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VERSION 4.00 OF THE MINTEQ GEOCHEMICAL CODE

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SUMMARY

The MINTEQ code is a thermodynamic model that can be used to calculate solution equilibria for geochemical applications. Included in the MINTEQ code are formulations for ionic speciation, ion exchange, adsorption, solubility, redox, gas-phase equilibria, and the dissolution of finite amounts of specified solids. Since the initial development of the MINTEQ geochemical code (see Felmy et al. 1984a, 1984b), a number of undocumented versions of the source code and data files have come into use at the Pacific Northwest Laboratory (PNL). This report documents these changes, describes source code modifications made for the Aquifer Thermal Energy Storage (ATES) program, and provides comprehensive listings of the data files. A version number of 4.00 has been assigned to the MINTEQ source code and the individual data files described in this report.

The principal changes to the MINTEQ source code that are described in this report include

- the correction of equilibrium constants for pressure
- the correction of equilibrium constants for temperature
- the insertion of control words in the input data file to define output length and end-of-file points
- the incorporation of the extended-Debye-Huckel B-dot equation as the default method for calculating single ion activity coefficients.

This report is not intended to replace the MINTEQ user's guide by Peterson et al. (1987) but rather to provide supplementary documentation on the most current version of the MINTEQ geochemical code at PNL.

ACKNOWLEDGMENTS

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INTRODUCTION

The MINTEQ code is a thermodynamic model that can be used to calculate solution equilibria for geochemical applications. Included in the MINTEQ code are formulations for ionic speciation, ion exchange, adsorption, solubility, redox, gas-phase equilibria, and the dissolution of finite amounts of specified solids.

The MINTEQ code was developed by Felmy et al. (1984a, 1984b) from the mathematical structure of the MINEQL code (Westall et al. 1976) and originally used the database from the WATEQ3 code (Ball et al. 1979, 1980, 1981). Much of the current database was compiled by Krupka et al. (1988) and includes contributions from Cowan et al. (1985), Cowan (1988), Crecilius et al. (1986), Krupka and Jenne (1982), Peterson et al. (1986), and Sehmel (1989). Technical details on the mathematical structure of the code are given by Felmy et al. (1984a, 1984b). The MINTEQ User's Manual (Peterson et al. 1987) describes the input files, input options, database files, and methodology for using the MINTEQ geochemical model.

The earliest versions of the MINTEQ code were developed for mainframe computers, but in 1987 the code was converted to run on personal computers by K. M. Krupka at Pacific Northwest Laboratory (PNL). A specialized version of the MINTEQ code was developed by Smith (1988) to conduct equilibrium calculations for the 13-component system K_2O-Na_2O-CaO-MgO-FeO-Al_2O_3-SiO_2-CO_2-H_2O-HF-HCl-H_2S-H_2SO_4 at temperatures to 300°C. This version contained modified formulations for calculating activity coefficients of aqueous species and the effects of temperature on equilibrium constants in the personal computer version. Other derivatives of the MINTEQ code include MINTEQA1 and MINTEQA2, which were developed by the U.S. Environmental Protection Agency (EPA) (Brown and Allison 1987; Allison et al. 1991). These EPA versions include pre-processor codes (PRODEFA1 and PRODEFA2) that are used to define input files, and also have software improvements that reduce computational time and aid in error recovery.

The purpose of this report is to provide a comprehensive description of the changes recently made to the MINTEQ code at PNL as part of the Aquifer

Thermal Energy Storage (ATES) program sponsored by the U.S. Department of Energy (DOE). These changes include a major restructuring of the database components and minor modifications to the MINTEQ source code and to input and output formats since the publication of the MINTEQ User's Guide (Peterson et al. 1987). This report is a reference source for the thermodynamic data contained in the MINTEQ database, which currently contains thermodynamic data for nearly all of the major and minor elemental aqueous species and solids found in significant concentrations in natural groundwater systems.

The most important limitation of the database is the absence of formation constants for organometallic complexes. The database has evolved from a number of studies on groundwater chemistry that have been conducted at PNL since the construction of the MINTEQ code. This database has not been rigorously checked for internal consistency. Future efforts will be directed at checking the internal consistency of the data and making additions to the database that are warranted. Users of the MINTEQ code should carefully review data pertinent to their particular studies.

This report also describes the implementation of a version numbering scheme for the MINTEQ code and its database components. This report is not intended to replace the MINTEQ User's Guide, but rather to provide supplementary documentation on the most current version of the MINTEQ code at PNL. Details on the mathematical formulations, input variables, and modeling concepts for the MINTEQ code are provided by Felmy (1984a, 1984b) and Peterson et al. (1987).

VERSION NUMBERING

Starting with this report, version numbers have been assigned to the MINTEQ source FORTRAN code and to the various data files (Figure 1). These version numbers are printed to the output file for reference. The purpose of the version numbers is to provide a means for tracking changes to either the source code or the data files. When major changes to either the source code or the data files are made, new version numbers will be assigned and documented in subsequent PNL reports. The initial assignment of the version number for all portions of the code was arbitrarily set at 4.00 to reflect the presence of prior MINTEQ versions at PNL. In the following sections of this report, MINTEQ(4.00) will be used to refer to Version 4.00.

FILE STRUCTURE

The new file structure for MINTEQ(4.00) is shown in Figure 1. The default names for the input and output files remain SAMPLE.DAT(4.00) and MINOUT.DAT(4.00) as in previous versions (Figure 1). The FORTRAN portion of the MINTEQ(4.00) code has been broken into six parts (see files with the ".FOR" extension in Figure 1), so that each part can be compiled separately, and then the individual object modules can be linked together to create an executable file. A seventh file named COMMON.BLK(4.00) contains variable type declarations and common block definitions. Separate compilation of the FORTRAN components is required to use the MINTEQ(4.00) code on personal computers with random access memory (RAM) less than or equal to one megabyte, which is the minimum amount needed to run the MINTEQ(4.00) code.

The database structure has been changed so that all thermodynamic data pertaining to aqueous speciation reactions are contained in a file named AQUEOUS.DAT(4.00) (Figure 1). All thermodynamic data pertaining to solid-phase solubility reactions are contained in a file named SOLIDS.DAT(4.00). Additionally, the GAS-RDX.DAT(4.00) file now contains thermodynamic data on both gas-phase equilibria and redox reactions (Figure 1). The file TYPE6.DAT contained in previous MINTEQ versions (Peterson et al. 1987) is no longer used; it was replaced by the SOLIDS.DAT(4.00) file. Type 6 monitored species are specified in the SAMPLE.DAT(4.00) input file in the same manner as in earlier MINTEQ versions, but the thermodynamic data for such species are found in either the SOLIDS.DAT(4.00) or GAS-RDX.DAT(4.00) data files. Additions of thermodynamic data for new solids, gases, or redox reactions need only be made to the pertinent file, either SOLIDS.DAT or GAS-RDX.DAT(4.00).

The ANALYT.DAT(4.00) file, which contained coefficients for correcting equilibrium constants for temperature (Smith 1988), is no longer used. The coefficients are now contained in the individual thermodynamic data files (discussed below). The COMP.DAT(4.00), ALK.DAT(4.00), and PRCOEF.DAT(4.00) data files are unchanged from previous MINTEQ versions. The COMP.DAT(4.00) data file contains characteristic data for the basis species. The ALK.DAT(4.00) data file contains stoichiometric data for reactions that involve noncarbonate alkalinity. The PRCOEF.DAT(4.00) data file contains a

limited set of molar volume data that are used internally in the MINTEQ code to correct equilibrium constants for the effect of pressure.

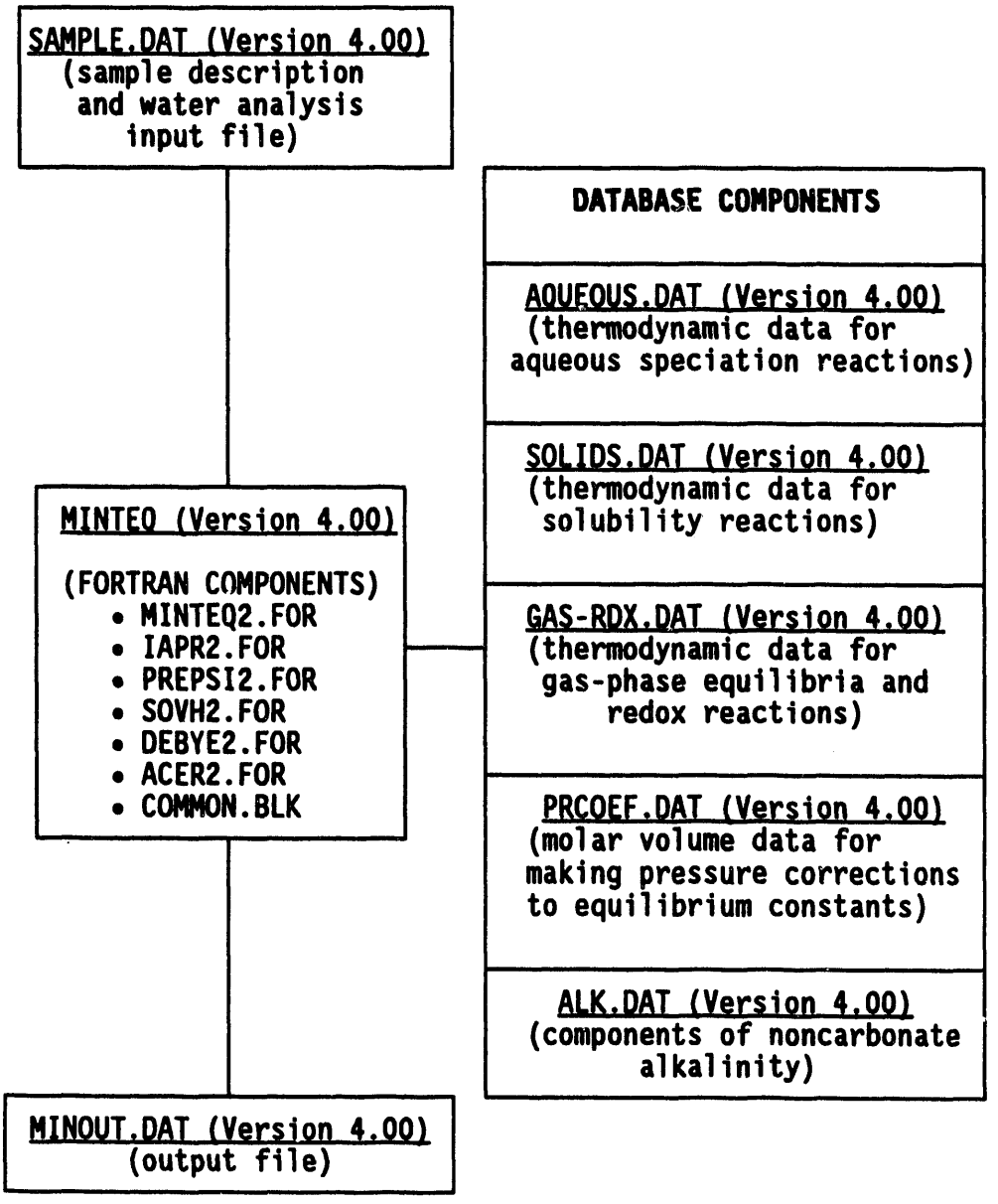

FIGURE 1. File Structure for the MINTEQ3 Geochemical Code

SOURCE CODE MODIFICATIONS

A number of changes have been made to the MINTEQ source code to improve its relevance to geochemical systems. These changes are described below.

ACTIVITY COEFFICIENT CALCULATION

The current version of the MINTEQ(4.00) code contains two forms of the Debye-Hückel equation to calculate activity coefficients of charged ionic species. One form is the extended-Debye-Huckel equation with B-dot described by Helgeson (1969):

$$\log \gamma_i = (-A\, z_i^2\, I^{0.5})/(1 + \mathring{a}_i\, B\, I^{0.5}) + B\dot{}\, I \qquad (1)$$

where γ_i, z_i, and $\mathring{a}_i$ are the activity coefficient, charge, and ion size of the ith ion. Also in Equation (1), I is the ionic strength and A and B are constants that are functions of the dielectric constant, temperature, and density of water. Functions for A and B are taken from Helgeson and Kirkham (1974) where the density of steam-saturated water is from Saul and Wagner (1987). The $B\dot{}$ in Equation (1) is the B-dot parameter of Helgeson (1969). The value of $B\dot{}$ is the same for all ions but is a function of temperature (Helgeson 1969). The details of these various functions are given by Smith (1988), who incorporated them into a high-temperature version of MINTEQ. The FORTRAN coding written by Smith (1988) was adapted to MINTEQ(4.00) with minor changes. The extended-Debye-Huckel equation with B-dot is now the default expression used to calculate activity coefficients in MINTEQ(4.00).

