C ==========================================================================|L18 0300
                                                                      L18 0310
      NL = SCREEN                                                     L18 0320
      CHOICE = -1                                                     L18 0330
                                                                      L18 0340
   10 CONTINUE                                                        L18 0350
      CALL CLEAR (NL)                                                 L18 0360
                                                                      L18 0370
      PRINT OPTION, '    ADDITIONAL IONS AND MINERALS MENU'           L18 0380
      PRINT *                                                         L18 0390
```

```
PRINT OPTION, '1)  Enter Anion #1'                                    L18 0400
PRINT *                                                               L18 0410
PRINT OPTION, '2)  Enter Complexs for Anion #1'                       L18 0420
PRINT *                                                               L18 0430
PRINT OPTION, '3)  Enter Anion #2'                                    L18 0440
PRINT *                                                               L18 0450
PRINT OPTION, '4)  Enter Complexs for Anion #2'                       L18 0460
PRINT *                                                               L18 0470
PRINT OPTION, '5)  Enter Additional Cation'                           L18 0480
PRINT *                                                               L18 0490
PRINT OPTION, '6)  Enter Cation Complexes'                            L18 0500
PRINT *                                                               L18 0510
PRINT OPTION, '7)  Enter Additional Minerals'                         L18 0520
PRINT *                                                               L18 0530
PRINT OPTION, '8)  Return to Options Menu'                            L18 0540
PRINT *                                                               L18 0550
PRINT *                                                               L18 0560
PRINT OPTION, '    Enter Choice (1-8) '                               L18 0570
                                                                      L18 0580
CALL IANSWR (CHOICE)                                                  L18 0590
                                                                      L18 0600
IF (CHOICE .LT. 1 .OR. CHOICE .GT. 8) THEN                            L18 0610
  PRINT *, 'Answer must be in the range [1-8] '                        L18 0620
  NL = SCREEN - 22                                                    L18 0630
  CHOICE = -1                                                         L18 0640
  GOTO 10                                                             L18 0650
END IF                                                                L18 0660
                                                                      L18 0670
IF      (CHOICE .EQ. 1) THEN                                          L18 0680
  NUM = 1                                                             L18 0690
  CALL ION (NUM)                                                      L18 0700
ELSE IF (CHOICE .EQ. 2) THEN                                          L18 0710
  NUM = 1                                                             L18 0720
  CALL COMPLX (NUM)                                                   L18 0730
ELSE IF (CHOICE .EQ. 3) THEN                                          L18 0740
  NUM = 16                                                            L18 0750
  CALL ION (NUM)                                                      L18 0760
ELSE IF (CHOICE .EQ. 4) THEN                                          L18 0770
  NUM = 16                                                            L18 0780
  CALL COMPLX (NUM)                                                   L18 0790
ELSE IF (CHOICE .EQ. 5) THEN                                          L18 0800
  NUM = 31                                                            L18 0810
  CALL ION (NUM)                                                      L18 0820
ELSE IF (CHOICE .EQ. 6) THEN                                          L18 0830
  CALL CATION                                                         L18 0840
ELSE IF (CHOICE .EQ. 7) THEN                                          L18 0850
  CALL MINERL                                                         L18 0860
ELSE IF (CHOICE .EQ. 8) THEN                                          L18 0870
  RETURN                                                              L18 0880
END IF                                                                L18 0890
                                                                      L18 0900
NL = SCREEN - 21                                                      L18 0910
CHOICE = -1                                                           L18 0920
GOTO 10                                                               L18 0930
```

```
                                                                        L23 0190
      CALL CLEAR (SCREEN)                                               L23 0200
      PRINT *, 'Enter the new value for the tolerance factor for'       L23 0210
      PRINT *, ' convergence on the distribution of the anions.'        L23 0220
      PRINT USING, '                [Current = ', CONV1(SAMP), '] '     L23 0230
                                                                        L23 0240
      CALL ANSWER (CONV1(SAMP))                                         L23 0250
                                                                        L23 0260
      PRINT *                                                           L23 0270
      PRINT *                                                           L23 0280
      PRINT *, 'Enter the new value for the tolerance factor for'       L23 0290
      PRINT *, ' the pH calculation using hydronium mass balance'       L23 0300
      PRINT USING, '  equation.     [Current = ', CONV2(SAMP), '] '     L23 0310
                                                                        L23 0320
      CALL ANSWER (CONV2(SAMP))                                         L23 0330
                                                                        L23 0340
      RETURN                                                            L23 0350
      END                                                               L23 0360


      SUBROUTINE MAJORS                                                 MAJ 0010
C ======================================================================|MAJ 0020
C     Display menu for entering values for major ion components         |MAJ 0030
C ----------------------------------------------------------------------|MAJ 0040
                                                                        MAJ 0050
      INTEGER MAX, SCREEN                                               MAJ 0060
      CHARACTER * 10 OPTION                                             MAJ 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)            MAJ 0080
                                                                        MAJ 0090
      INTEGER CHOICE, NL, SAMP                                          MAJ 0100
                                                                        MAJ 0110
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                         MAJ 0120
                                                                        MAJ 0130
      EXTERNAL CLEAR, IANSWR, LINE04, LINE05                            MAJ 0140
                                                                        MAJ 0150
      COMMON           SAMP                                             MAJ 0160
      COMMON /COM4   / CUNITS, TIC                                      MAJ 0170
                                                                        MAJ 0180
C ======================================================================|MAJ 0190
                                                                        MAJ 0200
      NL = SCREEN                                                       MAJ 0210
      CHOICE = -1                                                       MAJ 0220
                                                                        MAJ 0230
   10 CONTINUE                                                          MAJ 0240
      CALL CLEAR (NL)                                                   MAJ 0250
                                                                        MAJ 0260
      PRINT OPTION, '1)  ENTER: Na, K, Li, Ca, Mg, Fe, Al'              MAJ 0270
      PRINT *                                                           MAJ 0280
      PRINT OPTION, '2)  ENTER: SiO2, Cl, SO4, H2S, HCO3, CO3, TIC'     MAJ 0290
      PRINT *                                                           MAJ 0300
      PRINT OPTION, '3)  Return to Basic Parameters Menu'               MAJ 0310
```

```
      PRINT *                                                          MAJ 0320
      PRINT *                                                          MAJ 0330
      PRINT OPTION, '    Enter Choice (1-3) '                          MAJ 0340
                                                                       MAJ 0350
      CALL IANSWR (CHOICE)                                             MAJ 0360
                                                                       MAJ 0370
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 3) THEN                       MAJ 0380
        PRINT *, 'Answer must be in the range [1-3] '                  MAJ 0390
        NL = SCREEN - 10                                               MAJ 0400
        CHOICE = -1                                                    MAJ 0410
        GOTO 10                                                        MAJ 0420
      END IF                                                           MAJ 0430
                                                                       MAJ 0440
      IF      (CHOICE .EQ. 1) THEN                                     MAJ 0450
        CALL LINE04                                                    MAJ 0460
      ELSE IF (CHOICE .EQ. 2) THEN                                     MAJ 0470
        CALL LINE05                                                    MAJ 0480
      ELSE IF (CHOICE .EQ. 3) THEN                                     MAJ 0490
        RETURN                                                         MAJ 0500
      END IF                                                           MAJ 0510
                                                                       MAJ 0520
      NL = SCREEN - 9                                                  MAJ 0530
      CHOICE = -1                                                      MAJ 0540
      GOTO 10                                                          MAJ 0550
                                                                       MAJ 0560
      END                                                              MAJ 0570
```

```
      SUBROUTINE MAMENU (CHOICE)                                       MAM 0010
C ==========================================================================|MAM 0020
C     Display main menu                                                  |MAM 0030
C --------------------------------------------------------------------------|MAM 0040
                                                                       MAM 0050
      INTEGER SCREEN                                                   MAM 0060
      CHARACTER * 10 OPTION                                            MAM 0070
      PARAMETER (OPTION = '(10X, A)', SCREEN = 24)                     MAM 0080
                                                                       MAM 0090
      INTEGER CHOICE, SAMP                                             MAM 0100
                                                                       MAM 0110
      EXTERNAL CLEAR, IANSWR                                           MAM 0120
                                                                       MAM 0130
      COMMON          SAMP                                             MAM 0140
                                                                       MAM 0150
C ==========================================================================|MAM 0160
                                                                       MAM 0170
      CHOICE = 0                                                       MAM 0180
                                                                       MAM 0190
   10 CONTINUE                                                         MAM 0200
      PRINT '(60X, A, I2)', 'Sample ', SAMP                            MAM 0210
      PRINT *                                                          MAM 0220
      PRINT *                                                          MAM 0230
```

```
      PRINT OPTION, '    MAIN MENU'                                          MAM 0240
      PRINT *                                                                MAM 0250
      PRINT *                                                                MAM 0260
      PRINT OPTION, '1)  Create/Edit Current Sample Data'                    MAM 0270
      PRINT *                                                                MAM 0280
      PRINT OPTION, '2)  Read an Existing Input File'                        MAM 0290
      PRINT *                                                                MAM 0300
      PRINT OPTION, '3)  Go to Next Sample'                                  MAM 0310
      PRINT *                                                                MAM 0320
      PRINT OPTION, '4)  Go to Previous Sample'                              MAM 0330
      PRINT *                                                                MAM 0340
      PRINT OPTION, '5)  Write All Samples to an Input File'                 MAM 0350
      PRINT *                                                                MAM 0360
      PRINT OPTION, '6)  Exit Program'                                       MAM 0370
      PRINT *                                                                MAM 0380
      PRINT *                                                                MAM 0390
      PRINT OPTION, '    Enter Choice (1-6) '                                MAM 0400
                                                                             MAM 0410
      CALL IANSWR (CHOICE)                                                   MAM 0420
                                                                             MAM 0430
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 6) THEN                             MAM 0440
        PRINT *, 'Answer must be in the range [1-6] '                        MAM 0450
        CHOICE = 0                                                           MAM 0460
        CALL CLEAR (SCREEN - 23)                                             MAM 0470
        GOTO 10                                                              MAM 0480
      END IF                                                                 MAM 0490
                                                                             MAM 0500
      RETURN                                                                 MAM 0510
      END                                                                    MAM 0520
```

```
      SUBROUTINE MASTRN                                                      MAS 0010
C ====================================================================|MAS 0020
C     Display mass transfer menu                                       |MAS 0030
C --------------------------------------------------------------------|MAS 0040
                                                                             MAS 0050
      INTEGER MAX, SCREEN                                                    MAS 0060
      CHARACTER * 12 OPTION                                                  MAS 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)                 MAS 0080
                                                                             MAS 0090
      INTEGER CHOICE, IBMIX(MAX), IDDP(MAX), IDMIX(50, MAX)                  MAS 0100
      INTEGER IDN(10,10,MAX), IDSAT(MAX), INMIX(MAX), INSP(MAX)              MAS 0110
      INTEGER IRXDP(10, MAX), ISCHG(10, MAX), ISCOMP(10,MAX), ITMIX(MAX)MAS 0120
      INTEGER ITT(MAX), NL, SAMP                                             MAS 0130
                                                                             MAS 0140
      CHARACTER *  1 ADEX(MAX)                                               MAS 0150
      CHARACTER * 10 SPN(10,MAX)                                             MAS 0160
      CHARACTER * 80 MIXFLE(MAX), OUTIN(MAX)                                 MAS 0170
                                                                             MAS 0180
      DOUBLE PRECISION AMOL(50, MAX), CEC(MAX), COEF(10,10,MAX)              MAS 0190
      DOUBLE PRECISION DFRAC1(MAX), DP(MAX), FBOIL(MAX), INC(MAX)            MAS 0200
```