An alternative equation in MINTEQ(4.00) for calculating activity coefficients of charged species is the Davies equation:

$$\log \gamma_i = -A\, z_i^2\, [(I^{0.5}/1 + I^{0.5}) - 0.3\, I] \qquad (2)$$

The Davies equation can be selected by setting the appropriate option in the input file. The Davies equation is also selected automatically for species that do not have ionic size parameters ($\mathring{a}_i$) in the thermodynamic data files.

TEMPERATURE CORRECTION FOR EQUILIBRIUM CONSTANTS

Previous versions of MINTEQ used either the van't Hoff equation or analytical expressions that represent empirical fits of the change in equilibrium constants with temperature. The van't Hoff equation

$$\log K_T/K_{298} = -(\Delta H_r^\circ/2.303R)\ (1/T - 1/298) \qquad (3)$$

where ΔH_r° is the standard enthalpy of reaction at 298K (25°C), T is the temperature in K, R is the ideal gas constant, and K is the equilibrium constant, is retained in MINTEQ(4.00). This expression can be expected to be accurate only between 0 and 80°C (Smith 1988). For temperatures outside this range, analytical expressions that are based on Maier-Kelley power functions are used to describe the effect of temperature on the equilibrium constants (Maier and Kelley 1932). These expressions have the following form:

$$\log K_T = a_0 + a_1/T + a_2T + a_3 \log_{10}(T) + a_4/T^2 \qquad (4)$$

where T is in K and a_0, a_1, a_2, a_3, and a_4 are empirical coefficients. If values for the empirical constants are present in the thermodynamic data files for a specific reaction, then the MINTEQ(4.00) code automatically uses the analytical expression in Equation (4) to calculate the equilibrium constant. The exception is when the solution temperature is specified as 25°C, in which case the 25°C-values of the equilibrium constant in thermodynamic data files are used. If empirical data do not exist for the temperature dependence of the equilibrium constants (and for many reactions they do not), then the code will use the van't Hoff expression in Equation (3), given that a value for ΔH_r° is present in the thermodynamic data files. If neither the empirical coefficients nor an ΔH_r° is present, then the MINTEQ(4.00) code defaults to the 25°C-value for the equilibrium constant and no temperature correction is made.

The current database contains empirical coefficients for correcting equilibrium constants for the effect of temperature (i.e., to 300°C) according to Equation (4) for all of the major species and solids relevant to ATES systems. The data for these species and solids came from Smith (1988), Wolery (1983), and Wolery and Daveler (1989).

PRESSURE CORRECTION FOR EQUILIBRIUM CONSTANTS

Formulations for correcting equilibrium constants for the effect of pressure were inserted into the MINTEQ code by Sass and Howden.[a] The effect of pressure on the equilibrium constant is described by

$$[\partial(\ln K)/\partial P]_T = -\Delta V_r^\circ/RT \quad (5)$$

where ΔV_r° is the standard molar volume of reaction and P is the pressure. The pressure dependence of ΔV_r° can be related to the isothermal partial molar compressibility, $\Delta\kappa_r^\circ$ by

$$\Delta\kappa_r^\circ = -(\partial V_r^\circ/\partial P)_T \quad (6)$$

where $\Sigma V_r^\circ n_i = \Delta V_r^\circ$. The integration of Equation (6) from P°, which is the reference pressure to some other pressure, P, gives

$$V_P = V_{P^\circ} - \Delta\kappa_r^\circ (P - P^\circ) \quad (7)$$

(Lown et al. 1968). The substitution of Equation (7) into Equation (5) and integration at a constant temperature gives the following expression:

$$\log (K_P/K_{P^\circ}) = (- V_r P + \Delta\kappa_r^\circ P_2/2)/2.303RT \quad (8)$$

that relates the equilibrium constant to the partial molar volume of reaction.

The partial molar volumes, V_i° and compressibilities, $\Delta\kappa_i^\circ$, of individual aqueous species can be described as polynomial functions of temperature by

$$V_i^\circ = a_1 + b_1 T + c_1 T_2 \quad (9)$$

and

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[a] Sass, B. M. and W. M. Howden. 1984. MINTEQ Geochemical Model-Equilibrium Constant Calculations at Pressures Greater than 1 bar. (Unpublished Report, Pacific Northwest Laboratory, Richland, Washington.)

$$\Delta\kappa_i^\circ = a_2 + b_2T + c_2T^2 \qquad (10)$$

where a, b, and c are constants (Millero 1982). Equations (8-10) were incorporated into the MINTEQ(4.00) code to correct the equilibrium constants of specific reactions for pressure by Sass and Howden[(b)]. The system pressure, P, is entered in the MINTEQ(4.00) input file in feet of water (see following section). Values of a, b, and c for 21 aqueous species were obtained from Millero (1982) and were inserted in the PRCOEF.DAT(4.00) data file by Sass and Howden (1984). For solids, molar volume data were obtained from compilations by Robie et al. (1967, 1978) and inserted in the PRCOEF.DAT(4.00) data file by Sass and Howden. The compressibilities of all solids were set at zero.

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b Sass, B. M. and W. M. Howden. 1984. MINTEQ Geochemical Model-Equilibrium Constant Calculations at Pressures Greater than 1 bar. (Unpublished Report, Pacific Northwest Laboratory, Richland, Washington.)

INPUT FILE FORMATS

Formats for SAMPLE.DAT(4.00), MINOUT.DAT(4.00), COMP.DAT(4.00), AQUEOUS.DAT(4.00), SOLIDS.DAT(4.00), GAS-RDX.DAT(4.00), PRCOEF.DAT(4.00), and ALK.DAT(4.00) are described in this section.

THE SAMPLE.DAT(4.00) PROBLEM DEFINITION FILE

The SAMPLE.DAT(4.00) file is the user-input file that describes the water composition and defines various options for controlling the calculation modes used in MINTEQ(4.00). An example of an input file for the River Water Test Case Number One from Peterson et al. (1987) is given in Appendix A. The structure of the SAMPLE.DAT(4.00) is similar to that used in previous PNL versions of MINTEQ in that it is composed of three major sections: 1) basic input and control variables, 2) the water analysis, and 3) the type modifications. A few minor modifications have been made to the SAMPLE.DAT(4.00) file. These modifications are described below, along with a complete description of the basic input data and formats for the SAMPLE.DAT(4.00) file. Most of this description is taken directly from the MINTEQ User's Guide (Peterson et al. 1987).

The definitions of the species "types" in MINTEQ(4.00) are the same as those given in the User's Guide. Type 1 species are the basis components found in COMP.DAT(4.00) that are used to represent the water analysis. Water is automatically entered as a Type 1 species in the MINTEQ(4.00) code. Type 2 species are those aqueous species that are derived from the specified TYPE 1 basis species and are input to the MINTEQ(4.00) code through the SAMPLE.DAT(4.00) file. Type 3 species are those that have fixed activities in the geochemical calculations, such as gases with fixed partial pressures, solids that are present in infinite supply for dissolution, and components like H^+ or e^-(i.e., the pH and pe). Type 4 species are solids that are initially present in some finite mass and will be allowed to dissolve in the geochemical calculation. Type 5 species are solids from the MINTEQ database that are allowed to precipitate in the geochemical calculation. Type 6 species are monitored species that are excluded from the geochemical calculation but whose equilibria are calculated as an end result of the

model's speciation and solubility calculations and are printed to the output file. Type 6 species can be gases, aqueous complexes, or solids.

Multiple SAMPLE.DAT(4.00) files can be concatenated and run together but the individual files must be separated by two blank lines. The output from the MINTEQ(4.00) code for each SAMPLE.DAT(4.00) file will be appended to the end of the previous output.

A line-by-line description of the SAMPLE.DAT(4.00) input file is given in the following exhibit. Most of this description is taken from Peterson et al. (1987).

EXHIBIT 1. Description of the SAMPLE.DAT(4.00) Input File

Section 1: Basic Input and Control Variables.

Lines 1-9 (1 variable, A80). A maximum of nine lines of text can now be used to describe the water analysis and the model calculation. Previous versions allowed two lines of descriptive text.

Line 10 (1 variable, A5). The character string "STOP." must be placed in the first five spaces of the line immediately following the sample description. The "STOP." must be in capital letters and indicates the end of the sample description section and must be in line 10 or lower.

Line 11 (1 variable, A6). The word "SHORT." in capital letters should be placed here to produce a shortened output from MINTEQ(4.00) (see below). Any other character string will result in the full MINTEQ(4.00) output.

Line 12 (4 variables, free format). 1) Water temperature in °C, 2) the analytical units for the water analysis in capital letters and enclosed by single quotes (i.e., 'PPM', 'MG/L', 'MOL', or 'MEQ/L' for parts per million, milligram per liter, mole per liter, or milliequivalents per liter, respectively), 3) the hydrostatic pressure in feet of water[1], and 4) the fixed ionic strength designation. If 0.00 is entered for the fixed ionic strength designation, then MINTEQ(4.00) will compute the ionic strength (see also Option 7, Line 13). If a positive value other than 0.00 is entered, then the ionic strength will be fixed at this value for all calculations.

Line 13 (8 variables, 8(I1,1X)). This line contains 8 run-specific options.

Option 1. The total inorganic carbon input option.
- (0) = total inorganic carbon.
- (1) = total alkalinity.

Option 2. The debug print option. This option should be used only when modifications have been made to the code, or the values of certain arrays need to be checked.
- (0) = No debug printout.
- (1) = Print the values of the IDX, C, IDY, GAMMA, and Y arrays.
- (2) = Not used.
- (3) = Print the NNN, NN(1), NN(2), and the IDY, GK, GK1 arrays in subroutine KCORR.
- (4) = Print the IDX, X, IDY, L, and GK arrays every iteration in subroutine SOLID and print the saturation index for the solid added to the phase assemblage in subroutine SOLIDX.

Option 3. The charge balance option.
- (0) = Terminate execution if the initial charge imbalance is greater than 30%.
- (1) = Do not terminate execution regardless of the initial charge imbalance.

EXHIBIT 1. (continued)

Option 4. Considered solids and print option.
- (0) = Do not allow all of the solids in the database to precipitate or dissolve. The solids considered will be those entered as Type 3 solids. Print the problem results after the initial aqueous speciation plus solids problem is solved and after all Type 5 solids are either in equilibrium or are undersaturated.
- (1) = Allow all solids in the database to precipitate if they become oversaturated, that is, designate all solids in the database as Type 5 solids. Print the problem results only after the entire problem has been solved.
- (2) = Consider all solids in the database. Print the problem results after the initial user-specified problem has been solved and again after all Type 5 solids are undersaturated or are in equilibrium with the solution.
- (3) = Consider all solids in the database. Print the problem results following the selection of every solid and after all of the solids are in equilibrium or are undersaturated.

Option 5. The total number of iterations option.
- (0) = Allow 40 iterations.
- (1) = Allow 10 iterations.
- (2) = Allow 100 iterations.
- (3) = Allow 200 iterations.

Option 6. The pH variation option.
- (0) = Do not allow the pH to automatically change during the precipitation or dissolution of solids.
- (1) = Allow the pH to change during the precipitation or dissolution of solids. (Note, for this option to work, all solid phases must be declared as Type 5 in option 4.)

Option 7. The fixed ionic strength option.
- (0) = Allow MINTEQ to compute the ionic strength.
- (1) = Fix the ionic strength at the value designated on Line 12.

Option 8. The numerical method option.
- (0) = Use only Newton-Raphson iteration.

Option 9. Activity model option.
- (0) = Not used.
- (1) = Use extended Debye-Huckel with B-dot equation to calculate activity coefficients.
- (2) = Use Davies equation to calculate activity coefficients.

EXHIBIT 1. (continued)

Option 10. Output option.
(0) = Do not print an initial listing of the thermodynamic data.
(1) = Print an initial listing of the thermodynamic data.

Option 11. Definition of pressure units option.
(0) = Enter hydrostatic pressure in bars.
(1) = Enter hydrostatic pressure in feet of water.

Line 14. [5 variables, I1,1X,4(F6.2,1X)]. This line is for specifying adsorption parameters other than the total mass of the adsorbent and the activity. The first parameter is an option switch to specify which adsorption model is to be used. The options are
(0) = No adsorption.
(1) = Activity K_d or activity Langmuir isotherm model.
(2) = Constant capacitance double-layer model.
(3) = Triple layer, site-binding model.

The next four inputs on this line are
(1) solid concentration in g/L,
(2) specific surface area in m^2/g,
(3) inner-layer capacitance in F/m^2, and
(4) outer-layer capacitance in F/m^2.

Section 2: Water Analysis

Lines 15-plus (3 variables, I7,1X,F9.3,1X,F6.2). These are the component input lines and there should be as many lines as components in the water analysis. The first variable is the component identification number. The second variable is the component concentration in the specified units. The third variable is the estimated log of the activity of the component. A blank line must follow the last component.

EXHIBIT 1. (continued)

Section 3: Type Modifications

This section is for changing the default species designations. The default-type specifications are described by Peterson et al. (1987). The first line contains the first species-type designation and the number of species of this type. The format is (I3,1X,I3). The type designations can be from two to six. For each species, a line must follow that includes three variables describing that species. The format is (I7,1X,E9.3,1X,F6.2). The first field specification is the species identification number. Identification numbers for component species are given in the COMP.DAT file. All other identification numbers for aqueous, solid, and gas species are given in the thermodynamic data files (see Appendices A, B, and C). The second field is for the new base 10 logarithmic value of the equilibrium constant (log K). The third field is for the enthalpy of reaction for the designated species. The equilibrium constant and the enthalpy of reaction are optional. If they are not entered, then the default values in the thermodynamic datafiles will be used. In the case of the Type 4 species, a fourth field is added to specify the initial mass of the species in moles/L. In the case of the Type 4 species, the format is (I7,1X,E9.3,1X,F6.2,1X,E10.3).

Last 2 lines: The end of the SAMPLE.DAT(4.00) file is indicated by two blank lines and a final line with the character string "END." in the first 4 spaces.

THE MINOUT.DAT(4.00) OUTPUT FILE

Computed output from MINTEQ(4.00) is written to a file with a default name of MINOUT.DAT. If the option for a short output is selected [see above discussion of the SAMPLE.DAT(4.00) input file], then the MINOUT.DAT(4.00) output file will consist of a copy of the input file, the computed speciated charge balance, alkalinity, noncarbonate alkalinity, ionic strength, total masses of dissolved salts, the total hydrogen ion mass (i.e., the proton condition), and a list of saturation indices (SI). The characters "##" next to the solids in the list of SI indicate solids with SI < 5% of their solubility product. A listing of the short output file for the River Water Test Case is given in Appendix B.

If the option for a long output is selected, then the output will consist of a copy of the input file, data from the iteration cycles, aqueous species concentrations and activities, distributions of aqueous species, computed speciated charge balance and alkalinity, total hydrogen ion mass, list of SI, and a table of mineral formulas. The changes made for the MINOUT.DAT(4.00) file compared to previous versions include 1) listings of output data in table form, 2) output of the pressure in feet of water and bars, 3) output of the total hydrogen ion mass, 4) output of the concentration of total dissolved solids, 5) alphabetization of the mineral saturation indices, and 6) output of a table of mineral formulas.

THE COMP.DAT(4.00) DATA FILE

The COMP.DAT(4.00) data file contains characteristic information for the Type 1 or component species as in previous MINTEQ versions, but now it can also contain an unlimited number of descriptive text lines at the top of the file. [A complete listing of COMP.DAT(4.00) is given in Appendix C.] The text lines must be followed immediately by the word "STOP." to signify the end of the description. The next line contains the version number. The next two lines contain headings to describe the columns of data in the main part of the data file. The remaining part of the file contains columns of data for the component species. From left to right, these data include 1) the species identification number, 2) the species name enclosed in single quotes to define

the character string, 3) the species ionic charge, 4) the species ionic radius in angstroms for the extended-Debye-Huckel equation, and 5) the species atomic weight in grams (see Appendix C).

The data in COMP.DAT(4.00) are read by the MINTEQ(4.00) code in free format, but the species name must be 18 characters or less. The major change in the COMP.DAT(4.00) file is the elimination of the extended parameter for ionic species, b_i, which was used for activity calculations with the extended-Debye-Huckel equation (Peterson et al. 1987; Truesdell and Jones 1974). The extended parameter is replaced by the B-dot parameter, which is calculated internally in the MINTEQ(4.00) source code, as described above.

THE AQUEOUS.DAT(4.00) THERMODYNAMIC DATA FILE

The AQUEOUS.DAT(4.00) data file contains thermodynamic and stoichiometric information for aqueous speciation reactions. The top lines of the AQUEOUS.DAT(4.00) data file contain information on the file history and contents. This section is ended by a line containing the word "STOP." The next line gives the version number. The data portion of the file follows.

Previous versions of MINTEQ used a two-line format to provide thermodynamic and stoichiometric data. For the current version, a four-line format has been adopted (Figure 2).

```
3301400 'HCO3-1'            -3.561    10.329          -1.00 4.00 0.00  61.0171
1.00 2     1.000 140     1.000 330
1.078871e+2  -5.15179e+3  3.2528e-2  -3.892561e+1  5.637139e+5
Nordstrom et al. 1990
```

FIGURE 2. Example of a Four-Line Input Section for HCO_3^- in AQUEOUS.DAT(4.00)

The following data are required in the AQUEOUS.DAT(4.00) four-line version.

Line 1: 1) Species identification number, 2) name enclosed by single quotes (A18), 3) the enthalpy of the formation reaction at 25°C, 4) the base 10 logarithm of the equilibrium constant at 25°C for the formation reaction, 5) ionic charge, 6) ionic radius in angstroms for the extended Debye-Huckel equation, 7) noncarbonate alkalinity factor, and 8) the atomic weight.

Line 2: 1) The alkalinity factor for the reaction, 2) the number of component species in the speciation reaction not counting the

formed species, and 3) the reaction stoichiometry in terms of the component species.

Line 3: Five empirical coefficients for correcting the equilibrium constant for temperature according to Eq. (4). For reaction where temperature extrapolations are not available, the number "999." is entered five times.

Line 4: A citation for the source of the enthalpy and equilibrium constant.

All the data in these four lines are read in free format. Therefore, an entry for each variable must be present even if it has a value of zero. Also, the species name must be less than or equal to 18 characters in length, not counting the enclosing single quotes.

The thermodynamic data must be consistent with the direction of the reaction specified by the stoichiometric variables in Line 2. In the MINTEQ(4.00) format, the aqueous speciation reactions are written as formation reactions with positive signs for the stoichiometric coefficients for the reactants and negative signs for the stoichiometric coefficients for the products. For example, data in the second line of Figure 2 indicate that the formation of HCO_3^- (#3301400) produces one equivalent of alkalinity and involves the reaction of two component species. These component species include one equivalent of CO_3^{2-} (#140) and one equivalent of H^+ (#140);

$$\begin{array}{lccccc} \text{I.D. Numbers} & 140 & & 330 & & 3301400 \\ & CO_3^{2-} & + & H^+ & = & HCO_3^- \end{array} \qquad (11)$$

A stoichiometric coefficient and identification number for the formed species, HCO_3^- for this example, are not included in the description of the speciation reaction in Line 2.

The end of the data portion of the AQUEOUS.DAT(4.00) file is signaled by two lines with zero values for the species identification number. The remainder of the file contains complete references for the citations. A complete listing of the AQUEOUS.DAT(4.00) is provided in Appendix D.

THE SOLIDS.DAT(4.00) THERMODYNAMIC DATA FILE

The SOLIDS.DAT(4.00) data file contains thermodynamic and stoichiometric information for solid-phase equilibrium solubility reactions. The top of the SOLIDS.DAT(4.00) data file contains information on the file history and contents. This section is ended by a line containing the word "STOP." The next line gives the version number. The data portion of the file follows.

Previous versions of MINTEQ used a two-line format to provide thermodynamic and stoichiometric data for each reaction. For the SOLIDS.DAT(4.00) file, a four-line format similar to that in the AQUEOUS.DAT(4.00) data file has been adopted (Figure 3).

```
6041002 'Jarosite-K'        31.2820   14.8012                          500.8105
5    -6.000 330     1.000 410     3.000 281     2.000 732     6.000 002
999.  999.  999.  999.  999.
Krupka et al. 1988                    KFe3(SO4)2(OH)6
```

FIGURE 3. Example of a Four-Line Input Section for Potassium-Jarosite in SOLIDS.DAT(4.00)

The following data are required in the four-line version.

Line 1: 1) Solid identification number, 2) name enclosed by single quotes (A18), 3) the enthalpy of reaction at 25°C, 4) the base 10 logarithm of the equilibrium constant at 25°C, and 5) the atomic weight of the solid.

Line 2: 1) The number of component species in the reaction not counting the formed solid, and 2) the reaction stoichiometry in terms of the component species.

Line 3: Five empirical coefficients for correcting the equilibrium constant for temperature according to Equation (4). For reactions where temperature extrapolations are not available, the number "999." is entered five times.

Line 4: 1) A citation for the source of the enthalpy and equilibrium constant, and 2) a chemical formula for the solid. The format for line 4 is (42X,A38).

The data in these four lines are read in free format, except for the fourth line which is read in format (42X,A38), where the 42X is the space for

the source and the A38 is for the character string that defines the chemical formula of the solid. Also, the name for the solid must be less than or equal to 18 characters in length. In Line 3 of Figure 3, the five values of "999." indicate that no empirical data were found for correcting the equilibrium constant for temperature by Equation (4).

The thermodynamic data must be consistent with the direction of the reaction specified by the stoichiometric variables in Line 2. In the MINTEQ(4.00) format, reactions involving solids are written as formation reactions with positive signs for the stoichiometric coefficients for the reactants and negative signs for the stoichiometric coefficients for the products. For example, data in the second line of Figure 3 indicate that one equivalent of K^+ (#410), three equivalents of Fe^{3+} (#281), two equivalents of SO_4^{2-} (#732), and six equivalents of H_2O (#002) are required to form one equivalent of potassium-jarosite (#6041002) and six equivalents of H^+ (#330):

I.D. Numbers	410		281		732		002		6041002		330	
	K^+	+	$3Fe^{3+}$	+	$2SO_4^{2-}$	+	$6H_2O$	=	$KFe_3(SO_4)_2:6H_2O$	+	$6H^+$	(12)

A stoichiometric coefficient and identification number for the formed solid, potassium-jarosite for this example, is not included in the description of the formation reaction in Line 2.

The end of the data portion of the SOLIDS.DAT(4.00) file is signaled by two lines with zero values for the species identification number. The remainder of the file contains complete references for the citations. A complete listing of the SOLIDS.DAT(4.00) is provided in Appendix E.

THE GAS-RDX.DAT(4.00) THERMODYNAMIC DATA FILE

The GAS-RDX.DAT(4.00) data file contains thermodynamic and stoichiometric information for redox and gas solubility reactions. The top of the GAS-RDX.DAT(4.00) data file contains information on the file history and contents.

This section is ended by a line containing the word "STOP." The next line gives the version number. The data portion of the file follows.

Previous versions of MINTEQ used a two-line format to provide thermodynamic and stoichiometric data for each reaction. For the GAS-RDX.DAT(4.00), a four-line format that is similar to those in the AQUEOUS.DAT(4.00) and SOLIDS.DAT(4.00) data files has been adopted (Figure 4). The following data are required in the four-line version:

Line 1: 1) Identification number for the redox couple or gas, 2) name of either the redox couple or gas enclosed by single quotes (A18), 3) the enthalpy of reaction at 25°C, 4) the base 10 logarithm of the equilibrium constant at 25°C, and 5) the atomic weight.

Line 2: 1) The number of component species in the redox or gas solubility reaction including both the reduced and oxidized components for redox reactions, and 2) the reaction stoichiometry in terms of the component species.

Line 3: Five empirical coefficients for correcting the equilibrium constant for temperature according to Equation (4). For reactions where temperature extrapolations are not available, the number "999." is entered five times.

Line 4: A citation for the source of the enthalpy and equilibrium constant.

The thermodynamic data must be consistent with the direction of the reaction specified by the stoichiometric variables in Line 2. The rules for writing the reaction stoichiometries for the redox and gas solubility reactions are the same as those described above for the AQUEOUS.DAT(4.00) and SOLIDS.DAT(4.00) data files. Additionally, all redox reactions have been written with the reduced component as the reactant and the oxidized component and electrons as the products. [This convention has been adopted to make the redox data internally consistent but it is not a requirement of the MINTEQ(4.00) code.] For example, the iron redox reaction (see Figure 4) is written as

I.D. Number	280		281		001	
	Fe^{2+}	=	Fe^{3+}	+	1 e^-	(13)

```
2802810 'Fe+2=>Fe+3'                9.68    -13.01        0.0000
3     1.000 280     -1.000 281     -1.000 001
9.06142e+3  -5.11520e+5  1.28888e+0  -3.26601e+3  3.00780e+7
EQ3/6 database: version mdas.3245

3301403 'CO2(g)'                  -0.962    18.149        41.0100
3     1.000 140     2.000 330     -1.000 002
3.54181e+2  -1.99751e+4  7.33674e-2  -1.24722e+2  1.57398e+6
Nordstrom et al. 1990
```

FIGURE 4. Example of Two Four-Line Input Sections for the Fe^{2+}/Fe^{3+} Redox Couple and $CO_2(g)$ Solubility in GAS-RDX.DAT(4.00)

The end of the data portion of the GAS-RDX.DAT(4.00) file is signaled by two lines with zero values for the species identification number. The remainder of the file contains complete references for the citations. A complete listing of the GAS-RDX.DAT(4.00) data file is provided in Appendix F.