```
      DOUBLE PRECISION KRXN(10,MAX), MBASE(10,MAX)                      MAS 0210
      DOUBLE PRECISION RXDP(10,MAX), SAREA(MAX), TAREA(MAX)             MAS 0220
                                                                        MAS 0230
      EXTERNAL BOILIT, CLEAR, DSLPPT, IANSWR, LINE14, MIXIT             MAS 0240
                                                                        MAS 0250
      COMMON           SAMP                                             MAS 0260
      COMMON /COM8   / ADEX, SPN                                        MAS 0270
      COMMON /COM9   / CEC, TAREA, SAREA, INSP, ISCHG, MBASE, KRXN,     MAS 0280
     &                 ISCOMP, COEF, IDN                              MAS 0290
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,        MAS 0300
     &                 IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL   MAS 0310
      COMMON /COM20 / MIXFLE, OUTIN                                     MAS 0320
                                                                        MAS 0330
C ======================================================================|MAS 0340
                                                                        MAS 0350
      NL = SCREEN                                                       MAS 0360
      CHOICE = -1                                                       MAS 0370
                                                                        MAS 0380
   10 CONTINUE                                                          MAS 0390
      CALL CLEAR (NL)                                                   MAS 0400
                                                                        MAS 0410
      PRINT OPTION, '    MASS TRANSFER MENU'                            MAS 0420
      PRINT *                                                           MAS 0430
      PRINT OPTION, '1)  Ion Exchange and Adsorption Option'            MAS 0440
      PRINT *                                                           MAS 0450
      PRINT OPTION, '2)  Dissolution/Precipitation Option'              MAS 0460
      PRINT *                                                           MAS 0470
      PRINT OPTION, '3)  Mixing Option'                                 MAS 0480
      PRINT *                                                           MAS 0490
      PRINT OPTION, '4)  Boiling and Dilution Option'                   MAS 0500
      PRINT *                                                           MAS 0510
      PRINT OPTION, '5)  Return to Options Menu'                        MAS 0520
      PRINT *                                                           MAS 0530
      PRINT *                                                           MAS 0540
      PRINT OPTION, '    Enter Choice (1-5) '                           MAS 0550
                                                                        MAS 0560
      CALL IANSWR (CHOICE)                                              MAS 0570
                                                                        MAS 0580
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 5) THEN                        MAS 0590
        PRINT *, 'Answer must be in the range [1-5] '                    MAS 0600
        NL = SCREEN - 16                                                MAS 0610
        CHOICE = -1                                                     MAS 0620
        GOTO 10                                                         MAS 0630
      END IF                                                            MAS 0640
                                                                        MAS 0650
      IF      (CHOICE .EQ. 1) THEN                                      MAS 0660
        CALL LINE14                                                     MAS 0670
      ELSE IF (CHOICE .EQ. 2) THEN                                      MAS 0680
        CALL DSLPPT                                                     MAS 0690
      ELSE IF (CHOICE .EQ. 3) THEN                                      MAS 0700
        CALL MIXIT                                                      MAS 0710
      ELSE IF (CHOICE .EQ. 4) THEN                                      MAS 0720
        CALL BOILIT                                                     MAS 0730
      ELSE IF (CHOICE .EQ. 5) THEN                                      MAS 0740
```

```
        RETURN                                                          MAS 0750
      END IF                                                            MAS 0760
                                                                        MAS 0770
      CHOICE = -1                                                       MAS 0780
      NL = SCREEN - 15                                                  MAS 0790
      GOTO 10                                                           MAS 0800
                                                                        MAS 0810
      END                                                               MAS 0820
```

```
      SUBROUTINE MINERL                                                 MIN 0010
C ================================================================     |MIN 0020
C     Display addition minerals menu                                    |MIN 0030
C ----------------------------------------------------------------     |MIN 0040
                                                                        MIN 0050
      INTEGER MAX, SCREEN                                               MIN 0060
      CHARACTER * 12 OPTION                                             MIN 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A, A)', SCREEN = 24)         MIN 0080
                                                                        MIN 0090
      INTEGER CHOICE, MININD(10,5,MAX), NL, SAMP                        MIN 0100
                                                                        MIN 0110
      CHARACTER *  8 MINAME(5,MAX)                                      MIN 0120
                                                                        MIN 0130
      DOUBLE PRECISION DENS(MAX), HITEMP(MAX), MINCO(10,5,MAX)          MIN 0140
      DOUBLE PRECISION MINLOG(2,5,MAX), PRESS(MAX), TEMP(MAX)           MIN 0150
                                                                        MIN 0160
      EXTERNAL CLEAR, IANSWR, LINE20                                    MIN 0170
                                                                        MIN 0180
      COMMON           SAMP                                             MIN 0190
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                         MIN 0200
      COMMON /COM18 / MINAME                                            MIN 0210
      COMMON /COM19 / MINCO, MININD, MINLOG                             MIN 0220
                                                                        MIN 0230
C ================================================================     |MIN 0240
                                                                        MIN 0250
      NL = SCREEN                                                       MIN 0260
      CHOICE = -1                                                       MIN 0270
                                                                        MIN 0280
   10 CONTINUE                                                          MIN 0290
      CALL CLEAR (NL)                                                   MIN 0300
                                                                        MIN 0310
      PRINT OPTION, '    Choose Mineral'                                MIN 0320
      PRINT *                                                           MIN 0330
      PRINT OPTION, '1)  ', MINAME(1,SAMP)                              MIN 0340
      PRINT *                                                           MIN 0350
      PRINT OPTION, '2)  ', MINAME(2,SAMP)                              MIN 0360
      PRINT *                                                           MIN 0370
      PRINT OPTION, '3)  ', MINAME(3,SAMP)                              MIN 0380
      PRINT *                                                           MIN 0390
      PRINT OPTION, '4)  ', MINAME(4,SAMP)                              MIN 0400
      PRINT *                                                           MIN 0410
```

```
      PRINT OPTION, '5)  ', MINAME(5,SAMP)                                  MIN 0420
      PRINT *                                                               MIN 0430
      PRINT OPTION, '6)  Return to previous menu'                           MIN 0440
      PRINT *                                                               MIN 0450
      PRINT *                                                               MIN 0460
      PRINT OPTION, '    Enter Choice (1-6) '                               MIN 0470
                                                                            MIN 0480
      CALL IANSWR(CHOICE)                                                   MIN 0490
                                                                            MIN 0500
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 6) THEN                            MIN 0510
        PRINT *, 'Answer must be in the range [1-6] '                        MIN 0520
        NL = SCREEN - 18                                                    MIN 0530
        CHOICE = -1                                                         MIN 0540
        GOTO 10                                                             MIN 0550
      END IF                                                                MIN 0560
                                                                            MIN 0570
      IF      (CHOICE .GE. 1 .AND. CHOICE .LE. 5) THEN                      MIN 0580
        CALL LINE20(CHOICE)                                                 MIN 0590
      ELSE IF (CHOICE .EQ. 6) THEN                                          MIN 0600
        RETURN                                                              MIN 0610
      END IF                                                                MIN 0620
                                                                            MIN 0630
      CHOICE = -1                                                           MIN 0640
      NL = SCREEN -17                                                       MIN 0650
      GOTO 10                                                               MIN 0660
                                                                            MIN 0670
      END                                                                   MIN 0680
```

```
      SUBROUTINE MINORS                                                     MIN 0010
C ----------------------------------------------------------------------|MIN 0020
C     Display menu to select values for minor ion components            |MIN 0030
C ----------------------------------------------------------------------|MIN 0040
                                                                            MIN 0050
      INTEGER MAX, SCREEN                                                   MIN 0060
      CHARACTER * 10 OPTION                                                 MIN 0070
      PARAMETER (MAX = 10, OPTION = '(10X, A)', SCREEN = 24)                MIN 0080
                                                                            MIN 0090
      INTEGER CHOICE, NL, SAMP                                              MIN 0100
                                                                            MIN 0110
      DOUBLE PRECISION CUNITS(35,MAX), TIC(MAX)                             MIN 0120
                                                                            MIN 0130
      EXTERNAL CLEAR, IANSWR, LINE06, LINE07, LINE08                        MIN 0140
                                                                            MIN 0150
      COMMON          SAMP                                                  MIN 0160
      COMMON /COM4  / CUNITS, TIC                                           MIN 0170
                                                                            MIN 0180
C ----------------------------------------------------------------------|MIN 0190
                                                                            MIN 0200
      NL = SCREEN                                                           MIN 0210
      CHOICE = -1                                                           MIN 0220
```

```
                                                                      MIN 0230
 10 CONTINUE                                                          MIN 0240
    CALL CLEAR (NL)                                                   MIN 0250
                                                                      MIN 0260
    PRINT OPTION, '1)  ENTER: F, PO4, NO3, NH3, B, Sr, Ba'            MIN 0270
    PRINT *                                                           MIN 0280
    PRINT OPTION, '2)  ENTER: Pb, Zn, Cu, Mn, Hg, Ag'                 MIN 0290
    PRINT *                                                           MIN 0300
    PRINT OPTION, '3)  ENTER: As, U, V'                               MIN 0310
    PRINT *                                                           MIN 0320
    PRINT OPTION, '4)  Return to Basic Parameters Menu'               MIN 0330
    PRINT *                                                           MIN 0340
    PRINT *                                                           MIN 0350
    PRINT OPTION, '    Enter Choice (1-4) '                           MIN 0360
                                                                      MIN 0370
    CALL IANSWR (CHOICE)                                              MIN 0380
                                                                      MIN 0390
    IF (CHOICE .LT. 1 .OR. CHOICE .GT. 4) THEN                        MIN 0400
      PRINT *, 'Answer must be in the range [1-4] '                    MIN 0410
      NL = SCREEN - 12                                                MIN 0420
      CHOICE = -1                                                     MIN 0430
      GOTO 10                                                         MIN 0440
    END IF                                                            MIN 0450
                                                                      MIN 0460
    IF      (CHOICE .EQ. 1) THEN                                      MIN 0470
      CALL LINE06                                                     MIN 0480
    ELSE IF (CHOICE .EQ. 2) THEN                                      MIN 0490
      CALL LINE07                                                     MIN 0500
    ELSE IF (CHOICE .EQ. 3) THEN                                      MIN 0510
      CALL LINE08                                                     MIN 0520
    ELSE IF (CHOICE .EQ. 4) THEN                                      MIN 0530
      RETURN                                                          MIN 0540
    END IF                                                            MIN 0550
                                                                      MIN 0560
    CHOICE = -1                                                       MIN 0570
    NL = SCREEN - 11                                                  MIN 0580
    GOTO 10                                                           MIN 0590
                                                                      MIN 0600
    END                                                               MIN 0610
```

```
      SUBROUTINE MIXIT                                                MIX 0010
C ============================================================================|MIX 0020
C     Selects the parameters for mixing two samples                           |MIX 0030
C ----------------------------------------------------------------------------|MIX 0040
                                                                      MIX 0050
      INTEGER MAX, SCREEN                                             MIX 0060
      PARAMETER (MAX = 10, SCREEN = 24)                               MIX 0070
                                                                      MIX 0080
      INTEGER ACTLEN, I, IBMIX(MAX), IDDP(MAX), IDMIX(50,MAX)         MIX 0090
      INTEGER IDSAT(MAX), INMIX(MAX), IRXDP(10,MAX), ITMIX(MAX)       MIX 0100
```