THE PRCOEFF.DAT(4.00) DATA FILE

The PRCOEF.DAT(4.00) data file contains molar volume and compressibility data for a limited number of species. In PRCOEF.DAT(4.00) there are two lines for each species that contain the following data:

Line 1: 1) Species identification number, 2) the species name, and 3) values of a_1, b_1, and c_1 that are used to relate partial molar volumes to temperature [see Equation (10)].

Line 2: Values of a_2, b_2, and c_2 that are used to relate compressibilities to temperature [see Equation (11)].

The principal sources of these data are Millero (1982) and Robie et al. (1967, 1978). A complete listing of the PRCOEF.DAT(4.00) data file is given in Appendix G.

THE ALK.DAT(4.00) DATA FILE

The ALK.DAT(4.00) data file contains stoichiometric information for aqueous speciation reactions, other than those involving carbonate species, that contribute to the titration alkalinity. For example, the protonation of $H_3SiO_4^-$, which is described by

$$H_3SiO_4^- + H^+ = H_4SiO_4^0 \quad (14)$$

contributes one equivalent to the titration alkalinity and must be considered in the alkalinity balance equations used in MINTEQ(4.00). In the ALK.DAT(4.00) data file, there is entry of 1.0 for $H_3SiO_4^-$ (#330770) to specify its noncarbonate contribution to the titration alkalinity. A complete listing of the ALK.DAT(4.00) data file is given in Appendix H.

PORTABILITY

Several minor changes have been made to the MINTEQ code so that it will run on a number of different computers without alteration. Most importantly, calls to nonstandard intrinsic functions and VAX-FORTRAN extensions have been eliminated. Currently, the MINTEQ(4.00) code has been installed on IBM personal computers and IBM-compatible computers using the Microsoft FORTRAN 4.2 and 5.1 compiler versions and a VAX-8350 mainframe computer. The same MINTEQ code has also been installed on UNIX machines, including a SUN Sparkstation 2 and DEC Station 3100, using SUN-FORTRAN-77 and VAX-FORTRAN-77 compilers, respectively. No alterations to the code are necessary to operate it on these computers.

CONCLUSION

Since the development of the MINTEQ geochemical code by Felmy et al. (1984a, 1984b), a number of undocumented versions of the source code and data files have come into use at PNL. This report documents changes made to the source code for the ATES program and provides comprehensive listings of the data files. A version number of 4.00 has been assigned to the MINTEQ source code and to each of the individual data files described in this report. The initiation of a version numbering scheme provides a mechanism for documenting and referencing any changes that may be made to the source codes and data files in the future.

The principal changes made to the MINTEQ source code that have been made since Felmy et al. (1984a, 1984b) include

- the correction of equilibrium constants for pressure
- the correction of equilibrium constants for temperature
- the insertion of control words in the input data file to define output length and end-of-file points
- the incorporation of the extended-Debye-Huckel B-dot equation as the default method for calculating single ion activity coefficients. (The Davies method is retained as an option.)

The database structure of the MINTEQ code has also been changed so that thermodynamic data for aqueous speciation, dissolution/precipitation, redox, and gas solubility reactions are consolidated into separate files. The TYPE6.DAT data file used in earlier MINTEQ version has been eliminated. Within the thermodynamic data files, individual reactions are now described by four lines of data that include coefficients for describing the effect of temperature on the equilibrium constant and a reference for the source of the data. The thermodynamic data for MINTEQ(4.00) were compiled from literature sources and from PNL researchers who have used MINTEQ for various water-quality-related projects. Additionally, the formats and structures of the MINTEQ(4.00) thermodynamic data files are now interchangeable with those used by the Geochemical Model (GM) of the Chemical Transport Model (CTM) developed

by Erikson et al. (1990) so that the same thermodynamic data files can be used for making calculations with either code.

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APPENDIX A

LISTING OF THE SAMPLE.DAT(4.00) INPUT FILE FOR THE RIVER WATER TEST CASE

APPENDIX A

LISTING OF THE SAMPLE.DAT(4.00) INPUT FILE FOR THE RIVER WATER TEST CASE

```
River water test case from Nordstrom et al. (1979).
Sample input #1 Peterson et al. (1987).
STOP.
SHORT.
 9.5 'MG/L' 0.0   0.0
0 0 0 0 2 0 0 0 0 1 0
0   0.00   0.00   0.00   0.00
    500 1.200e+01   0.00          Na+
    410 1.400e+00   0.00          K+
    150 1.220e+01   0.00          Ca+2
    460 7.500e+00   0.00          Mg+2
    770 2.913e+01   0.00          Si(OH)4
    140 7.397e+01   0.00          CO3-2
    180 9.900e+00   0.00          Cl-
    732 7.700e+00   0.00          SO4-2
    090 2.860e-01   0.00          B(OH)3
    130 6.000e-03   0.00          Br-
    270 1.000e-01   0.00          F-
    580 2.100e-01   0.00          PO4-3
    492 8.980e-01   0.00          NO3-
    491 1.900e-02   0.00          NO2-
    490 1.440e-01   0.00          NH4+
    280 1.500e-02   0.00          Fe+2
    281 7.000e-04   0.00          Fe+3
    470 4.400e-03   0.00          Mn+2
    471 0.000e+00   0.00          Mn+3
    030 5.000e-03   0.00          Al+3
    950 4.900e-04   0.00          Zn+2
    160 1.000e-04   0.00          Cd+2
    600 3.000e-05   0.00          Pb+2
    230 0.000e+00   0.00          Cu+
    231 5.000e-04   0.00          Cu+2
    540 1.800e-03   0.00          Ni+2
    020 4.000e-05   0.00          Ag+
    060 3.362e-03   0.00          H3AsO3
    061 0.000e+00   0.00          H3AsO4
    001 0.000e+00  -7.43          e-
    330 0.000e+00  -8.01          H+

  3   8
    330 8.01
    001 7.43
2802810
2302310
4704710
4904920
4914920
0600610
```

APPENDIX B

LISTING OF THE MINTEQ.DAT(4.00) OUTPUT FILE (SHORT FORMAT)

APPENDIX B

LISTING OF THE MINOUT.DAT(4.00) OUTPUT FILE (SHORT FORMAT)

```
-------------------------------------------------------------------------------
   MINTEQ Code Version: 4.00 (PC-DOS Microsoft FORTRAN 4.1)
-------------------------------------------------------------------------------
     Echo of input file (sample.dat)

This is the River Water Test Case modified from Nordstrom et al.
(1979).  Inorganic carbon option-elements not in the EPA data
base are excluded.
Sample input #1 in MINTEQ's Users Manual (Peterson et al. 1987)
SHORT.
 T =   9.50 MG/L      0.00   0.00
 0 0 0 0 2 0 0 0 0 1 0
 0   0.00   0.00   0.00   0.00
     500  1.200E+01   0.00
     410  1.400E+00   0.00
     150  1.220E+01   0.00
     460  7.500E+00   0.00
     770  2.913E+01   0.00
     140  7.397E+01   0.00
     180  9.900E+00   0.00
     732  7.700E+00   0.00
      90  2.860E-01   0.00
     130  6.000E-03   0.00
     380  1.800E-03   0.00
     270  1.000E-01   0.00
     580  2.100E-01   0.00
     492  8.980E-01   0.00
     491  1.900E-02   0.00
     490  1.440E-01   0.00
     280  1.500E-02   0.00
     281  7.000E-04   0.00
     470  4.400E-03   0.00
     471  0.000E+00   0.00
      30  5.000E-03   0.00
     950  4.900E-04   0.00
     160  1.000E-04   0.00
     600  3.000E-05   0.00
     230  0.000E+00   0.00
     231  5.000E-04   0.00
     540  1.800E-03   0.00
      20  4.000E-05   0.00
      60  3.362E-03   0.00
      61  0.000E+00   0.00
       1  0.000E+00  -7.43
     330  0.000E+00  -8.01
  H2O HAS BEEN INSERTED AS A COMPONENT
   3   8
     330  8.010E+00   0.00
       1  7.430E+00   0.00
 2802810  0.000E+00   0.00
 2302310  0.000E+00   0.00
 4704710  0.000E+00   0.00
 4904920  0.000E+00   0.00
 4914920  0.000E+00   0.00
  600610  0.000E+00   0.00
```

START OF MINTEQ OUTPUT

-----MINTEQ FORTRAN Code Version: 4.000 (PC-DOS Microsoft FORTRAN 4.1)----------
-----COMP.DAT (basis components) Version: 4.000----------
-----AQUEOUS.DAT (aqueous species thermodynamic data) Version: 4.000----------
-----SOLIDS.DAT (solids thermodynamic data) Version: 4.000----------
-----GAS_RDX.DAT (gas and redox species thermodynamic data) Version: 4.000------

Unspeciated Charge Balance
  Sum of Cations= 1.793E-03 Sum of Anions = 2.932E-03
  Percent Difference = 2.410E+01 (anions - cations)/(anions + cations)*100

Speciated Charge Balance
  Sum of Cations = 1.764E-03 Sum of Anions = 1.663E-03
  Percent Difference = -2.951E+00 (anions - cations)/(anions + cations)*100

Noncarbonate Alkalinity = 0.000E+00
Ionic Strength = 2.396E-03
Total Dissolved Solids = 179.802 mg/liter
Total H+ mass = 0.12558E-02 (sum of H+ as free H+ plus as aqueous species)
Temperature = 9.50 C or 282.66 K
Pressure = 0.000 feet of water or 0.000 bars

SATURATION INDICES FOR ALL MINERALS AND SOLIDS
  (Solids with ID = 0000009 do not have Log K values)

ID	Name	EQ-BD	Sat Index	Log K	5%*Log K	Log IAP	Del H
2000	Ag(metal)		-2.536	14.522	0.726	-17.058	-25.275
5002000	Ag2CO3		-13.232	11.455	0.573	-24.687	-9.600
2002000	Ag2O		-16.219	-12.984	0.649	-3.235	10.344
6002000	Ag2SO4		-18.379	5.089	0.254	-23.468	-4.329
7002000	Ag3PO4		-21.828	17.542	0.877	-39.371	0.000
4202000	AgF:4H2O		-15.322	-0.388	0.019	-14.934	-4.325
2002001	AgO		-18.244	-32.067	1.603	13.822	40.137
8015005	Akermanite		-17.829	-48.001	2.400	30.172	74.132
2003000	Al(OH)3(am)		-2.259	-11.865	0.593	9.606	26.500
6003002	Al2(SO4)3		-61.995	-20.509	1.025	-41.487	0.000
6003003	Al2(SO4)3:6H2O		-43.173	-1.686	0.084	-41.487	0.000
7203000	AlAsO4:2H2O		-42.936	-3.665	0.183	-39.271	0.000
6003000	AlOHSO4		-7.397	3.230	0.162	-10.627	0.000
6041000	Alum-K		-21.324	5.995	0.300	-27.319	-7.220
6003001	Alunite		-8.727	-0.620	0.031	-8.107	50.250
8450001	Analcime		1.415	-5.852	0.293	7.266	21.944
6060003	Anglesite		-10.520	7.989	0.399	-18.509	-2.144
6015000	Anhydrite		-3.493	4.336	0.217	-7.829	1.710
8641001	Annite		-15.133	-30.855	1.543	15.722	65.770
8415001	Anorthite		-2.891	-27.463	1.373	24.571	70.680
4115000	Antarcticite		-14.892	-4.122	0.206	-10.770	0.000
6023100	Antlerite		-12.286	-8.753	0.438	-3.533	0.000
6050003	Aphthitalite		-21.712	3.426	0.171	-25.138	0.000
5015000	Aragonite		-0.795	8.253	0.413	-9.048	2.589
6041003	Arcanite		-11.094	2.056	0.103	-13.151	0.000
3006000	Arsenolite		-117.353	1.698	0.085	-119.052	-7.185
5046000	Artinite		-7.049	-10.413	0.521	3.364	28.532
3006100	As2O5		-106.009	-8.255	0.413	-97.754	0.000
4306000	AsI3		-111.251	-4.081	0.204	-107.170	-1.892
4123101	Atacamite		-8.543	-8.089	0.404	-0.454	18.687
5023102	Azurite		-15.537	10.668	0.533	-26.204	23.765
6003001	Basaluminite		-4.310	-22.500	1.125	18.190	0.000

6095005	Bianchite		-29.515	1.759	0.088	-31.275	0.163
2047102	Birnessite		-4.708	-18.068	0.903	13.361	0.000
4146000	Bischofite		-15.192	-4.426	0.221	-10.766	0.000
3047100	Bixbyite		-4.361	-0.202	0.010	-4.159	29.746
6050004	Bloedite		-16.260	2.388	0.119	-18.649	0.000
2003001	Boehmite	##	0.073	-9.533	0.477	9.606	26.194
6023101	Brochantite		-14.976	-17.009	0.850	2.033	0.000
4002000	Bromyrite		-3.693	13.082	0.654	-16.775	-20.213
2046000	Brucite		-4.966	-17.374	0.869	12.408	27.240
2054001	Bunsenite		-5.217	-13.404	0.670	8.188	23.935
5050002	Burkeite		-32.881	0.810	0.040	-33.691	0.000
8615002	Ca-Montmorillonite		6.424	-1.672	0.084	8.095	0.000
8615001	Ca-Nontronite		16.986	11.708	0.585	5.279	0.000
8015001	Ca-Olivine		-18.646	-39.932	1.997	21.286	54.743
4115003	Ca2Cl2(OH)2:3H2O		-24.889	-26.522	1.326	1.634	0.000
7215001	Ca3(AsO4)2		-84.572	-24.030	1.201	-60.543	32.207
7215000	Ca3(AsO4)2:4H2O		-82.010	-21.467	1.073	-60.543	0.000
8015007	Ca3SiO5		-44.493	-78.183	3.909	33.689	106.386
4115002	Ca4Cl2(OH)6:19H2O		-42.260	-68.701	3.435	26.441	0.000
4115001	CaCl2:4H2O		-16.470	-5.700	0.285	-10.770	0.000
5015001	Calcite		-0.639	8.409	0.420	-9.048	2.297
4141000	Carnallite		-23.242	-4.430	0.222	-18.812	0.000
5216000	Cd(BO2)2		-13.803	-9.837	0.492	-3.966	0.000
2016001	Cd(OH)2(c)		-7.121	-13.860	0.693	6.739	0.000
16000	Cd(alpha)		-38.358	-14.217	0.711	-24.141	18.000
16001	Cd(gamma)		-38.467	-14.326	0.716	-24.141	18.141
6016001	Cd3(OH)2(SO4)2		-26.950	-6.702	0.335	-20.248	0.000
6016000	Cd3(OH)4SO4		-22.541	-22.526	1.126	-0.015	0.000
7016000	Cd3(PO4)2		-16.222	32.596	1.630	-48.817	0.000
6016002	Cd4(OH)6(SO4)		-21.677	-28.401	1.420	6.724	0.000
4016000	CdBr2:4H2O		-20.869	2.706	0.135	-23.575	-7.227
4116000	CdCl2		-15.938	0.497	0.025	-16.435	4.474
4116002	CdCl2:2.5H2O		-14.430	2.005	0.100	-16.435	-1.707
4116001	CdCl2:H2O		-14.795	1.640	0.082	-16.435	1.819
4216000	CdF2		-17.304	2.590	0.129	-19.894	9.721
4316000	CdI2		-21.247	3.776	0.189	-25.024	-4.067
4116003	CdOHCl		-8.661	-3.813	0.191	-4.848	7.407
6016003	CdSO4		-13.891	-0.397	0.020	-13.494	12.403
6016005	CdSO4:2.7H2O		-11.947	1.546	0.077	-13.494	4.526
6016004	CdSO4:H2O		-12.138	1.355	0.068	-13.494	7.517
8216000	CdSiO3		-4.924	-8.142	0.407	3.217	14.577
4102000	Cerargyrite		-2.824	10.381	0.519	-13.205	-15.693
5060000	Cerrusite		-5.875	13.853	0.693	-19.728	-4.844
6023105	Chalcanthite		-11.982	2.684	0.134	-14.666	-1.433
2077000	Chalcedony		0.554	4.076	0.204	-3.522	-4.620
6023104	Chalcocyanite		-18.258	-3.592	0.180	-14.666	17.482
8628001	Chlorite-Fe-1		25.081	-23.725	1.186	48.806	0.000
8628002	Chlorite-Fe-2		22.059	-22.497	1.125	44.556	0.000
8646008	Chlorite-Mg		-9.393	-80.080	4.004	70.687	158.620
8646009	Chlorite-Mg-Fe-1		5.055	-53.205	2.660	58.260	0.000
8646007	Chlorite-Mg-Fe-2		8.247	-51.814	2.591	60.061	0.000
8646000	Chrysotile		-4.042	-34.222	1.711	30.181	46.800
7060001	Cl-Pyromorphite		-22.089	84.430	4.221	-106.519	0.000
3006001	Claudetite		557.297	676.348	33.817	-119.052	-6.665
4160000	Cotunnite		-16.457	4.993	0.250	-21.450	-5.591
2077001	Cristobalite		0.250	3.772	0.189	-3.522	-4.780
4250000	Cryolite		-21.974	34.205	1.710	-56.179	-9.090
2023100	Cu(OH)2		-3.103	-8.670	0.433	5.566	0.000
23000	Cu-metal		-13.376	9.445	0.472	-22.821	-17.130
5123100	Cu2(OH)3NO3		-10.952	-9.403	0.470	-1.549	15.081
6023000	Cu2SO4		-33.225	1.770	0.089	-34.995	4.561
7223100	Cu3(AsO4)2.6H2O		-85.712	-4.657	0.233	-81.055	0.000
7023100	Cu3(PO4)2		-15.482	36.853	1.843	-52.335	0.000
7023101	Cu3(PO4)2:3H2O		-17.217	35.118	1.756	-52.335	0.000
4023000	CuBr		-13.810	8.728	0.436	-22.538	-13.079

5023100	CuCO3		-6.252	9.633	0.482	-15.885	0.000
4223000	CuF		-28.272	-7.575	0.379	-20.698	12.370
4223100	CuF2		-20.980	0.086	0.004	-21.066	13.320
4223101	CuF2:2H2O		-16.662	4.404	0.220	-21.066	3.650
4323000	CuI		-10.556	12.707	0.635	-23.263	-20.144
6023103	CuOCuSO4		-9.965	-0.865	0.043	-9.100	20.096
3023100	Cupricferrite		10.644	-7.917	0.396	18.561	50.269
2023000	Cuprite		-12.600	2.162	0.108	-14.762	-6.241
3023000	Cuprousferrite		7.888	8.772	0.439	-0.884	3.796
2003002	Diaspore		0.997	-8.609	0.430	9.606	24.394
8215000	Diopside		-4.536	-22.304	1.115	17.768	35.199
2023102	Dioptase		-4.437	-6.482	0.324	2.045	8.670
5015003	Dolomite(d)		-1.998	16.094	0.805	-18.092	11.090
5015002	Dolomite(o)	##	-0.174	17.918	0.896	-18.092	9.436
8246000	Enstatite		-3.411	-12.297	0.615	8.886	22.294
6046000	Epsomite		-5.572	2.252	0.113	-7.825	-2.824
6015002	Ettringite		-29.315	-62.250	3.112	32.935	88.287
7015002	FCO3-Apatite		9.916	115.983	5.799	-106.067	-39.390
2028001	Fe(OH)2(ppt)		-8.176	-12.557	0.628	4.380	21.935
4128100	Fe(OH)2:7Cl		6.062	3.041	0.152	3.021	0.000
2028100	Fe(OH)3(am)		0.815	-5.683	0.284	6.497	19.835
2028107	Fe(OH)3(ppt)		2.273	-4.224	0.211	6.497	19.835
2028106	Fe(OH)3(soil)		3.811	-2.686	0.134	6.497	0.000
6028100	Fe2(SO4)3		-53.229	-5.525	0.276	-47.703	58.150
2028101	Fe3(OH)8		-2.847	-20.222	1.011	17.375	0.000
6028001	FeSO4(s)		-19.185	-3.332	0.167	-15.852	0.000
7015004	Fluorapatite		6.798	61.647	3.082	-54.850	14.127
4215000	Fluorite		-3.425	10.804	0.540	-14.229	-4.690
8046000	Forsterite		-8.497	-29.792	1.490	21.294	53.379
5015005	Gaylussite		-11.649	9.442	0.472	-21.091	0.000
8015006	Gehlenite		-18.622	-59.119	2.956	40.497	109.361
2003003	Gibbsite(c)		0.579	-9.026	0.451	9.606	22.800
2003005	Gibbsite(uc)		-0.729	-10.335	0.517	9.606	24.500
6050005	Glauberite		-13.383	5.269	0.263	-18.653	0.000
2028102	Goethite		6.913	0.416	0.021	6.497	14.540
6095006	Goslarite		-29.183	2.092	0.105	-31.275	-3.293
8628000	Greenalite		-18.074	-24.171	1.209	6.097	0.000
6015001	Gypsum		-3.237	4.592	0.230	-7.829	0.109
8633000	H-Montronite		15.977	12.738	0.637	3.239	0.000
4150000	Halite		-8.407	-1.524	0.076	-6.883	-0.951
8603000	Halloysite		1.596	-10.572	0.529	12.168	39.758
2047000	Hausmannite		-8.048	-65.075	3.254	57.027	100.640
2028105	Hematite		11.656	-1.338	0.067	12.995	31.135
3028001	Hercynite		-6.787	-30.378	1.519	23.592	78.375
6046001	Hexahydrite		-6.159	1.666	0.083	-7.825	0.000
8450003	High-Albite	##	0.133	-3.612	0.181	3.744	19.974
8441003	High-Sanidine		2.417	-0.164	0.008	2.581	14.462
7060004	Hinsdalite		-21.710	2.499	0.125	-24.209	0.000
5015004	Huntite		-6.118	30.061	1.503	-36.179	29.239
5060003	Hydrocerrusite		-18.870	18.862	0.943	-37.732	0.000
5046001	Hydromagnesite		-15.515	8.251	0.413	-23.767	58.061
7015003	Hydroxyapatite		-2.782	38.752	1.938	-41.533	38.938
5095002	Hydrozincite		-110.793	-12.681	0.634	-98.113	0.000
8641003	Illite		6.698	-8.295	0.415	14.993	49.855
4302000	Iodyrite	##	-0.352	17.147	0.857	-17.499	-26.864
6028101	Jarosite-H		-11.088	9.886	0.494	-20.974	55.147
6041002	Jarosite-K		-3.889	13.544	0.677	-17.433	31.282
6050000	Jarosite-Na		-6.524	9.745	0.487	-16.269	36.182
6003002	Jurbanite		-6.827	3.800	0.190	-10.627	0.000
8441002	K-Feldspar		3.728	1.147	0.057	2.581	12.520
8641004	K-Montmorillonite		19.320	12.103	0.605	7.217	0.000
8641002	K-Montronite		16.511	12.103	0.605	4.408	0.000
5041004	K-Trona		-22.265	8.852	0.443	-31.118	0.000
5041001	K2CO3:1.5H2O		-17.663	-3.293	0.165	-14.370	0.000
6041010	K3H(SO4)2		-26.675	3.167	0.158	-29.843	0.000