```
      INTEGER ITT(MAX), LEN, LENGTH, SAMP                                MIX 0110
                                                                         MIX 0120
      CHARACTER * 80 ANSWR, MIXFLE(MAX), OUTIN(MAX)                      MIX 0130
                                                                         MIX 0140
      DOUBLE PRECISION AMOL(50,MAX), DFRAC1(MAX), DP(MAX), FBOIL(MAX)    MIX 0150
      DOUBLE PRECISION INC(MAX), RXDP(10,MAX)                            MIX 0160
                                                                         MIX 0170
      EXTERNAL ANSWER, CLEAR, DSLPPT, IANSWR, LENGTH                     MIX 0180
                                                                         MIX 0190
      COMMON           SAMP                                              MIX 0200
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,         MIX 0210
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL      MIX 0220
      COMMON /COM20 / MIXFLE, OUTIN                                      MIX 0230
                                                                         MIX 0240
C ========================================================================|MIX 0250
                                                                         MIX 0260
      CALL CLEAR (SCREEN)                                                MIX 0270
                                                                         MIX 0280
C ------------------------------------------------------------------------|MIX 0290
C     Clear other options using these variables                          |MIX 0300
C ------------------------------------------------------------------------|MIX 0310
                                                                         MIX 0320
      IBMIX(SAMP)  = 2                                                   MIX 0330
      ITMIX(SAMP)  = 0                                                   MIX 0340
      IDDP(SAMP)   = 0                                                   MIX 0350
      IDSAT(SAMP)  = 0                                                   MIX 0360
      ITT(SAMP)    = 0                                                   MIX 0370
      DP(SAMP)     = 0.0                                                 MIX 0380
      FBOIL(SAMP)  = 0.0                                                 MIX 0390
                                                                         MIX 0400
      DO 40 I = 1, 10                                                    MIX 0410
        RXDP (I,SAMP) = 0.0                                              MIX 0420
        IRXDP(I,SAMP) = 0                                                MIX 0430
   40 CONTINUE                                                           MIX 0440
                                                                         MIX 0450
      DO 50 I = 1, 50                                                    MIX 0460
        IDMIX(I,SAMP) = 0                                                MIX 0470
        AMOL(I,SAMP)  = 0.0                                              MIX 0480
   50 CONTINUE                                                           MIX 0490
                                                                         MIX 0500
      PRINT *, 'Total number of mixtures of the two solutions',          MIX 0510
     &         ' to be mixed ?'                                          MIX 0520
      PRINT '(35X, A, I4, A)', ' [Current = ', INMIX(SAMP), '] '         MIX 0530
      CALL IANSWR (INMIX(SAMP))                                          MIX 0540
                                                                         MIX 0550
      PRINT *                                                            MIX 0560
      PRINT *, 'Smallest fraction of solution 1 to be mixed',            MIX 0570
     &         ' with solution 2 ?'                                      MIX 0580
      PRINT '(35X, A, E10.4, A)', ' [Current = ', DFRAC1(SAMP), '] '     MIX 0590
      CALL ANSWER (DFRAC1(SAMP))                                         MIX 0600
                                                                         MIX 0610
      PRINT *                                                            MIX 0620
      PRINT *, 'Increment of solution 1 to be added/subtracted ?'        MIX 0630
      PRINT '(35X, A, E10.4, A)', ' [Current = ', INC(SAMP), '] '        MIX 0640
```

```
      CALL ANSWER (INC(SAMP))                                                  MIX 0650
                                                                               MIX 0660
      PRINT *                                                                  MIX 0670
      PRINT *, 'Pathname of the file that has the sample to be',               MIX 0680
     &         ' mixed with this one.'                                         MIX 0690
      PRINT *, 'Leave blank if the sample follows this one.'                   MIX 0700
      ACTLEN = 80                                                              MIX 0710
      LEN = LENGTH(MIXFLE(SAMP), ACTLEN)                                       MIX 0720
      PRINT '(1X,A,A,A)', '     [Current = ', MIXFLE(SAMP)(1:LEN), '] '        MIX 0730
                                                                               MIX 0740
      READ '(A80)', ANSWR                                                      MIX 0750
                                                                               MIX 0760
      IF (ANSWR .NE. ' ') THEN                                                 MIX 0770
        MIXFLE(SAMP) = ANSWR                                                   MIX 0780
      END IF                                                                   MIX 0790
                                                                               MIX 0800
      IF (INMIX(SAMP) .LE. 0) THEN                                             MIX 0810
        IBMIX(SAMP) = 0                                                        MIX 0820
      END IF                                                                   MIX 0830
                                                                               MIX 0840
      RETURN                                                                   MIX 0850
      END                                                                      MIX 0860
```

```
      SUBROUTINE NSAMP (MAXSAM)                                                NSA 0010
C ============================================================================|NSA 0020
C     Increments the current sample                                            |NSA 0030
C ----------------------------------------------------------------------------|NSA 0040
                                                                               NSA 0050
      INTEGER MAX                                                              NSA 0060
      PARAMETER (MAX = 10)                                                     NSA 0070
                                                                               NSA 0080
      INTEGER MAXSAM, SAMP                                                     NSA 0090
      CHARACTER * 1 ANS                                                        NSA 0100
                                                                               NSA 0110
      COMMON          SAMP                                                     NSA 0120
                                                                               NSA 0130
C ============================================================================|NSA 0140
                                                                               NSA 0150
      IF (SAMP .EQ. MAX) THEN                                                  NSA 0160
        PRINT *, 'SAMPLE must be in the range [1-10]'                          NSA 0170
        PRINT *, '     Hit return to continue '                                NSA 0180
        READ '(A1)', ANS                                                       NSA 0190
      ELSE                                                                     NSA 0200
        SAMP = SAMP + 1                                                        NSA 0210
        IF (MAXSAM .LT. SAMP) MAXSAM = SAMP                                    NSA 0220
      END IF                                                                   NSA 0230
                                                                               NSA 0240
      RETURN                                                                   NSA 0250
      END                                                                      NSA 0260
```

```
      SUBROUTINE OPTION                                                      OPT 0010
C ============================================================================|OPT 0020
C     Selects item from option menu                                          |OPT 0030
C ----------------------------------------------------------------------------|OPT 0040
                                                                             OPT 0050
      INTEGER MAX                                                            OPT 0060
      PARAMETER (MAX = 10)                                                   OPT 0070
                                                                             OPT 0080
      INTEGER ALK(MAX), ANSR(3,MAX), CHOICE, FLAGS(6,MAX), GEOTH(MAX)        OPT 0090
      INTEGER IBMIX(MAX), ICCSAT(MAX), IDDP(MAX), IDMIX(50, MAX)             OPT 0100
      INTEGER IDN(10,10,MAX), IDSAT(MAX), IMCO3(MAX)                         OPT 0110
      INTEGER INFORM(MAX), INMIX(MAX), INSP(MAX), IPIT(MAX)                  OPT 0120
      INTEGER IPRIN1(MAX), IPRIN2(MAX), IRXDP(10, MAX), ISCHG(10, MAX)       OPT 0130
      INTEGER ISCOMP(10,MAX), ITIC(MAX), ITMIX(MAX), ITT(MAX)                OPT 0140
      INTEGER MININD(10,5,MAX), ND(2,45,MAX), NDUM(12,MAX)                   OPT 0150
      INTEGER NUFLAG(MAX), RATIO(MAX), SAMP, Z(3,MAX)                        OPT 0160
                                                                             OPT 0170
      CHARACTER *  1 ADEX(MAX), ODUM(12,MAX)                                 OPT 0180
      CHARACTER *  5 UNITS(MAX)                                              OPT 0190
      CHARACTER *  8 MINAME(5,MAX), PAGE(45,MAX)                             OPT 0200
      CHARACTER * 10 SPN(10,MAX)                                             OPT 0210
      CHARACTER * 80 FLNAME, MIXFLE(MAX), OUTIN(MAX), TITLE(MAX)             OPT 0220
                                                                             OPT 0230
      DOUBLE PRECISION AMOL(50, MAX), CEC(MAX), COEF(10,10,MAX)              OPT 0240
      DOUBLE PRECISION CONC(3,MAX), CONV1(MAX), CONV2(MAX)                   OPT 0250
      DOUBLE PRECISION CUNITS(35, MAX), DCH4(MAX), DCO2(MAX)                 OPT 0260
      DOUBLE PRECISION DENS(MAX), DFRAC1(MAX), DH2S(MAX), DHA(3,MAX)         OPT 0270
      DOUBLE PRECISION DNA(45,MAX), DNH3(MAX), DP(MAX), EHM(MAX)             OPT 0280
      DOUBLE PRECISION EHMC(MAX), EMFZSC(MAX), FBOIL(MAX), FCCSAT(MAX)       OPT 0290
      DOUBLE PRECISION FIXIT(MAX), GFW(3,MAX), HITEMP(MAX), INC(MAX)         OPT 0300
      DOUBLE PRECISION KCH4OL(MAX), KCO2OL(MAX), KH2SOL(MAX)                 OPT 0310
      DOUBLE PRECISION KRXN(10,MAX), MBASE(10,MAX), MINCO(10,5,MAX)          OPT 0320
      DOUBLE PRECISION MINLOG(2,5,MAX), PH(MAX), DSEP(MAX), PRESS(MAX)       OPT 0330
      DOUBLE PRECISION RXDP(10,MAX), SAREA(MAX), TAREA(MAX), TCH4M(MAX)      OPT 0340
      DOUBLE PRECISION TCO2M(MAX), TEMP(MAX), TH2SM(MAX), TIC(MAX)           OPT 0350
      DOUBLE PRECISION WROIL(MAX), XD(2,45,MAX), XDUM(12,MAX)                OPT 0360
                                                                             OPT 0370
      EXTERNAL BASIC, FLAG, GAPHCO, LINE16, LINE18, MASTRN, OPMENU           OPT 0380
                                                                             OPT 0390
      COMMON           SAMP                                                  OPT 0400
      COMMON /COM1  / TITLE, UNITS, FLNAME                                   OPT 0410
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                              OPT 0420
      COMMON /COM3  / PH, EHM, EHMC, EMFZSC                                  OPT 0430
      COMMON /COM4  / CUNITS, TIC                                            OPT 0440
      COMMON /COM5  / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2                  OPT 0450
      COMMON /COM6  / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,          OPT 0460
     &                FCCSAT                                                OPT 0470
      COMMON /COM7  / TCO2M, TCH4M, TH2SM, WROIL,                            OPT 0480
     &                KCO2OL, KCH4OL, KH2SOL, DSEP                          OPT 0490
      COMMON /COM8  / ADEX, SPN                                              OPT 0500
      COMMON /COM9  / CEC, TAREA, SAREA, INSP, ISCHG, MBASE, KRXN,           OPT 0510
     &                ISCOMP, COEF, IDN                                     OPT 0520
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,             OPT 0530
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL          OPT 0540
```

```
      COMMON /COM11 / ODUM                                                  OPT 0550
      COMMON /COM12 / NDUM, XDUM                                            OPT 0560
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2                  OPT 0570
      COMMON /COM14 / FLAGS                                                 OPT 0580
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                               OPT 0590
      COMMON /COM16 / PAGE                                                  OPT 0600
      COMMON /COM17 / ND, XD, DNA                                           OPT 0610
      COMMON /COM18 / MINAME                                                OPT 0620
      COMMON /COM19 / MINCO, MININD, MINLOG                                 OPT 0630
      COMMON /COM20 / MIXFLE, OUTIN                                         OPT 0640
                                                                            OPT 0650
C ============================================================================|OPT 0660
                                                                            OPT 0670
                                                                            OPT 0680
   10 CONTINUE                                                              OPT 0690
      CALL OPMENU (CHOICE)                                                  OPT 0700
                                                                            OPT 0710
      IF      (CHOICE .EQ. 1) THEN                                          OPT 0720
        CALL BASIC                                                          OPT 0730
      ELSE IF (CHOICE .EQ. 2) THEN                                          OPT 0740
        CALL FLAG                                                           OPT 0750
      ELSE IF (CHOICE .EQ. 3) THEN                                          OPT 0760
        CALL GAPHCO                                                         OPT 0770
      ELSE IF (CHOICE .EQ. 4) THEN                                          OPT 0780
        CALL MASTRN                                                         OPT 0790
      ELSE IF (CHOICE .EQ. 5) THEN                                          OPT 0800
        CALL LINE16                                                         OPT 0810
      ELSE IF (CHOICE .EQ. 6) THEN                                          OPT 0820
        CALL LINE18                                                         OPT 0830
      ELSE IF (CHOICE .EQ. 7) THEN                                          OPT 0840
        GOTO 20                                                             OPT 0850
      END IF                                                                OPT 0860
                                                                            OPT 0870
      GOTO 10                                                               OPT 0880
                                                                            OPT 0890
   20 CONTINUE                                                              OPT 0900
      RETURN                                                                OPT 0910
      END                                                                   OPT 0920
```

```
      SUBROUTINE OPMENU (CHOICE)                                            OPM 0010
C ============================================================================|OPM 0020
C     Prints option menu                                                    |OPM 0030
C ----------------------------------------------------------------------------|OPM 0040
                                                                            OPM 0050
      INTEGER SCREEN                                                        OPM 0060
      CHARACTER * 10 OPTION                                                 OPM 0070
      PARAMETER (OPTION = '(10X, A)', SCREEN = 24)                          OPM 0080
                                                                            OPM 0090
      INTEGER CHOICE, NL                                                    OPM 0100
                                                                            OPM 0110
```

```
      EXTERNAL CLEAR, IANSWR                                                OPM 0120
                                                                            OPM 0130
C ============================================================================|OPM 0140
                                                                            OPM 0150
      NL = SCREEN                                                           OPM 0160
      CHOICE = 0                                                            OPM 0170
                                                                            OPM 0180
   10 CONTINUE                                                              OPM 0190
      CALL CLEAR (NL)                                                       OPM 0200
                                                                            OPM 0210
      PRINT OPTION, '    OPTIONS MENU'                                      OPM 0220
      PRINT *                                                               OPM 0230
      PRINT OPTION, '1)  Enter Basic Parameters'                            OPM 0240
      PRINT *                                                               OPM 0250
      PRINT OPTION, '2)  Enter Program Option Flags'                        OPM 0260
      PRINT *                                                               OPM 0270
      PRINT OPTION, '3)  Enter pH Options'                                  OPM 0280
      PRINT *                                                               OPM 0290
      PRINT OPTION, '4)  Enter Mass Transfer Options'                       OPM 0300
      PRINT *                                                               OPM 0310
      PRINT OPTION, '5)  Enter User Log K Option'                           OPM 0320
      PRINT *                                                               OPM 0330
      PRINT OPTION, '6)  Enter Additional Ions and Minerals Option'         OPM 0340
      PRINT *                                                               OPM 0350
      PRINT OPTION, '7)  Return to Main Menu'                               OPM 0360
      PRINT *                                                               OPM 0370
      PRINT *                                                               OPM 0380
      PRINT OPTION, '    Enter Choice (1-7) '                               OPM 0390
                                                                            OPM 0400
      CALL IANSWR (CHOICE)                                                  OPM 0410
                                                                            OPM 0420
      IF (CHOICE .LT. 1 .OR. CHOICE .GT. 7) THEN                            OPM 0430
        PRINT *, 'Answer must be in the range [1-7] '                        OPM 0440
        CHOICE = 0                                                          OPM 0450
        NL = SCREEN - 20                                                    OPM 0460
        GOTO 10                                                             OPM 0470
      END IF                                                                OPM 0480
                                                                            OPM 0490
      RETURN                                                                OPM 0500
      END                                                                   OPM 0510
```

```
      SUBROUTINE PRNTOT                                                     PRN 0010
C ============================================================================|PRN 0020
C     Select printout options                                               |PRN 0030
C ----------------------------------------------------------------------------|PRN 0040
                                                                            PRN 0050
      INTEGER MAX, SCREEN                                                   PRN 0060
      CHARACTER * 10 USING                                                  PRN 0070
      PARAMETER (MAX = 10, SCREEN = 24, USING = '(1X, A)')                  PRN 0080
                                                                            PRN 0090
```

```
      INTEGER ACTLEN, GEOTH(MAX), INFORM(MAX), IPRIN1(MAX), IPRIN2(MAX) PRN 0100
      INTEGER LEN, LENGTH, NL, RATIO(MAX), SAMP                         PRN 0110
                                                                        PRN 0120
      CHARACTER *  1 ANS                                                PRN 0130
      CHARACTER * 80 MIXFLE(MAX), OUTIN(MAX)                            PRN 0140
                                                                        PRN 0150
      EXTERNAL CLEAR, LENGTH                                            PRN 0160
                                                                        PRN 0170
      COMMON           SAMP                                             PRN 0180
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2              PRN 0190
      COMMON /COM20 / MIXFLE, OUTIN                                     PRN 0200
                                                                        PRN 0210
C ----------------------------------------------------------------------|PRN 0220
                                                                        PRN 0230
      NL = SCREEN                                                       PRN 0240
                                                                        PRN 0250
   10 CONTINUE                                                          PRN 0260
      CALL CLEAR (NL)                                                   PRN 0270
                                                                        PRN 0280
      PRINT *, 'Do you want to print the aqueous log K values in the'   PRN 0290
      PRINT *, ' data base at the temperatures of interest ? (Y/N)'     PRN 0300
                                                                        PRN 0310
      IF      (INFORM(SAMP) .EQ. 0) THEN                                PRN 0320
        PRINT USING, '     [Current =  N] '                             PRN 0330
      ELSE IF (INFORM(SAMP) .EQ. 1) THEN                                PRN 0340
        PRINT USING, '     [Current =  Y] '                             PRN 0350
      END IF                                                            PRN 0360
                                                                        PRN 0370
      READ '(A)', ANS                                                   PRN 0380
                                                                        PRN 0390
      IF (ANS .NE. ' ') THEN                                            PRN 0400
        IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                   PRN 0410
          INFORM(SAMP) = 1                                              PRN 0420
        ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                   PRN 0430
          INFORM(SAMP) = 0                                              PRN 0440
        ELSE                                                            PRN 0450
          PRINT *, 'Answer must be in [Y, y, N, n] '                    PRN 0460
          NL = SCREEN - 5                                               PRN 0470
          GOTO 10                                                       PRN 0480
        END IF                                                          PRN 0490
      END IF                                                            PRN 0500
                                                                        PRN 0510
      NL = 2                                                            PRN 0520
                                                                        PRN 0530
   20 CONTINUE                                                          PRN 0540
      CALL CLEAR (NL)                                                   PRN 0550
      PRINT *, 'Do you want to print out the analytical and calculated' PRN 0560
      PRINT *, ' activity ratios of the major elements? (Y/N)'          PRN 0570
                                                                        PRN 0580
      IF      (RATIO(SAMP) .EQ. 0) THEN                                 PRN 0590
        PRINT USING, '     [Current =  N] '                             PRN 0600
      ELSE IF (RATIO(SAMP) .EQ. 1) THEN                                 PRN 0610
        PRINT USING, '     [Current =  Y] '                             PRN 0620
      END IF                                                            PRN 0630
```

```
                                                                        PRN 0640
   READ '(A)', ANS                                                      PRN 0650
                                                                        PRN 0660
   IF (ANS .NE. ' ') THEN                                               PRN 0670
     IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                      PRN 0680
       RATIO(SAMP) = 1                                                  PRN 0690
     ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                      PRN 0700
       RATIO(SAMP) = 0                                                  PRN 0710
     ELSE                                                               PRN 0720
       PRINT *, 'Answer must be in [Y, y, N, n] '                       PRN 0730
       NL = SCREEN - 5                                                  PRN 0740
       GOTO 20                                                          PRN 0750
     END IF                                                             PRN 0760
   END IF                                                               PRN 0770
                                                                        PRN 0780
   NL = 2                                                               PRN 0790
                                                                        PRN 0800
30 CONTINUE                                                             PRN 0810
   CALL CLEAR (NL)                                                      PRN 0820
   PRINT *, 'Do you want to print out the temperature estimates'        PRN 0830
   PRINT *, ' from the chemical geothermometers? (Y/N)'                 PRN 0840
                                                                        PRN 0850
   IF      (GEOTH(SAMP) .EQ. 0) THEN                                    PRN 0860
     PRINT USING, '     [Current =  N] '                                PRN 0870
   ELSE IF (GEOTH(SAMP) .EQ. 1) THEN                                    PRN 0880
     PRINT USING, '     [Current =  Y] '                                PRN 0890
   END IF                                                               PRN 0900
                                                                        PRN 0910
   READ '(A)', ANS                                                      PRN 0920
                                                                        PRN 0930
   IF (ANS .NE. ' ') THEN                                               PRN 0940
     IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                      PRN 0950
       GEOTH(SAMP) = 1                                                  PRN 0960
     ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                      PRN 0970
       GEOTH(SAMP) = 0                                                  PRN 0980
     ELSE                                                               PRN 0990
       PRINT *, 'Answer must be in [Y, y, N, n] '                       PRN 1000
       NL = SCREEN - 5                                                  PRN 1010
       GOTO 30                                                          PRN 1020
     END IF                                                             PRN 1030
   END IF                                                               PRN 1040
                                                                        PRN 1050
   NL = 2                                                               PRN 1060
                                                                        PRN 1070
40 CONTINUE                                                             PRN 1080
   CALL CLEAR (NL)                                                      PRN 1090
   PRINT *, 'Do you want to print out the data on the iteration'        PRN 1100
   PRINT *, ' of the anions? (Y/N)'                                     PRN 1110
                                                                        PRN 1120
   IF      (IPRIN1(SAMP) .EQ. 0) THEN                                   PRN 1130
     PRINT USING, '     [Current =  N] '                                PRN 1140
   ELSE IF (IPRIN1(SAMP) .EQ. 1) THEN                                   PRN 1150
     PRINT USING, '     [Current =  Y] '                                PRN 1160
   END IF                                                               PRN 1170
```

```
                                                                      PRN 1180
   READ '(A)', ANS                                                    PRN 1190
                                                                      PRN 1200
   IF (ANS .NE. ' ') THEN                                             PRN 1210
     IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                    PRN 1220
       IPRIN1(SAMP) = 1                                               PRN 1230
     ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                    PRN 1240
       IPRIN1(SAMP) = 0                                               PRN 1250
     ELSE                                                             PRN 1260
       PRINT *, 'Answer must be in [Y, y, N, n] '                     PRN 1270
       NL = SCREEN - 5                                                PRN 1280
       GOTO 40                                                        PRN 1290
     END IF                                                           PRN 1300
   END IF                                                             PRN 1310
                                                                      PRN 1320
   NL = 2                                                             PRN 1330
                                                                      PRN 1340
50 CONTINUE                                                           PRN 1350
   CALL CLEAR (NL)                                                    PRN 1360
   PRINT *, 'Do you want to print out the data on the mass balance'    PRN 1370
   PRINT *, ' on Hydrogen whenever a new pH is calculated? (Y/N)'     PRN 1380
                                                                      PRN 1390
   IF      (IPRIN2(SAMP) .EQ. 0) THEN                                 PRN 1400
     PRINT USING, '     [Current =  N] '                              PRN 1410
   ELSE IF (IPRIN2(SAMP) .EQ. 1) THEN                                 PRN 1420
     PRINT USING, '     [Current =  Y] '                              PRN 1430
   END IF                                                             PRN 1440
                                                                      PRN 1450
   READ '(A)', ANS                                                    PRN 1460
                                                                      PRN 1470
   IF (ANS .NE. ' ') THEN                                             PRN 1480
     IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                    PRN 1490
       IPRIN2(SAMP) = 1                                               PRN 1500
     ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                    PRN 1510
       IPRIN2(SAMP) = 0                                               PRN 1520
     ELSE                                                             PRN 1530
       PRINT *, 'Answer must be in [Y, y, N, n] '                     PRN 1540
       NL = SCREEN - 5                                                PRN 1550
       GOTO 50                                                        PRN 1560
     END IF                                                           PRN 1570
   END IF                                                             PRN 1580
                                                                      PRN 1590
   PRINT *                                                            PRN 1600
   PRINT *                                                            PRN 1610
   PRINT *, 'Name of a new input file to be created based upon',      PRN 1620
  &         ' the output of this sample.'                             PRN 1630
   ACTLEN = 80                                                        PRN 1640
   LEN = LENGTH(OUTIN(SAMP), ACTLEN)                                  PRN 1650
   PRINT '(1X,A,A,A)', '     [Current = ', OUTIN(SAMP)(1:LEN),'] '    PRN 1660
   READ '(A80)', OUTIN(SAMP)                                          PRN 1670
                                                                      PRN 1680
   RETURN                                                             PRN 1690
   END                                                                PRN 1700
```