5041002	K8H4(CO3)6:3H2O		-67.062	33.322	1.666	-100.384	0.000
5041003	KNaCO3:6H2O		-13.205	0.002	0.000	-13.207	0.000
6041004	Kainite		-15.783	0.088	0.004	-15.871	0.000
5041000	Kalicinite		-7.980	9.931	0.497	-17.911	0.000
8441000	Kalsilite		-1.304	-10.929	0.546	9.625	29.029
8603001	Kaolinite		3.476	-8.691	0.435	12.168	35.300
8646010	Kerolite		-2.653	-25.790	1.290	23.137	0.000
6046002	Kieserite		-7.682	0.142	0.007	-7.825	0.000
6050006	Labile-Salt		-23.760	5.716	0.286	-29.477	0.000
6023102	Langite		-16.813	-18.846	0.942	2.033	39.677
6060000	Larnakite		-16.767	0.018	0.001	-16.785	6.448
8015002	Larnite		-19.322	-40.608	2.030	21.286	57.286
8415002	Laumontite		4.179	-13.348	0.667	17.528	0.000
4160003	Laurionite		-10.484	-0.622	0.031	-9.863	0.000
8415000	Leonhardite		15.059	-19.997	1.000	35.055	85.417
6041005	Leonite		-17.226	3.749	0.187	-20.975	0.000
2028103	Lepidocrocite		5.134	-1.363	0.068	6.497	0.000
8441001	Leucite		-1.541	-7.644	0.382	6.103	22.245
2015000	Lime		-22.040	-34.443	1.722	12.404	46.264
2060001	Litharge		-11.551	-13.275	0.664	1.724	16.381
8450002	Low-Albite		1.580	-2.165	0.108	3.744	17.374
8450000	Magadiite		-5.643	14.306	0.715	-19.949	0.000
2028104	Maghemite		6.621	-6.373	0.319	12.995	0.000
5046002	Magnesite		-1.258	7.785	0.389	-9.044	7.340
3028000	Magnetite		4.843	-12.532	0.627	17.375	51.075
5023101	Malachite		-6.492	3.827	0.191	-10.319	16.210
2047101	Manganite		49.496	25.340	1.267	24.156	0.000
2047001	Manganosite		-10.376	-19.091	0.955	8.716	0.000
8615000	Margarite	##	1.671	-42.112	2.106	43.783	0.000
2060000	Massicot		-11.856	-13.580	0.679	1.724	16.780
4160001	Matlockite		-13.443	9.736	0.487	-23.179	-7.938
4123100	Melanothallite		-21.808	-4.201	0.210	-17.607	11.819
6028000	Melanterite		-13.435	2.417	0.121	-15.853	-4.910
6041006	Mercallite		-15.410	1.282	0.064	-16.692	0.000
8015004	Merwinite		-29.978	-72.554	3.628	42.576	107.208
3046001	Mg-Ferrite		5.963	-19.440	0.972	25.403	66.619
8646006	Mg-Montmorillonite		6.502	-1.594	0.080	8.096	0.000
8646005	Mg-Montronite		17.001	11.722	0.586	5.279	0.000
4146001	Mg2Cl(OH)3:7H2O		-12.820	-26.049	1.302	13.229	0.000
3060001	Minium		-41.764	-77.816	3.891	36.052	102.776
6050001	Mirabilite		-8.849	1.975	0.099	-10.824	-18.987
6041007	Misenite		-103.468	9.834	0.492	-113.301	0.000
6047100	Mn2(SO4)3		-60.666	4.190	0.210	-64.857	39.063
7247000	Mn3(AsO4)2:8H2O		-81.804	-10.196	0.510	-71.608	0.000
7047000	Mn3(PO4)2		-18.982	23.906	1.195	-42.888	-2.105
4147000	MnCl2:4H2O		-17.273	-2.815	0.141	-14.458	2.627
7047001	MnHPO4(c)	##	-0.522	25.280	1.264	-25.802	0.000
2047105	MnO2(beta)		-4.184	-17.545	0.877	13.361	39.340
6047000	MnSO4		-14.815	-3.298	0.165	-11.517	15.481
2016002	Monteponite		-9.352	-16.091	0.805	6.739	24.745
8015003	Monticellite		-10.131	-31.421	1.571	21.290	49.470
6054002	Morenosite		-9.861	2.184	0.109	-12.045	-2.924
8641000	Muscovite		8.920	-12.872	0.644	21.792	59.425
8650002	Na-Montmorillonite		6.007	-1.594	0.080	7.601	0.000
8650001	Na-Montronite		16.501	11.710	0.585	4.792	0.000
5050005	Na2CO3:7H2O		-11.560	0.484	0.024	-12.043	0.000
6050007	Na3H(SO4)2		-25.506	0.846	0.042	-26.352	0.000
5050003	Nahcolite		-5.997	10.751	0.538	-16.748	0.000
4123000	Nantokite		-11.803	7.165	0.358	-18.968	-9.970
3050000	Natron		-10.099	1.944	0.097	-12.043	-15.745
8450004	Nepheline		-3.295	-14.083	0.704	10.788	33.224
5046003	Nesquehonite		-4.065	4.979	0.249	-9.044	5.789
2054000	Ni(OH)2		-5.466	-13.654	0.683	8.188	22.940
8054000	Ni2SiO4		-2.857	-15.710	0.786	12.853	33.070
7054000	Ni3(PO4)2		-13.152	31.320	1.566	-44.472	0.000

6054000	Ni4(OH)6SO4		-23.165	-35.683	1.784	12.517	93.451
5054000	NiCO3		-6.822	6.442	0.322	-13.264	10.050
5054001	NiCO3:6H2O		-0.804	12.461	0.623	-13.264	0.000
2047103	Nsutite		-4.121	-17.482	0.874	13.361	0.000
7060002	OH-Pyromorphite		-32.141	62.791	3.140	-94.932	0.000
5016000	Otavite		-2.496	12.217	0.611	-14.713	0.583
8650000	Paragonite		5.828	-17.128	0.856	22.956	0.000
5260000	Pb(BO2)2		-16.906	-7.925	0.396	-8.981	6.358
2060004	Pb(OH)2(c)		-6.981	-8.705	0.435	1.724	13.986
60000	Pb(metal)		-33.452	-4.296	0.215	-29.156	0.406
4160004	Pb2(OH)3Cl		-16.932	-8.794	0.440	-8.139	0.000
2060005	Pb2O(OH)2		-22.751	-26.199	1.310	3.448	0.000
3060000	Pb2O3		-26.710	-61.038	3.052	34.328	0.000
5060001	Pb2OCO3		-17.957	0.047	0.002	-18.004	11.464
8060000	Pb2SiO4		-19.303	-19.229	0.961	-0.074	23.973
7060007	Pb3(PO4)2		-19.291	44.571	2.229	-63.863	-5.380
5060002	Pb3O2CO3		-28.364	-12.084	0.604	-16.280	26.428
6060001	Pb3O2SO4		-26.771	-11.710	0.586	-15.060	20.776
6060004	Pb4(OH)6SO4		-34.434	-21.097	1.055	-13.337	0.000
6060002	Pb4O3SO4		-36.844	-23.508	1.175	-13.336	35.099
4060000	PbBr2		-23.085	5.506	0.275	-28.590	-8.103
4060001	PbBrF		-18.267	8.483	0.424	-26.749	0.000
4260000	PbF2		-18.789	6.119	0.306	-24.909	0.706
7060006	PbHPO4		-8.564	24.229	1.211	-32.793	-10.568
4360000	PbI2		-21.359	8.679	0.434	-30.039	-15.153
2060002	PbO:1.33H2O		-11.119	-12.843	0.642	1.724	0.000
8260000	PbSiO3		-7.905	-6.107	0.305	-1.798	7.212
2046001	Periclase		-10.374	-22.782	1.139	12.408	36.085
8450005	Phillipsite		2.873	-3.452	0.173	6.325	0.000
8646001	Phlogopite	##	0.488	-39.317	1.966	39.806	42.300
4160002	Phosgenite		-21.369	19.809	0.990	-41.178	0.000
6041008	Picromerite		-16.873	4.102	0.205	-20.975	0.000
5050004	Pirssonite		-11.834	9.258	0.463	-21.091	0.000
2060003	Plattnerite		-19.529	-52.133	2.607	32.604	70.736
7060003	Plumbogummite		-5.707	32.787	1.639	-38.494	0.000
6041009	Polyhalite		-23.104	13.529	0.676	-36.633	0.000
2015001	Portlandite		-11.398	-23.802	1.190	12.404	31.000
8615002	Prehnite		-2.782	-36.236	1.812	33.453	78.059
8215003	Ps-Wollastonite		-5.894	-14.776	0.739	8.882	21.117
2047003	Pyrochroite		-6.484	-15.200	0.760	8.716	0.000
2047104	Pyrolusite		-4.401	-43.997	2.200	39.596	65.110
8603002	Pyrophyllite		5.809	0.685	0.034	5.124	28.415
2077002	Quartz		1.274	4.796	0.240	-3.522	-5.400
6054001	Retgersite		-9.951	2.095	0.105	-12.045	-1.088
5047000	Rhodochrosite		-2.244	10.493	0.525	-12.736	2.060
8447000	Rhodonite		-5.116	-10.310	0.516	5.194	0.000
8646004	Sepiolite(am)		-4.523	-18.774	0.939	14.251	0.000
8646003	Sepiolite(c)		-3.222	-31.723	1.586	28.501	0.000
2077003	SiO2(am)		-0.581	2.941	0.147	-3.522	-3.910
2077004	SiO2(ppt)		-0.495	3.027	0.151	-3.522	-3.910
5028000	Siderite		-6.692	10.379	0.519	-17.072	2.480
5095000	Smithsonite		-22.754	9.740	0.487	-32.494	4.361
3046000	Spinel		-8.355	-39.975	1.999	31.620	89.109
7028100	Strengite		-2.377	25.643	1.282	-28.020	6.396
4141001	Sylvite		-9.075	-1.029	0.051	-8.046	0.000
6041011	Syngenite		-13.775	7.205	0.360	-20.980	0.000
4146002	Tachyhydrite		-49.619	-17.317	0.866	-32.302	0.000
8646002	Talc	##	0.746	-22.391	1.120	23.137	43.346
2023101	Tenorite		-2.712	-8.279	0.414	5.567	15.235
6050002	Thenardite		-10.552	0.272	0.014	-10.824	0.411
5050001	Thermonatrite		-12.281	-0.238	0.012	-12.043	2.802
8215001	Tremolite		-6.120	-64.794	3.240	58.673	109.523
5050007	Trona		-17.386	11.405	0.570	-28.791	0.000
7060005	Tsumebite		-15.711	9.792	0.490	-25.503	0.000
7028001	Vivianite		-19.893	36.001	1.800	-55.894	0.000

8415003	Wairakite	##	-0.718	-18.246	0.912	17.528	63.176
8095000	Willemite		-40.697	-15.092	0.755	-25.605	31.322
8215002	Wollastonite		-5.571	-14.453	0.723	8.882	19.547
2095006	Zincite		-23.105	-12.063	0.603	-11.042	21.856
6095003	Zincosite		-35.566	-4.292	0.215	-31.274	19.207
5295000	Zn(BO2)2		-30.036	-8.289	0.414	-21.747	0.000
5195000	Zn(NO3)2:6H2O		-38.698	-2.291	0.115	-36.407	-6.637
2095000	Zn(OH)2(am)		-23.494	-12.452	0.623	-11.042	0.000
2095002	Zn(OH)2(beta)		-23.726	-12.684	0.634	-11.042	19.991
2095001	Zn(OH)2(c)		-23.241	-12.199	0.610	-11.042	0.000
2095004	Zn(OH)2(eps)		-23.441	-12.400	0.620	-11.042	19.671
2095003	Zn(OH)2(gamma)		-22.871	-11.829	0.591	-11.042	0.000
95000	Zn(metal)		-69.163	-27.241	1.362	-41.922	36.781
6095000	Zn2(OH)2SO4		-49.817	-7.501	0.375	-42.316	0.000
4195001	Zn2(OH)3Cl		-48.847	-15.176	0.759	-33.671	0.000
7095000	Zn3(PO4)2:4H2O		-69.978	32.182	1.609	-102.160	0.000
6095002	Zn3O(SO4)2		-95.103	-21.512	1.076	-73.591	62.009
6095001	Zn4(OH)6SO4		-92.799	-28.399	1.420	-64.400	0.000
4195002	Zn5(OH)8Cl2		-116.882	-38.499	1.925	-78.383	0.000
4095000	ZnBr2:2H2O		-46.868	-5.511	0.276	-41.356	7.517
5095001	ZnCO3:H2O		-22.228	10.266	0.513	-32.494	0.000
4195000	ZnCl2		-41.946	-7.731	0.387	-34.216	17.486
4295000	ZnF2		-51.369	-13.695	0.685	-37.674	378.477
4395000	ZnI2		-54.569	-11.764	0.588	-42.805	112.883
6095004	ZnSO4:H2O		-31.129	0.146	0.007	-31.275	10.636
8295000	ZnSiO3		-18.142	-3.579	0.179	-14.564	16.221

OUTPUT DATA FOR SOLIDS WITH LOG K VARYING WITH pH
(Solids with ID = 0000009 do not have Log K values)

ID	Name	EQ-BD	Sat Index	Log K	5X*Log K	Log IAP
8603003	Allophane(A)	##	-0.234	-7.757	0.388	7.523
8603004	Allophane(F)		0.748	-6.775	0.339	7.523

OUTPUT DATA FOR SOLIDS WITH IAP VARYING WITH ACTIVITES OF EXCHANGEABLE CATIONS
(Solids with ID = 0000009 do not have Log K values)

ID	Name	EQ-BD	Sat Index	Log K	5X*Log K	Log IAP
8603005	Beidellite		1.490	-10.018	0.501	11.508
8646006	Montmorillonite-BF		6.567	-1.427	0.071	7.994
8646007	MONT-AB		6.085	-4.122	0.206	10.207
	9 Clinoptilolite					-1.632
	9 Mordenite					0.129