```
      SUBROUTINE PSAMP                                                  PSA 0010
C ================================================================== |PSA 0020
C     Decrements the current sample                                   |PSA 0030
C ------------------------------------------------------------------ |PSA 0040
                                                                        PSA 0050
      INTEGER SAMP                                                      PSA 0060
      CHARACTER * 1 ANS                                                 PSA 0070
                                                                        PSA 0080
      COMMON          SAMP                                              PSA 0090
                                                                        PSA 0100
C ================================================================== |PSA 0110
                                                                        PSA 0120
      IF (SAMP .EQ. 1) THEN                                             PSA 0130
        PRINT *, 'SAMPLE must be in the range [1-10] '                  PSA 0140
        PRINT *, '       Hit return to continue'                        PSA 0150
        READ '(A1)', ANS                                                PSA 0160
      ELSE                                                              PSA 0170
        SAMP = SAMP - 1                                                 PSA 0180
      END IF                                                            PSA 0190
                                                                        PSA 0200
      RETURN                                                            PSA 0210
      END                                                               PSA 0220
```

```
      SUBROUTINE READFL (MAXSAM)                                        REA 0010
C ================================================================== |REA 0020
C     This routine reads the input file                               |REA 0030
C ------------------------------------------------------------------ |REA 0040
                                                                        REA 0050
      INTEGER MAX, SCREEN, UN                                           REA 0060
      PARAMETER (MAX = 10, SCREEN = 24, UN = 20)                        REA 0070
                                                                        REA 0080
      LOGICAL HERE                                                      REA 0090
                                                                        REA 0100
      INTEGER ACTLEN, ACTUAL, ALK(MAX), ANSR(3,MAX), NUFLAG(MAX)        REA 0110
      INTEGER FLAGS(6,MAX), GEOTH(MAX), I                               REA 0120
      INTEGER IBMIX(MAX), ICCSAT(MAX), IDDP(MAX), IDMIX(50,MAX)         REA 0130
      INTEGER IDN(10,10,MAX), IDSAT(MAX), IMCO3(MAX), INDEX             REA 0140
      INTEGER INFORM(MAX), INMIX(MAX), INSP(MAX), IPIT(MAX)             REA 0150
      INTEGER IPRIN1(MAX), IPRIN2(MAX), IRXDP(10,MAX), ISCHG(10,MAX)    REA 0160
      INTEGER ISCOMP(10,MAX), ITIC(MAX), ITMIX(MAX), ITT(MAX), J, LEN   REA 0170
      INTEGER LENGTH, MAXSAM, MININD(10,5,MAX), ND(2,45,MAX)            REA 0180
      INTEGER NDUM(12,MAX), NUMINS, RATIO(MAX), SAMP, Z(3,MAX)          REA 0190
                                                                        REA 0200
      CHARACTER *  1 ADEX(MAX), ODUM(12,MAX)                            REA 0210
      CHARACTER *  5 UNITS(MAX)                                         REA 0220
      CHARACTER *  8 MINAME(5,MAX), NAME, PAGE(45,MAX)                  REA 0230
      CHARACTER * 10 SPN(10,MAX)                                        REA 0240
      CHARACTER * 20 ANSWR                                              REA 0250
      CHARACTER * 80 FLNAME, MIXFLE(MAX), OUTIN(MAX), TITLE(MAX)        REA 0260
                                                                        REA 0270
```

```
      DOUBLE PRECISION AMOL(50,MAX), CEC(MAX), COEF(10,10,MAX)          REA 0280
      DOUBLE PRECISION CONC(3,MAX), CONV1(MAX), CONV2(MAX)              REA 0290
      DOUBLE PRECISION CUNITS(35,MAX), DA, DCH4(MAX), DCO2(MAX)         REA 0300
      DOUBLE PRECISION DENS(MAX), DFRAC1(MAX), DH2S(MAX), DNH3(MAX)     REA 0310
      DOUBLE PRECISION DHA(3,MAX), DNA(45,MAX), DP(MAX), EHM(MAX)       REA 0320
      DOUBLE PRECISION EHMC(MAX), EMFZSC(MAX), FBOIL(MAX), FCCSAT(MAX)  REA 0330
      DOUBLE PRECISION FIXIT(MAX), GFW(3,MAX), HIGHKT, HITEMP(MAX)      REA 0340
      DOUBLE PRECISION INC(MAX), KCH4OL(MAX), KCO2OL(MAX), KH2SOL(MAX)  REA 0350
      DOUBLE PRECISION KRXN(10,MAX), LOWKT, MBASE(10,MAX)               REA 0360
      DOUBLE PRECISION MINCO(10,5,MAX), MINLOG(2,5,MAX), PH(MAX)        REA 0370
      DOUBLE PRECISION DSEP(MAX), PRESS(MAX), RXDP(10,MAX), SAREA(MAX)  REA 0380
      DOUBLE PRECISION TAREA(MAX), TCH4M(MAX), TCO2M(MAX), TEMP(MAX)    REA 0390
      DOUBLE PRECISION TH2SM(MAX), TIC(MAX), WROIL(MAX), XD(2,45,MAX)   REA 0400
      DOUBLE PRECISION XDUM(12,MAX)                                     REA 0410
                                                                        REA 0420
      EXTERNAL CLEAR, LENGTH                                            REA 0430
                                                                        REA 0440
      COMMON           SAMP                                             REA 0450
      COMMON /COM1  / TITLE, UNITS, FLNAME                              REA 0460
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                         REA 0470
      COMMON /COM3  / PH, EHM, EHMC, EMFZSC                             REA 0480
      COMMON /COM4  / CUNITS, TIC                                       REA 0490
      COMMON /COM5  / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2             REA 0500
      COMMON /COM6  / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,     REA 0510
     &                FCCSAT                                           REA 0520
      COMMON /COM7  / TCO2M, TCH4M, TH2SM, WROIL,                       REA 0530
     &                KCO2OL, KCH4OL, KH2SOL, DSEP                     REA 0540
      COMMON /COM8  / ADEX, SPN                                         REA 0550
      COMMON /COM9  / CEC, TAREA, SAREA, INSP, ISCHG, MBASE,            REA 0560
     &                KRXN, ISCOMP, COEF, IDN                          REA 0570
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,        REA 0580
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL     REA 0590
      COMMON /COM11 / ODUM                                              REA 0600
      COMMON /COM12 / NDUM, XDUM                                        REA 0610
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2              REA 0620
      COMMON /COM14 / FLAGS                                             REA 0630
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                           REA 0640
      COMMON /COM16 / PAGE                                              REA 0650
      COMMON /COM17 / ND, XD, DNA                                       REA 0660
      COMMON /COM18 / MINAME                                            REA 0670
      COMMON /COM19 / MINCO, MININD, MINLOG                             REA 0680
      COMMON /COM20 / MIXFLE, OUTIN                                     REA 0690
                                                                        REA 0700
C ----------------------------------------------------------------------|REA 0710
                                                                        REA 0720
      CALL CLEAR (SCREEN)                                               REA 0730
                                                                        REA 0740
      PRINT *, 'What is the name of the file you want to read ?'        REA 0750
      ACTLEN = 80                                                       REA 0760
      LEN = LENGTH(FLNAME, ACTLEN)                                      REA 0770
      PRINT '(1X,A,A,A)', '     [Current = ', FLNAME(1:LEN), '] '       REA 0780
                                                                        REA 0790
      READ '(A)', ANSWR                                                 REA 0800
                                                                        REA 0810
```

```
      IF (ANSWR .NE. ' ') THEN                                          REA 0820
        FLNAME = ANSWR                                                  REA 0830
      END IF                                                            REA 0840
                                                                        REA 0850
      INQUIRE (FILE = FLNAME, EXIST = HERE, ERR = 100)                  REA 0860
                                                                        REA 0870
      IF (HERE) THEN                                                    REA 0880
        OPEN (UNIT = UN, FILE = FLNAME, STATUS = 'OLD', ERR = 100)      REA 0890
      ELSE                                                              REA 0900
        PRINT *, FLNAME, ' does not exists.  Can not open.'             REA 0910
        PRINT *, ' Hit Return to continue'                              REA 0920
        READ '(A)', ANSWR                                               REA 0930
        RETURN                                                          REA 0940
      END IF                                                            REA 0950
                                                                        REA 0960
      MAXSAM = 1                                                        REA 0970
      SAMP   = 1                                                        REA 0980
                                                                        REA 0990
   10 CONTINUE                                                          REA 1000
      READ (UN, 9010, END = 90) TITLE(SAMP)                             REA 1010
      PRINT *, 'Reading File ...'                                       REA 1020
                                                                        REA 1030
      READ (UN, 9030) TEMP(SAMP), HITEMP(SAMP), DENS(SAMP), PRESS(SAMP) REA 1040
      READ (UN, 9030) PH(SAMP), EHM(SAMP), EHMC(SAMP), EMFZSC(SAMP),    REA 1050
     &                UNITS(SAMP)                                       REA 1060
      READ (UN, 9080) (CUNITS(I,SAMP), I =  1,  7)                      REA 1070
      READ (UN, 9080) (CUNITS(I,SAMP), I =  8, 13), TIC(SAMP)           REA 1080
      READ (UN, 9080) (CUNITS(I,SAMP), I = 14, 20)                      REA 1090
      READ (UN, 9080) (CUNITS(I,SAMP), I = 21, 26)                      REA 1100
      READ (UN, 9080) (CUNITS(I,SAMP), I = 27, 29)                      REA 1110
      READ (UN, 9080) (CUNITS(I,SAMP), I = 30, 33)                      REA 1120
      READ (UN, 9100) ALK(SAMP), ITIC(SAMP)                             REA 1130
      READ (UN, 9080) DCO2(SAMP), DH2S(SAMP), DNH3(SAMP), DCH4(SAMP)    REA 1140
      READ (UN, 9100) ICCSAT(SAMP), IMCO3(SAMP), FIXIT(SAMP),           REA 1150
     &                FCCSAT(SAMP)                                      REA 1160
      READ (UN, 9080) TCO2M(SAMP), TCH4M(SAMP), TH2SM(SAMP),            REA 1170
     &                WROIL(SAMP), KCO2OL(SAMP), KCH4OL(SAMP),          REA 1180
     &                KH2SOL(SAMP), DSEP(SAMP)                          REA 1190
      READ (UN, 9160) ADEX(SAMP)                                        REA 1200
      IF (ADEX(SAMP) .EQ. 'a') ADEX(SAMP) = 'A'                         REA 1210
      IF (ADEX(SAMP) .EQ. 'e') ADEX(SAMP) = 'E'                         REA 1220
                                                                        REA 1230
      IF (ADEX(SAMP) .EQ. 'A' .OR. ADEX(SAMP) .EQ. 'E') THEN            REA 1240
        READ (UN, 9150) CEC(SAMP), TAREA(SAMP), SAREA(SAMP), INSP(SAMP) REA 1250
        DO 20 I = 1, INSP(SAMP)                                         REA 1260
          READ (UN, 9200) ISCHG(I,SAMP), MBASE(I,SAMP), SPN(I,SAMP)     REA 1270
          READ (UN, 9210) KRXN(I,SAMP), ISCOMP(I,SAMP), (COEF(I,J,SAMP),REA 1280
     &                    IDN(I,J,SAMP), J = 1, ISCOMP(I,SAMP))         REA 1290
   20   CONTINUE                                                        REA 1300
      END IF                                                            REA 1310
                                                                        REA 1320
      READ (UN, 9100) IBMIX(SAMP), ITMIX(SAMP)                          REA 1330
      IF (IBMIX(SAMP) .EQ. 1) THEN                                      REA 1340
        IF (ITMIX(SAMP) .GT. 0) THEN                                    REA 1350
```

```
      DO 30 I = 1, ITMIX(SAMP)                                          REA 1360
        READ (UN, 9280) IDMIX(I,SAMP), AMOL(I,SAMP)                     REA 1370
30    CONTINUE                                                          REA 1380
     ELSE IF (ITMIX(SAMP) .EQ. 0) THEN                                  REA 1390
      READ (UN, 9270) IDSAT(SAMP), IDDP(SAMP), DP(SAMP)                 REA 1400
      IF (IDDP(SAMP) .EQ. 0) THEN                                       REA 1410
        READ (UN, 9270) ITT(SAMP)                                       REA 1420
        DO 40 I = 1, ITT(SAMP)                                          REA 1430
          READ (UN, 9280) IRXDP(I,SAMP), RXDP(I,SAMP)                   REA 1440
40      CONTINUE                                                        REA 1450
      END IF                                                            REA 1460
     ELSE                                                               REA 1470
      READ (UN, 9280) IDDP(SAMP), AMOL(1,SAMP)                          REA 1480
     END IF                                                             REA 1490
   ELSE IF (IBMIX(SAMP) .EQ. 2) THEN                                    REA 1500
     READ (UN, 9280) INMIX(SAMP), DFRAC1(SAMP), INC(SAMP),              REA 1510
  &                  MIXFLE(SAMP)                                      REA 1520
    ELSE IF (IBMIX(SAMP) .EQ. 3) THEN                                   REA 1530
     READ (UN, 9080) FBOIL(SAMP)                                        REA 1540
    END IF                                                              REA 1550
    READ (UN, 9180) (ODUM(I,SAMP), NDUM(I,SAMP), XDUM(I,SAMP),         REA 1560
  &                  I = 1,  6)                                        REA 1570
    READ (UN, 9180) (ODUM(I,SAMP), NDUM(I,SAMP), XDUM(I,SAMP),         REA 1580
  &                  I = 7, 12)                                        REA 1590
                                                                        REA 1600
    READ (UN, 9290) ANSR(1,SAMP), ANSR(2,SAMP)                          REA 1610
    IF (ANSR(1,SAMP) .EQ. 0 .AND. ANSR(2,SAMP) .NE. 0) THEN             REA 1620
      ANSR(1,SAMP) = ANSR(2,SAMP)                                       REA 1630
      ANSR(2,SAMP) = 0                                                  REA 1640
    END IF                                                              REA 1650
                                                                        REA 1660
    IF (ANSR(1,SAMP) .GT. 0) THEN                                       REA 1670
      READ (UN, 9350) CONC(1,SAMP), GFW(1,SAMP), Z(1,SAMP),             REA 1680
  &                   DHA(1,SAMP), PAGE(1,SAMP)                        REA 1690
      DO 50 I = 1, ANSR(1,SAMP)                                         REA 1700
        READ (UN, 9360) INDEX, DA, LOWKT, HIGHKT, NAME                  REA 1710
        PAGE(INDEX,SAMP) = NAME                                         REA 1720
        DNA(INDEX, SAMP) = DA                                           REA 1730
        ND(1,INDEX,SAMP) = INDEX                                        REA 1740
        ND(2,INDEX,SAMP) = INDEX                                        REA 1750
        XD(1,INDEX,SAMP) = LOWKT                                        REA 1760
        XD(2,INDEX,SAMP) = HIGHKT                                       REA 1770
50    CONTINUE                                                          REA 1780
    END IF                                                              REA 1790
                                                                        REA 1800
    IF (ANSR(2,SAMP) .GT. 0) THEN                                       REA 1810
      READ (UN, 9350) CONC(2,SAMP), GFW(2,SAMP), Z(2,SAMP),             REA 1820
  &                   DHA(2,SAMP), PAGE(16,SAMP)                       REA 1830
      DO 60 I = 1, ANSR(2,SAMP)                                         REA 1840
        READ (UN, 9360) INDEX, DA, LOWKT, HIGHKT, NAME                  REA 1850
        ACTUAL = INDEX + 15                                             REA 1860
        PAGE(ACTUAL,SAMP) = NAME                                        REA 1870
        DNA (ACTUAL,SAMP) = DA                                          REA 1880
        ND(1,ACTUAL,SAMP) = INDEX                                       REA 1890
```

```
        ND(2,ACTUAL,SAMP) = INDEX                                          REA 1900
        XD(1,ACTUAL,SAMP) = LOWKT                                          REA 1910
        XD(2,ACTUAL,SAMP) = HIGHKT                                         REA 1920
 60   CONTINUE                                                             REA 1930
    END IF                                                                 REA 1940
                                                                           REA 1950
    READ (UN, 9500) ANSR(3,SAMP), Z(3,SAMP), DHA(3,SAMP), GFW(3,SAMP),REA 1960
   &               CONC(3,SAMP), PAGE(31,SAMP)                           REA 1970
    IF (ANSR(3,SAMP) .GT. 0) THEN                                          REA 1980
      DO 70 I = 1, ANSR(3,SAMP)                                            REA 1990
        READ  (UN, 9360) INDEX, DA, LOWKT, HIGHKT, NAME                    REA 2000
        ACTUAL = INDEX + 30                                                REA 2010
        PAGE(ACTUAL,SAMP) = NAME                                           REA 2020
        DNA (ACTUAL,SAMP) = DA                                             REA 2030
        ND(1,ACTUAL,SAMP) = INDEX                                          REA 2040
        ND(2,ACTUAL,SAMP) = INDEX                                          REA 2050
        XD(1,ACTUAL,SAMP) = LOWKT                                          REA 2060
        XD(2,ACTUAL,SAMP) = HIGHKT                                         REA 2070
 70   CONTINUE                                                             REA 2080
    END IF                                                                 REA 2090
                                                                           REA 2100
    READ (UN, '(I2)') NUMINS                                               REA 2110
    DO 80 I = 1, NUMINS                                                    REA 2120
      READ (UN, 9560) MINLOG(1,I,SAMP), MINLOG(2,I,SAMP),                 REA 2130
   &                  MINCO(10,I,SAMP), MINAME(I,SAMP)                    REA 2140
      READ (UN, 9210) (MINCO(J,I,SAMP), MININD(J,I,SAMP), J = 1, 9)       REA 2150
 80 CONTINUE                                                               REA 2160
                                                                           REA 2170
    READ (UN, 9290) NUFLAG(SAMP), IPIT(SAMP), (FLAGS(I,SAMP),              REA 2180
   &                I = 1, 6)                                              REA 2190
                                                                           REA 2200
    READ (UN, 9300) INFORM(SAMP), RATIO(SAMP), GEOTH(SAMP),                REA 2210
   &                IPRIN1(SAMP), IPRIN2(SAMP), OUTIN(SAMP)               REA 2220
    READ (UN, 9080) CONV1(SAMP), CONV2(SAMP)                               REA 2230
                                                                           REA 2240
    SAMP = SAMP + 1                                                        REA 2250
    IF (SAMP .EQ. MAX) THEN                                                REA 2260
      PRINT *, 'Only ', MAX, ' samples can be read'                        REA 2270
      GOTO 90                                                              REA 2280
    ELSE                                                                   REA 2290
      GOTO 10                                                              REA 2300
    END IF                                                                 REA 2310
                                                                           REA 2320
 90 CONTINUE                                                               REA 2330
                                                                           REA 2340
    MAXSAM = SAMP - 1                                                      REA 2350
    SAMP = 1                                                               REA 2360
                                                                           REA 2370
    CLOSE (UN)                                                             REA 2380
    RETURN                                                                 REA 2390
                                                                           REA 2400
100 CONTINUE                                                               REA 2410
    PRINT *, FLNAME, ' is not valid.  Can not open.'                       REA 2420
    PRINT *, ' Hit Return to continue'                                     REA 2430
```

```
      READ '(A)', ANSWR                                                  REA 2440
      RETURN                                                             REA 2450
                                                                         REA 2460
C -----------------------------------------------------------------------|REA 2470
C     Format Statements                                                  |REA 2480
C --------------------                                                   |REA 2490
                                                                         REA 2500
 9010 FORMAT (A80)                                                       REA 2510
 9030 FORMAT (4E10.4, A5)                                                REA 2520
 9080 FORMAT (8E10.4)                                                    REA 2530
 9100 FORMAT (2I2, 2E10.4)                                               REA 2540
 9150 FORMAT (3E10.4, I3)                                                REA 2550
 9160 FORMAT (A1)                                                        REA 2560
 9180 FORMAT (6(A1, I4, E10.4))                                          REA 2570
 9200 FORMAT (I4, E10.4, A10)                                            REA 2580
 9210 FORMAT (11(E10.4, I3))                                             REA 2590
 9270 FORMAT (2I4, E10.4)                                                REA 2600
 9280 FORMAT (I4, 2E10.4, A80)                                           REA 2610
 9290 FORMAT (8I2)                                                       REA 2620
 9300 FORMAT (5I2, A80)                                                  REA 2630
 9350 FORMAT (2E10.4, I2, E10.4, A8)                                     REA 2640
 9360 FORMAT (I2, 3E10.4, A8)                                            REA 2650
 9500 FORMAT (2I2, 3E10.4, A8)                                           REA 2660
 9560 FORMAT (3E10.4, A8)                                                REA 2670
                                                                         REA 2680
      END                                                                REA 2690
```

```
      SUBROUTINE REDOX                                                   RED 0010
C =================================================================     |RED 0020
C     Set the redox flags                                                |RED 0030
C -----------------------------------------------------------------     |RED 0040
                                                                         RED 0050
      INTEGER MAX, SCREEN                                                RED 0060
      CHARACTER * 15 USING                                               RED 0070
      PARAMETER (MAX = 10, SCREEN = 24, USING = '(1X, A, I2, A)')        RED 0080
                                                                         RED 0090
      INTEGER FLAGS(6,MAX), I, NL, SAMP                                  RED 0100
                                                                         RED 0110
      CHARACTER * 1 ANS                                                  RED 0120
      CHARACTER * 2 REDION(6)                                            RED 0130
                                                                         RED 0140
      EXTERNAL CLEAR                                                     RED 0150
                                                                         RED 0160
      COMMON           SAMP                                              RED 0170
      COMMON /COM14 / FLAGS                                              RED 0180
                                                                         RED 0190
      DATA REDION /'Fe', 'Cu', 'Hg', 'Mn', 'U ', 'V '/                   RED 0200
                                                                         RED 0210
C =================================================================     |RED 0220
                                                                         RED 0230
```