APPENDIX C

COMPLETE LISTING OF THE COMP.DAT(4.00) DATA FILE

APPENDIX C

COMPLETE LISTING OF THE COMP.DAT(4.00) DATA FILE

```
COMP.DAT(4.00)  Basis Component List
Created 9-20-91 by Ted Eary
STOP.
Version 4.00
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ID	Name	Charge	Size (a)	Molecular wt.
003	'O2(aq)'	0.0	3.0	32.000
005	'CH4(aq)'	0.0	3.0	16.0426
020	'Ag+'	1.0	3.0	107.8680
030	'Al+3'	3.0	9.0	26.9815
100	'Ba+2'	2.0	5.0	137.3400
130	'Br-'	-1.0	4.0	79.9040
140	'CO3-2'	-2.0	5.0	60.0094
143	'CN-'	-1.0	4.0	26.018
144	'OCN-'	-1.0	4.0	42.017
150	'Ca+2'	2.0	6.0	40.0800
160	'Cd+2'	2.0	6.0	112.3994
170	'Ce+3'	3.0	9.0	140.12
171	'Ce+4'	4.0	9.0	140.12
180	'Cl-'	-1.0	3.0	35.4530
181	'ClO4-'	-1.0	3.0	99.451
200	'Co+2'	2.0	4.5	58.933
201	'Co+3'	3.0	5.0	58.993
211	'CrOH+2'	2.0	4.5	69.0033
210	'Cr+2'	2.0	4.5	51.996
212	'CrO4-2'	-2.0	4.0	115.994
220	'Cs+'	1.0	2.5	132.9050
230	'Cu+1'	1.0	4.0	63.5460
231	'Cu+2'	2.0	6.0	63.5460
001	'e-'	-1.0	0.0	0.0000
270	'F-'	-1.0	4.0	18.9984
141	'Fulvate'	-2.0	0.0	400.0000
280	'Fe+2'	2.0	6.0	55.8470
281	'Fe+3'	3.0	9.0	55.8470
330	'H+'	1.0	9.0	1.0080
002	'H2O'	0.0	0.0	18.0153
060	'H3AsO3'	0.0	3.0	125.9437
061	'H3AsO4'	0.0	3.0	141.9431
090	'H3BO3'	0.0	4.0	61.8331
770	'H4SiO4'	0.0	3.0	96.1155
142	'Humate'	-2.0	0.0	2000.0000
361	'Hg(OH)2'	0.0	4.5	234.61
360	'Hg2+2'	2.0	4.5	401.18
380	'I-'	-1.0	4.0	126.9044
410	'K+'	1.0	3.0	39.1020
440	'Li+'	1.0	4.0	6.9390
460	'Mg+2'	2.0	8.0	24.3120
470	'Mn+2'	2.0	6.0	54.9380
471	'Mn+3'	3.0	5.0	54.9380
472	'MnO4-1'	-1.0	4.0	118.9830
473	'MnO4-2'	-2.0	4.0	118.9830
480	'Mo+3'	3.0	5.0	95.94
481	'MoO4-2'	-2.0	4.0	159.94
490	'NH4+'	1.0	3.0	18.0386
491	'NO2-'	-1.0	4.0	46.0055
492	'NO3-'	-1.0	3.0	62.0049
500	'Na+'	1.0	4.0	22.9898

540	'Ni+2'	2.0	4.5	58.7100
580	'PO4-3'	-3.0	4.0	94.9714
600	'Pb+2'	2.0	5.0	207.1899
670	'Re+2'	2.0	4.5	266.0
680	'Rb+'	1.0	4.0	85.4699
730	'HS-'	-1.0	3.0	33.0720
731	'S'	0.0	0.0	32.0640
732	'SO4-2'	-2.0	4.0	96.0616
733	'SO3-2'	-2.0	4.0	80.0622
734	'SCN-'	-1.0	4.0	58.0819
735	'S2O3-2'	-2.0	4.0	112.1262
990	'SOH1'	0.0	0.0	0.0
991	'SOH2'	0.0	0.0	0.0
740	'Sb(OH)3'	0.0	3.0	172.7719
741	'Sb(OH)6-'	-1.0	4.0	223.7938
760	'HSe-1'	-1.0	4.0	79.968
761	'HSeO3-1'	-1.0	4.0	127.966
762	'SeO4-2'	-2.0	4.0	142.958
800	'Sr+2'	2.0	5.0	87.6200
850	'Th+4'	4.0	5.5	232.038
871	'Tl(OH)3'	0.0	3.0	255.39
870	'Tl+1'	1.0	2.5	204.37
890	'U+3'	3.0	5.0	238.0290
891	'U+4'	4.0	5.5	238.0290
892	'UO2+'	1.0	4.0	270.0278
893	'UO2+2'	2.0	4.5	270.0278
900	'V+2'	2.0	4.5	50.94
901	'V+3'	3.0	5.0	50.94
902	'VO+2'	2.0	4.5	66.939
903	'VO2+1'	1.0	4.0	82.939
992	'XPSIO'	0.0	0.0	0.0
993	'XPSIB'	0.0	0.0	0.0
994	'XPSID'	0.0	0.0	0.0
950	'Zn+2'	2.0	6.0	65.3699

APPENDIX D

COMPLETE LISTING OF THE AQUEOUS.DAT(4.00) DATA FILE

APPENDIX D

COMPLETE LISTING OF THE AQUEOUS.DAT(4.00) DATA FILE

```
AQUEOUS.DAT:  Thermochemical data for Aqueous Species
File History:
Date      Version   Person   Action
9-20-91    4.00     T. Eary  A four-line database created for use by both
                             the GM and MINTEQ geochemical models. Data
                             included are as follows.
                             Line 1: ID#, name, del H(rxn), logK(25C), charge,
                                     ion size (angstroms), noncarbonate
                                     alkalinity factor, and molecular wt.
                             Line 2: carbonate alkalinity factor, number of
                                     reactants in formation reaction,
                                     reaction stoichiometry and species ID
                                     number (same as in old GM and MINTEQ)
                             Line 3: Coefficients for temperature dependence
                                     of the log K i.e., log K = a0 + a1/T +
                                     a2*T + a3*log(T) + a4/T**2 where T is
                                     in degrees K.  Values of 999. indicate
                                     no temperature data available.  In such
                                     cases, the enthalpy of reaction, if
                                     available, will be used to calculate
                                     log K values for temperatures other than
                                     25 C using the Van't Hoff equation.  If
                                     the enthalpy of reaction is absent, then
                                     the codes will default to the 25C-logK
                                     value.
                              Line 4: Reference for source of data.  Full
                                      citations are given at the bottom of
                                      the file.