```
      NL = SCREEN                                                       RED 0240
                                                                        RED 0250
      DO 20 I = 1, 6                                                    RED 0260
   10   CONTINUE                                                        RED 0270
        CALL CLEAR (NL)                                                 RED 0280
        PRINT *, 'Do you want to distribute ', REDION(I),               RED 0290
     &           ' using Eh? (Y/N)'                                     RED 0300
        IF      (FLAGS(I,SAMP) .EQ. 0) THEN                             RED 0310
          PRINT USING, '           [Current =  N] '                     RED 0320
        ELSE IF (FLAGS(I,SAMP) .EQ. 1) THEN                             RED 0330
          PRINT USING, '           [Current =  Y] '                     RED 0340
        END IF                                                          RED 0350
                                                                        RED 0360
        READ '(A)', ANS                                                 RED 0370
                                                                        RED 0380
        IF (ANS .NE. ' ') THEN                                          RED 0390
          IF      (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                 RED 0400
            FLAGS(I,SAMP) = 1                                           RED 0410
          ELSE IF (ANS. EQ. 'N' .OR. ANS .EQ. 'n') THEN                 RED 0420
            FLAGS(I,SAMP) = 0                                           RED 0430
          ELSE                                                          RED 0440
            PRINT *, 'Answer must be in [Y, y, N, n] '                  RED 0450
            NL = SCREEN - 4                                             RED 0460
            GOTO 10                                                     RED 0470
          END IF                                                        RED 0480
        END IF                                                          RED 0490
                                                                        RED 0500
        NL = 2                                                          RED 0510
                                                                        RED 0520
   20 CONTINUE                                                          RED 0530
                                                                        RED 0540
      RETURN                                                            RED 0550
      END                                                               RED 0560
```

```
      SUBROUTINE STORE (MAXSAM, WRTFLE)                                 STO 0010
C ==================================================================== STO 0020
C     Store the data in memory into the input file                      |STO 0030
C --------------------------------------------------------------------- STO 0040
                                                                        STO 0050
      INTEGER MAX, SCREEN, UN                                           STO 0060
      DOUBLE PRECISION CPUMIN                                           STO 0070
      PARAMETER (CPUMIN = 1.0D-35, MAX = 10, SCREEN = 24, UN = 20)      STO 0080
                                                                        STO 0090
      LOGICAL HERE                                                      STO 0100
                                                                        STO 0110
      INTEGER ACTLEN, ALK(MAX), ANSR(3,MAX), FLAGS(6,MAX), GEOTH(MAX)   STO 0120
      INTEGER I, IBMIX(MAX), ICCSAT(MAX), IDDP(MAX), IDMIX(50,MAX)      STO 0130
      INTEGER IDN(10,10,MAX), IDSAT(MAX), IMCO3(MAX)                    STO 0140
      INTEGER INFORM(MAX), INMIX(MAX), INSP(MAX), IPIT(MAX)             STO 0150
      INTEGER IPRIN1(MAX), IPRIN2(MAX), IRXDP(10,MAX), ISCHG(10,MAX)    STO 0160
```

```
      INTEGER ISCOMP(10,MAX), ITIC(MAX), ITMIX(MAX), ITT(MAX), J, L      STO 0170
      INTEGER LEN, LENGTH, MAXSAM, MININD(10,5,MAX), ND(2,45,MAX)       STO 0180
      INTEGER NDUM(12,MAX), NUFLAG(MAX), NUMINS, RATIO(MAX), SAMP       STO 0190
      INTEGER WRTFLE, Z(3,MAX)                                          STO 0200
                                                                        STO 0210
      CHARACTER *  1 ADEX(MAX), ANS, ODUM(12,MAX)                       STO 0220
      CHARACTER *  2 HOLD(14)                                           STO 0230
      CHARACTER *  4 ANHOLD(13)                                         STO 0240
      CHARACTER *  5 UNITS(MAX)                                         STO 0250
      CHARACTER *  8 MINAME(5,MAX), PAGE(45,MAX)                        STO 0260
      CHARACTER * 10 SPN(10,MAX)                                        STO 0270
      CHARACTER * 20 ANSWR                                              STO 0280
      CHARACTER * 80 FLNAME, MIXFLE(MAX), OUTIN(MAX), TITLE(MAX)        STO 0290
                                                                        STO 0300
      DOUBLE PRECISION AMOL(50,MAX), CEC(MAX), COEF(10,10,MAX)          STO 0310
      DOUBLE PRECISION CONC(3,MAX), CONV1(MAX), CONV2(MAX)              STO 0320
      DOUBLE PRECISION CUNITS(35,MAX), DCH4(MAX), DCO2(MAX)             STO 0330
      DOUBLE PRECISION DENS(MAX), DFRAC1(MAX), DH2S(MAX), DHA(3,MAX)    STO 0340
      DOUBLE PRECISION DNA(45,MAX), DNH3(MAX), DP(MAX), EHM(MAX)        STO 0350
      DOUBLE PRECISION EHMC(MAX), EMFZSC(MAX), FBOIL(MAX), FCCSAT(MAX)  STO 0360
      DOUBLE PRECISION FIXIT(MAX), GFW(3,MAX), HITEMP(MAX), INC(MAX)    STO 0370
      DOUBLE PRECISION KCH4OL(MAX), KCO2OL(MAX), KH2SOL(MAX)            STO 0380
      DOUBLE PRECISION KRXN(10,MAX), MBASE(10,MAX), MINCO(10,5,MAX)     STO 0390
      DOUBLE PRECISION MINLOG(2,5,MAX), PH(MAX), DSEP(MAX), PRESS(MAX)  STO 0400
      DOUBLE PRECISION RXDP(10,MAX), SAREA(MAX), TAREA(MAX), TCH4M(MAX) STO 0410
      DOUBLE PRECISION TCO2M(MAX), TEMP(MAX), TH2SM(MAX), TIC(MAX)      STO 0420
      DOUBLE PRECISION WROIL(MAX), XD(2,45,MAX), XDUM(12,MAX)           STO 0430
                                                                        STO 0440
      INTRINSIC DABS                                                    STO 0450
                                                                        STO 0460
      EXTERNAL CLEAR, IANSWR, LENGTH                                    STO 0470
                                                                        STO 0480
      COMMON           SAMP                                             STO 0490
      COMMON /COM1  / TITLE, UNITS, FLNAME                              STO 0500
      COMMON /COM2  / TEMP, HITEMP, DENS, PRESS                         STO 0510
      COMMON /COM3  / PH, EHM, EHMC, EMFZSC                             STO 0520
      COMMON /COM4  / CUNITS, TIC                                       STO 0530
      COMMON /COM5  / ALK, ITIC, NUFLAG, IPIT, CONV1, CONV2             STO 0540
      COMMON /COM6  / DCH4, DCO2, DH2S, DNH3, ICCSAT, IMCO3, FIXIT,     STO 0550
     &                FCCSAT                                           STO 0560
      COMMON /COM7  / TCO2M, TCH4M, TH2SM, WROIL,                       STO 0570
     &                KCO2OL, KCH4OL, KH2SOL, DSEP                     STO 0580
      COMMON /COM8  / ADEX, SPN                                         STO 0590
      COMMON /COM9  / CEC, TAREA, SAREA, INSP, ISCHG, MBASE,            STO 0600
     &                KRXN, ISCOMP, COEF, IDN                          STO 0610
      COMMON /COM10 / IBMIX, ITMIX, IDSAT, IDDP, ITT, DP, IRXDP,        STO 0620
     &                IDMIX, INMIX, RXDP, AMOL, DFRAC1, INC, FBOIL     STO 0630
      COMMON /COM11 / ODUM                                              STO 0640
      COMMON /COM12 / NDUM, XDUM                                        STO 0650
      COMMON /COM13 / INFORM, RATIO, GEOTH, IPRIN1, IPRIN2              STO 0660
      COMMON /COM14 / FLAGS                                             STO 0670
      COMMON /COM15 / ANSR, CONC, DHA, GFW, Z                           STO 0680
      COMMON /COM16 / PAGE                                              STO 0690
      COMMON /COM17 / ND, XD, DNA                                       STO 0700
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      COMMON /COM18 / MINAME                                                  STO 0710
      COMMON /COM19 / MINCO, MININD, MINLOG                                   STO 0720
      COMMON /COM20 / MIXFLE, OUTIN                                           STO 0730
                                                                              STO 0740
      DATA HOLD /'H', 'H2', 'Al', 'Ba', 'Ca', 'Cu', 'Fe', ' K', 'Mg',         STO 0750
     &          'Mn', 'Na', 'Pb', 'Sr', 'Zn'/                                STO 0760
      DATA ANHOLD /'Cl', 'SO4', 'HCO3', 'OH', 'PO4', 'F', 'Ace', 'CO3',       STO 0770
     &            'HS', 'Oxy', 'Suc', ' ', ' '/                             STO 0780
                                                                              STO 0790
C ------------------------------------------------------------------------|  STO 0800
                                                                              STO 0810
      CALL CLEAR (SCREEN)                                                     STO 0820
                                                                              STO 0830
      PRINT *, 'What do you want to call this file?'                          STO 0840
      ACTLEN = 80                                                             STO 0850
      LEN = LENGTH(FLNAME, ACTLEN)                                            STO 0860
      PRINT '(1X,A,A,A)', '     [Current = ', FLNAME(1:LEN), '] '             STO 0870
                                                                              STO 0880
      READ '(A)', ANSWR                                                       STO 0890
                                                                              STO 0900
      IF (ANSWR .NE. ' ') THEN                                                STO 0910
        FLNAME = ANSWR                                                        STO 0920
      END IF                                                                  STO 0930
                                                                              STO 0940
      INQUIRE (FILE = FLNAME, EXIST = HERE, ERR = 110)                        STO 0950
                                                                              STO 0960
      IF (HERE) THEN                                                          STO 0970
        PRINT *, FLNAME, ' already exists.  Do you wish to overwrite?'        STO 0980
        READ '(A)', ANS                                                       STO 0990
        IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') THEN                              STO 1000
          OPEN (UNIT = UN, FILE = FLNAME, STATUS = 'UNKNOWN', ERR = 110)      STO 1010
        ELSE                                                                  STO 1020
          RETURN                                                              STO 1030
        END IF                                                                STO 1040
      ELSE                                                                    STO 1050
          OPEN (UNIT = UN, FILE = FLNAME, STATUS = 'NEW', ERR = 110)          STO 1060
      END IF                                                                  STO 1070
                                                                              STO 1080
      WRTFLE = 1                                                              STO 1090
                                                                              STO 1100
      PRINT '(1X, A, I2, A)', 'Will write out ', MAXSAM, ' sample(s).'        STO 1110
      PRINT *, 'Enter a <CR> for ok or a number indicating how many',         STO 1120
     &         ' samples you want written out. '                            STO 1130
                                                                              STO 1140
      CALL IANSWR(MAXSAM)                                                     STO 1150
                                                                              STO 1160
      DO 100 L = 1, MAXSAM                                                    STO 1170
        PRINT *, 'Writing file ...'                                           STO 1180
        WRITE (UN, 9010) TITLE(L)                                             STO 1190
        WRITE (UN, 9030) TEMP(L), HITEMP(L), DENS(L), PRESS(L)                STO 1200
        WRITE (UN, 9030) PH(L), EHM(L), EHMC(L), EMFZSC(L), UNITS(L)          STO 1210
        WRITE (UN, 9080) (CUNITS(I,L), I =  1,  7)                            STO 1220
        WRITE (UN, 9080) (CUNITS(I,L), I =  8, 13), TIC(L)                    STO 1230
        WRITE (UN, 9080) (CUNITS(I,L), I = 14, 20)                            STO 1240
```

```
      WRITE (UN, 9080) (CUNITS(I,L), I = 21, 26)                        STO 1250
      WRITE (UN, 9080) (CUNITS(I,L), I = 27, 29)                        STO 1260
      WRITE (UN, 9080) (CUNITS(I,L), I = 30, 33)                        STO 1270
      WRITE (UN, 9100) ALK(L), ITIC(L)                                  STO 1280
      WRITE (UN, 9080) DCO2(L), DH2S(L), DNH3(L), DCH4(L)               STO 1290
      WRITE (UN, 9100) ICCSAT(L), IMCO3(L), FIXIT(L), FCCSAT(L)         STO 1300
      WRITE (UN, 9080) TCO2M(L), TCH4M(L), TH2SM(L), WROIL(L),          STO 1310
     &                 KCO2OL(L), KCH4OL(L), KH2SOL(L), DSEP(L)       STO 1320
                                                                        STO 1330
      WRITE (UN, 9160) ADEX(L)                                          STO 1340
      IF (ADEX(L) .EQ. 'A' .OR. ADEX(L) .EQ. 'E') THEN                  STO 1350
        WRITE (UN, 9150) CEC(L), TAREA(L), SAREA(L), INSP(L)            STO 1360
        DO 10 I = 1, INSP(L)                                            STO 1370
          WRITE (UN, 9200) ISCHG(I,L), MBASE(I,L), SPN(I,L)             STO 1380
          WRITE (UN, 9210) KRXN(I,L), ISCOMP(I,L), (COEF(I,J,L),        STO 1390
     &                     IDN(I,J,L), J = 1, ISCOMP(I,L))            STO 1400
10      CONTINUE                                                        STO 1410
      END IF                                                            STO 1420
                                                                        STO 1430
      WRITE (UN, 9100) IBMIX(L), ITMIX(L)                               STO 1440
      IF (IBMIX(L) .EQ. 1) THEN                                         STO 1450
        IF      (ITMIX(L) .LT. 0) THEN                                  STO 1460
          WRITE (UN, 9280) IDDP(L), AMOL(1,L)                           STO 1470
        ELSE IF (ITMIX(L) .EQ. 0) THEN                                  STO 1480
          WRITE (UN, 9270) IDSAT(L), IDDP(L), DP(L)                     STO 1490
          IF (IDDP(L) .EQ. 0) THEN                                      STO 1500
            WRITE (UN, 9270) ITT(L)                                     STO 1510
            DO 20 I = 1, ITT(L)                                         STO 1520
              WRITE (UN, 9280) IRXDP(I,L), RXDP(I,L)                    STO 1530
20          CONTINUE                                                    STO 1540
          END IF                                                        STO 1550
        ELSE IF (ITMIX(L) .GT. 0) THEN                                  STO 1560
          DO 30 I = 1, ITMIX(L)                                         STO 1570
            WRITE (UN, 9280) IDMIX(I,L), AMOL(I,L)                      STO 1580
30        CONTINUE                                                      STO 1590
        END IF                                                          STO 1600
      ELSE IF (IBMIX(L) .EQ. 2) THEN                                    STO 1610
        WRITE (UN, 9280) INMIX(L), DFRAC1(L), INC(L), MIXFLE(SAMP)      STO 1620
      ELSE IF (IBMIX(L) .EQ. 3) THEN                                    STO 1630
        WRITE (UN, 9080) FBOIL(L)                                       STO 1640
      END IF                                                            STO 1650
      WRITE (UN, 9180) (ODUM(I,L), NDUM(I,L), XDUM(I,L), I = 1,  6)     STO 1660
      WRITE (UN, 9180) (ODUM(I,L), NDUM(I,L), XDUM(I,L), I = 7, 12)     STO 1670
      WRITE (UN, 9290) ANSR(1,L), ANSR(2,L)                             STO 1680
      IF (ANSR(1,L) .GT. 0) THEN                                        STO 1690
        WRITE (UN, 9350) CONC(1,L), GFW(1,L), Z(1,L), DHA(1,L),         STO 1700
     &                   PAGE(1,L)                                      STO 1710
        DO 40 I = 2, 15                                                 STO 1720
          IF      (ND(1,I,L) .GT. 0) THEN                               STO 1730
            WRITE (UN, 9360) ND(1,I,L), DNA(I,L), XD(1,I,L),            STO 1740
     &                       XD(2,I,L), HOLD(I-1) // PAGE(1,L)          STO 1750
          ELSE IF (ND(2,I,L) .GT. 0) THEN                               STO 1760
            WRITE (UN, 9360) ND(1,I,L), DNA(I,L), XD(1,I,L),            STO 1770
     &                       XD(2,I,L), HOLD(I-1) // PAGE(1,L)          STO 1780
```

```
        END IF                                                          STO 1790
40      CONTINUE                                                        STO 1800
      END IF                                                            STO 1810
      IF (ANSR(2,L) .GT. 0) THEN                                        STO 1820
        WRITE (UN, 9350) CONC(2,L), GFW(2,L), Z(2,L), DHA(2,L),         STO 1830
     &                   PAGE(16,L)                                     STO 1840
        DO 50 I = 2, 15                                                 STO 1850
          IF      (ND(1,I+15,L) .GT. 0) THEN                            STO 1860
            WRITE (UN, 9360) ND(1,I+15,L), DNA(I+15,L), XD(1,I+15,L),   STO 1870
     &                       XD(2,I+15,L), HOLD(I-1) // PAGE(16,L)      STO 1880
          ELSE IF (ND(2,I+15,L) .GT. 0) THEN                            STO 1890
            WRITE (UN, 9360) ND(2,I+15,L), DNA(I+15,L), XD(1,I+15,L),   STO 1900
     &                       XD(2,I+15,L), HOLD(I-1) // PAGE(16,L)      STO 1910
          END IF                                                        STO 1920
50      CONTINUE                                                        STO 1930
      END IF                                                            STO 1940
                                                                        STO 1950
      IF (ANSR(3,L) .GT. 0) THEN                                        STO 1960
        WRITE (UN, 9500) ANSR(3,L), Z(3,L), DHA(3,L), GFW(3,L),         STO 1970
     &                   CONC(3,L), PAGE(31,L)                          STO 1980
        IF (ANSR(3,L) .GT. 0) THEN                                      STO 1990
          ANHOLD(12) = PAGE(1,L)                                        STO 2000
          ANHOLD(13) = PAGE(16,L)                                       STO 2010
          ACTLEN = 8                                                    STO 2020
          LEN = LENGTH(PAGE(31,L), ACTLEN)                              STO 2030
          DO 60 I = 2, 14                                               STO 2040
            IF      (ND(1,I+30,L) .GT. 0) THEN                          STO 2050
              WRITE (UN, 9360) ND(1,I+30,L), DNA(I+30,L),               STO 2060
     &          XD(1,I+30,L), XD(2,I+30,L), PAGE(31,L)(1:LEN) //        STO 2070
     &          ANHOLD(I-1)                                           STO 2080
            ELSE IF (ND(2,I+15,L) .GT. 0) THEN                          STO 2090
              WRITE (UN, 9360) ND(2,I+30,L), DNA(I+30,L),               STO 2100
     &          XD(1,I+30,L), XD(2,I+30,L), PAGE(31,L)(1:LEN) //        STO 2110
     &          ANHOLD(I-1)                                           STO 2120
            END IF                                                      STO 2130
60        CONTINUE                                                      STO 2140
        END IF                                                          STO 2150
      ELSE                                                              STO 2160
        WRITE (UN, 9500) ANSR(3,L)                                      STO 2170
      END IF                                                            STO 2180
                                                                        STO 2190
      NUMINS = 0                                                        STO 2200
      DO 70 I = 1, 5                                                    STO 2210
        IF (DABS(MINLOG(1,I,L)) .GT. CPUMIN .OR.                        STO 2220
     &      DABS(MINLOG(2,I,L)) .GT. CPUMIN) THEN                       STO 2230
          NUMINS = NUMINS + 1                                           STO 2240
        END IF                                                          STO 2250
70    CONTINUE                                                          STO 2260
                                                                        STO 2270
      WRITE (UN, 9360) NUMINS                                           STO 2280
      DO 80 I = 1, NUMINS                                               STO 2290
        IF (DABS(MINLOG(1,I,L)) .GT. CPUMIN .OR.                        STO 2300
     &      DABS(MINLOG(2,I,L)) .GT. CPUMIN) THEN                       STO 2310
          WRITE (UN, 9560) MINLOG(1,I,L), MINLOG(2,I,L),                STO 2320
```

```
     &                        MINCO(10,I,L), MINAME(I,L)                    STO 2330
           WRITE (UN, 9210) (MINCO(J,I,L), MININD(J,I,L), J = 1, 9)         STO 2340
         END IF                                                             STO 2350
  80   CONTINUE                                                            STO 2360
                                                                           STO 2370
       WRITE (UN, 9290) NUFLAG(L), IPIT(L), (FLAGS(I,L), I = 1, 6)         STO 2380
       WRITE (UN, 9300) INFORM(L), RATIO(L), GEOTH(L),                     STO 2390
     &                  IPRIN1(L), IPRIN2(L), OUTIN(L)                    STO 2400
       WRITE (UN, 9080) CONV1(L), CONV2(L)                                 STO 2410
                                                                           STO 2420
 100 CONTINUE                                                              STO 2430
                                                                           STO 2440
       CLOSE (UN)                                                          STO 2450
       RETURN                                                              STO 2460
                                                                           STO 2470
 110 CONTINUE                                                              STO 2480
       PRINT *, FLNAME, ' is not valid.  Can not open.'                    STO 2490
       PRINT *, 'Hit return to continue'                                   STO 2500
       READ '(A)', ANS                                                     STO 2510
                                                                           STO 2520
       RETURN                                                              STO 2530
                                                                           STO 2540
C ------------------------------------------------------------------------|STO 2550
C      Format Statements                                                   |STO 2560
C ---------------------                                                    |STO 2570
                                                                           STO 2580
 9010 FORMAT (A80)                                                         STO 2590
 9030 FORMAT (4E10.4, A5)                                                  STO 2600
 9080 FORMAT (8E10.4)                                                      STO 2610
 9100 FORMAT (2I2, 2E10.4)                                                 STO 2620
 9150 FORMAT (3E10.4, I3)                                                  STO 2630
 9160 FORMAT (A1)                                                          STO 2640
 9180 FORMAT (6(A1, I4, E10.4))                                            STO 2650
 9200 FORMAT (I4, E10.4, A10)                                              STO 2660
 9210 FORMAT (11(E10.4, I3))                                               STO 2670
 9270 FORMAT (2I4, E10.4)                                                  STO 2680
 9280 FORMAT (I4, 2E10.4, A80)                                             STO 2690
 9290 FORMAT (8I2)                                                         STO 2700
 9300 FORMAT (5I2, A80)                                                    STO 2710
 9350 FORMAT (2E10.4, I2, E10.4, A8)                                       STO 2720
 9360 FORMAT (I2, 3E10.4, A8)                                              STO 2730
 9500 FORMAT (2I2, 3E10.4, A8)                                             STO 2740
 9560 FORMAT (3E10.4, A8)                                                  STO 2750
                                                                           STO 2760
       END                                                                 STO 2770




       SUBROUTINE UPCASE (STRING, ACTLEN)                                  UPC 0010
C ======================================================================|UPC 0020
C      This subroutine converts the characters in the given string to     |UPC 0030
C      upper case.  Uses function length                                  |UPC 0040
```

```
C ------------------------------------------------------------------------|UPC 0050
                                                                          UPC 0060
      INTEGER ACTLEN, I, L, LENGTH                                        UPC 0070
                                                                          UPC 0080
      CHARACTER *  1  LCHAR                                               UPC 0090
      CHARACTER * (*) STRING                                              UPC 0100
                                                                          UPC 0110
      INTRINSIC CHAR, ICHAR                                               UPC 0120
                                                                          UPC 0130
      EXTERNAL LENGTH                                                     UPC 0140
                                                                          UPC 0150
C =======================================================================|UPC 0160
                                                                          UPC 0170
      L = LENGTH (STRING, ACTLEN)                                         UPC 0180
                                                                          UPC 0190
      DO 10 I = 1, L                                                      UPC 0200
        LCHAR = STRING(I:I)                                               UPC 0210
        IF (LCHAR .LE. 'z' .AND. LCHAR .GE. 'a') THEN                     UPC 0220
          LCHAR = CHAR(ICHAR(LCHAR) - (ICHAR('a') - ICHAR('A')))          UPC 0230
          STRING(I:I) = LCHAR                                             UPC 0240
        END IF                                                            UPC 0250
   10 CONTINUE                                                            UPC 0260
                                                                          UPC 0270
      RETURN                                                              UPC 0280
      EN                                                                  UPC 0290
```


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