                              Note:  All data is read in FREE FORMAT with all
                                     names as 18 character length strings.
STOP.
Version 4.00
3300020 'OH-1'              13.3620    -14.00            -1.00 3.00 1.00  17.0073
 0.00 2     1.000 002    -1.000 330
      -2.83971e+2  1.33230e+4  -5.069842e-2  1.0224447e+2  -1.119669e+6
      Nordstrom et al. 1990
3304900 'NH3(aq)'           12.4810   -9.2517             0.00 3.00 0.00  17.0306
 0.00 2     1.000 490    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3304910 'HNO2(aq)'          -3.4900    3.2207             0.00 3.00 0.00  47.0135
 0.00 2     1.000 330     1.000 491
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4907320 'NH4SO4-1'           0.0000    1.1119            -1.00 4.00 0.00 114.1021
 0.00 2     1.000 490     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3301400 'HCO3-1'            -3.561    10.329             -1.00 4.00 0.00  61.0171
 1.00 2     1.000 140     1.000 330
      1.078871e+2  -5.15179e+3  3.2528e-2  -3.892561e+1  5.637139e+5
      Nordstrom et al. 1990
3301401 'H2CO3(aq)'         -5.738     16.68             0.00 3.00 0.00  62.0251
 0.00 2     1.000 140     2.000 330
      5.19613e+2  -3.02174e+4  1.00821e-1  -1.85554e+2  2.44400e+6
      Nordstrom et al. 1990
3301800 'HCl(aq)'           0.0000     -0.67             0.00 3.00 0.00  36.4610
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 0.00 2     1.000 180     1.000 330
      2.01122e+3  -1.08495e+5  3.13714e-1  -7.32023e+2  6.20320e+6
      EQ3/6 version: mdas.3245
3307320 'HSO4-1'              3.85      1.988            -1.00 4.00 1.00  97.0715
 0.00 2     1.000 732     1.000 330
      -5.6889e+1  2.3079e+3  6.473e-3  1.98858e+1  0.00
      Nordstrom et al. 1990
3302700 'HF(aq)'              3.18      3.18              0.00 3.00 0.00  20.0063
 0.00 2     1.000 270     1.000 330
      -2.033e+0  4.2901e+2  1.2645e-2  0.0000  0.0000
      Nordstrom et al. 1990
3302701 'HF2-1'               4.55      3.67             -1.00 4.00 0.00  39.0047
 0.00 2     2.000 270     1.000 330
      2.31903e+3  -1.29395e+5  3.44527e-1  -8.36289e+2  7.57693e+6
      EQ3/6 version: mdas.3245
3302702 'H2F2(aq)'          0.0000    6.7698             0.00 3.00 0.00  40.0127
 0.00 2     2.000 270     2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3305800 'HPO4-2'            -3.5230     12.37            -2.00 4.00 2.00  95.9793
 0.00 2     1.000 580     1.000 330
      -4.27806e+1  5.45216e+3  1.24985e-2  1.41985e+1  -1.77525e+5
      Reed and Spycher 1989: SOLVEQ database
3305801 'H2PO4-1'           -4.5150     19.57            -1.00 4.00 1.00  96.9872
 0.00 2     1.000 580     2.000 330
      1.29977e+3  -7.41422e+4  2.01096e-1  -4.63855e+2  5.00485e+6
      Smith et al. 1986
3305802 'H3PO4(aq)'         -2.6150     21.70             0.00 3.00 0.00  97.9952
 0.00 2     1.000 580     3.000 330
      1.94380e+3  -1.12417e+5  2.96897e-1  -6.94209e+2  7.48728e+6
      Smith et al. 1986
3307300 'H2S(aq)'           -5.2820      6.99             0.00 3.00 0.00  34.0819
 0.00 2     1.000 730     1.000 330
      7.54093e+2  -4.20616e+4  1.19704e-1  -2.71998e+2  2.78406e+6
      EQ3/6 version: mdas.3245
3307301 'S-2'               12.1180    -12.94            -2.00 3.00 2.00  32.0660
 0.00 2     1.000 730    -1.000 330
      6.00274e+2  -5.46305e+4  3.70756e-2  -1.98632e+2  4.47896e+6
      EQ3/6 version: mdas.3245
7317305 'S2-2'              11.4010    -11.81            -2.00 4.00 0.00  64.1320
 0.00 3     1.000 730     1.000 731    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
7317301 'S3-2'              10.3970  -10.7954            -2.00 4.00 0.00  96.1980
 0.00 3     1.000 730     2.000 731    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
7317302 'S4-2'               9.7040   -9.9891            -2.00 4.00 0.00 128.2640
 0.00 3     1.000 730     3.000 731    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
7317303 'S5-2'               9.2980   -9.3939            -2.00 4.00 0.00 160.3300
 0.00 3     1.000 730     4.000 731    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
7317304 'S6-2'               0.0000   -9.8828            -2.00 4.00 0.00 192.3960
 0.00 3     1.000 730     2.000 731    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3307330 'HSO3-1'             2.2200    7.1700            -1.00 4.00 1.00  81.0721
 0.00 2     1.000 733     1.000 330
      1.55725e+2  -2.37867e+3  7.05294e-2  -6.53100e+1  -4.54976e-5
      Goldberg and Parker 1985
3307331 'H2SO3(aq)'          6.3800    9.0303             0.00 3.00 0.00  82.0801
 0.00 2     1.000 733     2.000 330
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     -1.35603e+2  8.24311e+3  2.05742e-2  4.58914e+1  -2.40594e+5
     Goldberg and Parker 1985
3307340 'HSCN(aq)'          0.0000   -0.8495            0.00 3.00 0.00  59.0917
 0.00 2     1.000 734     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
3307350 'HS2O3-1'           5.7000    1.7225           -1.00 4.00 1.00 113.1381
 0.00 2     1.000 330     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
3307351 'H2S2O3(aq)'       10.5500    2.3236            0.00 3.00 0.00 114.1461
 0.00 2     2.000 330     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0201400 'AgCO3-1'           0.0000    1.8735           -1.00 4.00 0.00 167.8774
 2.00 2     1.000 020     1.000 140
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0201300 'AgBr(aq)'          0.0000    4.2279            0.00 3.00 0.00 187.7722
 0.00 2     1.000 020     1.000 130
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0201301 'AgBr2-1'           0.0000    7.2837           -1.00 4.00 0.00 267.6762
 0.00 2     1.000 020     2.000 130
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0201800 'AgCl(aq)'         -2.7230      3.38            0.00 3.00 0.00 143.3209
 0.00 2     1.000 020     1.000 180
     1.17952e+2  -5.10617e+3  1.90297e-2 -4.29289e+1  2.54070e+5
     Reed and Spycher 1989: SOLVEQ database
0201801 'AgCl2-1'          -3.9710      5.17            -1.00 4.00 0.00 178.7736
 0.00 2     1.000 020     2.000 180
     1.94514e+3  -1.19031e+5  2.60564e-1  -6.91093e+2  8.14642e+6
     Reed and Spycher 1989: SOLVEQ database
0201802 'AgCl3-2'           0.0000      5.21            -2.00 4.00 0.00 214.2263
 0.00 2     1.000 020     3.000 180
     2.30029e+3  -1.50236e+5  2.78653e-1  -8.07536e+2  1.10174e+7
     Reed and Spycher 1989: SOLVEQ database
0201803 'AgCl4-3'           0.0000      3.97            -3.00 4.00 0.00 249.6790
 0.00 2     1.000 020     4.000 180
     1.11750e+3  4.24587e+3  3.81681e-1  -4.80595e+2  -4.65874e+6
     Reed and Spycher 1989: SOLVEQ database
0202700 'AgF(aq)'          -2.8750      0.36            0.00 3.00 0.00 126.8666
 0.00 2     1.000 020     1.000 270
     -1.33472e+3  7.65951e+4  -1.93512e-1  4.80130e+2  -4.63803e+6
     Reed and Spycher 1989: SOLVEQ database
0207300 'AgHS(aq)'          0.0000     13.85            0.00 3.00 0.00 140.9421
 0.00 2     1.000 020     1.000 730
     1.69440e+3  -9.42486e+4  2.20825e-1  -6.04344e+2  5.79009e+6
     Reed and Spycher 1989: SOLVEQ database
0207301 'Ag(HS)2-1'         0.0000     17.71            -1.00 4.00 0.00 174.0161
 0.00 2     1.000 020     2.000 730
     -2.45934e+3  1.60089e+5  -2.81210e-1  8.63995e+2  -1.01304e+7
     Gammons and Barnes 1989
0203800 'AgI(aq)'           0.0000    6.5910            0.00 3.00 0.00 234.7727
 0.00 2     1.000 020     1.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0203801 'AgI2-1'            0.0000   10.6781           -1.00 4.00 0.00 361.6771
 0.00 2     1.000 020     2.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0203300 'AgOH(aq)'          0.0000  -11.9103            0.00 3.00 0.00 124.8755
 0.00 3     1.000 020     1.000 002    -1.000 330
     999.  999.  999.  999.  999.
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     Krupka et al. 1988
0203301 'Ag(OH)2-1'          0.0000  -23.9935            -1.00 4.00 0.00 141.8829
 0.00 3     1.000 020     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207320 'AgSO4-1'            1.4360    1.2893            -1.00 4.00 0.00 203.9318
 0.00 2     1.000 020     1.000 732
     2.52961e+2  -1.81988e+4  3.22102e-2   -3.74661e+1  1.44044e+6
     Reed and Spycher 1989: SOLVEQ database
0204920 'AgNO3(aq)'          0.0000    0.1473             0.00 0.00 0.00 169.8731
 0.00 2     1.000 020     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0204910 'Ag(NO2)2-1'         0.0000    3.9581            -1.00 4.00 0.00 199.8793
 0.00 2     1.000 020     2.000 491
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0201302 'AgBr3-2'            0.0000    8.7093            -2.00 4.00 0.00 347.5802
 0.00 2     1.000 020     3.000 130
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0203802 'AgI3-2'           -29.2010   13.3630            -2.00 4.00 0.00 488.5816
 0.00 2     1.000 020     3.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0203803 'AgI4-3'             0.0000   14.0865            -3.00 4.00 0.00 615.4861
 0.00 2     1.000 020     4.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207302 'Ag(S4)2-3'          0.0000    0.9895            -3.00 4.00 0.00 364.3962
 0.00 4     1.000 020     2.000 730    -2.000 330     6.000 731
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207303 'AgS4S5-3'           0.0000    0.6743            -3.00 4.00 0.00 396.4622
 0.00 4     1.000 020     2.000 730    -2.000 330     7.000 731
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207304 'Ag(HS)S4-2'         0.0000   10.4304            -2.00 4.00 0.00 269.2061
 0.00 4     1.000 020     2.000 730    -1.000 330     3.000 731
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207330 'AgSO3-1'            0.0000    5.5971            -1.00 4.00 0.00 187.9324
 0.00 2     1.000 020     1.000 733
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207331 'Ag(SO3)2-3'         0.0000    8.6756            -3.00 4.00 0.00 267.9966
 0.00 2     1.000 020     2.000 733
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207332 'Ag(SO3)3-5'         0.0000    8.9981            -5.00 4.00 0.00 348.0608
 0.00 2     1.000 020     3.000 733
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207340 'AgSCN(aq)'          0.0000    4.7483             0.00 3.00 0.00 165.9519
 0.00 2     1.000 020     1.000 734
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207341 'Ag(SCN)2-1'         0.0000    8.3062            -1.00 4.00 0.00 224.0357
 0.00 2     1.000 020     2.000 734
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0207342 'Ag(SCN)3-2'         0.0000    9.5141            -2.00 4.00 0.00 282.1194
 0.00 2     1.000 020     3.000 734
     999.  999.  999.  999.  999.
     Krupka et al. 1988
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0207343 'Ag(SCN)4-3'          0.0000    9.6959            -3.00 4.00 0.00 340.2032
 0.00 2     1.000 020     4.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207350 'AgS2O3-1'            0.0000    7.0704            -1.00 4.00 0.00 219.9984
 0.00 2     1.000 020     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207351 'Ag(S2O3)2-3'       -19.0950   13.4547            -3.00 4.00 0.00 332.1286
 0.00 2     1.000 020     2.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207600 'Ag2Se(aq)'           0.0000   34.0882             0.00 3.00 0.00 294.6964
 0.00 3     1.000 760     2.000 020    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207601 'AgOH(Se)2-4'         0.0000  -18.5804            -4.00 4.00 0.00 282.7955
 0.00 4     2.000 760     1.000 020     1.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207610 'AgSeO3-1'            0.0000   -5.5817            -1.00 4.00 0.00 234.8264
 0.00 3     1.000 761     1.000 020    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0207611 'Ag(SeO3)2-3'         0.0000  -10.9625            -3.00 4.00 0.00 361.7846
 0.00 3     2.000 761     1.000 020    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0303300 'AlOH+2'                11.49     -5.00             2.00 4.50 0.00  43.9889
 0.00 3     1.000 030     1.000 002    -1.000 330
     -3.8253e+1  -6.5627e+2  0.0000  1.4327e+1  0.0000
      Nordstrom et al. 1990
0303301 'Al(OH)2+1'             26.9    -10.11             1.00 4.00 0.00  60.9962
 0.00 3     1.000 030     2.000 002    -2.000 330
      8.8500e+1  -9.3916e+3  0.0000  -2.7121e+1  0.0000
      Nordstrom et al. 1990
0303303 'Al(OH)3(aq)'           39.89    -16.94             0.00 3.00 0.00  78.0036
 0.00 3     1.000 030     3.000 002    -3.000 330
      2.26374e+2  -1.82478e+4  0.0000  -7.3597e+1  0.0000
      Nordstrom et al. 1990
0303302 'Al(OH)4-1'             42.30    -22.67            -1.00 4.00 0.00  95.0109
 0.00 3     1.000 030     4.000 002    -4.000 330
      5.1578e+1  -1.11689e+4  0.0000  -1.4865e+1  0.0000
      Nordstrom et al. 1990
0303304 'Al2(OH)2+4'          17.6500   -7.6890             4.00 5.00 0.00  87.9778
 0.00 3     2.000 030     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0303305 'Al3(OH)4+5'          34.3900  -13.8607             5.00 5.00 0.00 148.9740
 0.00 3     3.000 030     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0302700 'AlF+2'                 1.06      7.00             2.00 4.50 0.00  45.9799
 0.00 2     1.000 030     1.000 270
      3.12133e+3  -1.72679e+5  4.65847e-1  -1.12665e+3  1.01100e+7
      EQ3/6 version: mdas.3245
0302701 'AlF2+1'                1.98     12.60             1.00 4.00 0.00  64.9783
 0.00 2     1.000 030     2.000 270
      4.30620e+3  -2.37929e+5  6.51142e-1  -1.5547e+3  1.39889e+7
      EQ3/6 version: mdas.3245
0302702 'AlF3(aq)'              2.16     16.70             0.00 3.00 0.00  83.9767
 0.00 2     1.000 030     3.000 270
      2.02361e+3  -9.10283e+4  4.24316e-1  -7.59007e+2  4.44431e+6
      EQ3/6 version: mdas.3245
0302703 'AlF4-1'                2.2      19.10            -1.00 4.00 0.00 102.9751
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 0.00 2     1.000 030     4.000 270
      6.71590e+3  -3.72626e+5  9.98634e-1  -2.42133e+3  2.19228e+7
      EQ3/6 version: mdas.3245
0302704 'AlF5-2'              1.84      20.97            -2.00 4.00 0.00 121.9735
 0.00 2     1.000 030     5.000 270
      7.78656e+3  -4.30218e+5  1.17663e+0  -2.81232e+3  2.53705e+7
      EQ3/6 version: mdas.3245
0302705 'AlF6-3'             -1.67      20.60            -3.00 4.00 0.00 140.9719
 0.00 2     1.000 030     6.000 270
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
0307320 'AlSO4+1'             2.1500      3.02             1.00 4.00 0.00 123.0451
 0.00 2     1.000 030     1.000 732
      3.97631e+3  -2.20177e+5  6.10821e-1  -1.44017e+3  1.30337e+7
      EQ3/6 version: mdas.3245
0307321 'Al(SO4)2-1'          2.84      4.90             -1.00 4.00 0.00 219.1087
 0.00 2     1.000 030     2.000 732
      5.80389e+3  -3.23819e+5  8.30936e-1  -2.09038e+3  1.88293e+7
      EQ3/6 version: mdas.3245
0307322 'AlHSO4+2'            0.0000      2.45             2.00 4.00 0.00 124.0511
 0.00 3     1.000 030     1.000 732     1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
0603300 'H2AsO3-1'            6.5500     -9.29            -1.00 4.00 1.00 124.9357
 0.00 2     1.000 060    -1.000 330
      -4.59183e+2  2.46851e+4  -7.32042e-2  1.64850e+2  -1.68781e+6
      Smith et al. 1986
0603301 'HAsO3-2'            12.6900    -21.36            -2.00 4.00 2.00 123.9277
 0.00 2     1.000 060    -2.000 330
      -9.03561e+1  -1.00048e+2  -5.45171e-2  3.67159e+1  -4.68039e+5
      Reed and Spycher 1989: SOLVEQ database
0603302 'AsO3-3'              0.0000    -34.76            -3.00 4.00 3.00 122.9197
 0.00 2     1.000 060    -3.000 330
      -4.86041e+1  -5.55236e+3  -6.70153e-2  2.25165e+1  -2.90503e+5
      Reed and Spycher 1989: SOLVEQ database
0613301 'H2AsO4-1'           -1.6900     -2.24            -1.00 4.00 1.00 140.9351
 0.00 2     1.000 061    -1.000 330
      -5.34357e+2  3.12410e+4  -8.25548e-2  1.91747e+2  -2.00187e+6
      Smith et al. 1986
0613302 'HAsO4-2'            -0.9200     -9.18            -2.00 4.00 2.00 139.9271
 0.00 2     1.000 061    -2.000 330
      -1.92980e+3  1.13925e+5  -2.78199e-1  6.88771e+2  -7.36647e+6
      Smith et al. 1986
0613303 'AsO4-3'              3.4300    -20.69            -3.00 4.00 3.00 138.9192
 0.00 2     1.000 061    -3.000 330
      -1.85715e+3  1.07477e+5  -2.86473e-1  6.63518e+2  -7.15104e+6
      Reed and Spycher 1989: SOLVEQ database
0603303 'AsO+1'               0.0000   -0.3049            1.00 4.00 0.00  90.9210
 0.00 3     1.000 060     1.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0612700 'AsO3F-2'             0.0000   38.5059            -2.00 4.00 0.00 141.9182
 0.00 4     1.000 061     1.000 270    -1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
0612701 'HAsO3F-1'            0.0000   44.3771            -1.00 4.00 0.00 142.9261
 0.00 3     1.000 061     1.000 270    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1003300 'BaOH+1'              0.0000   -13.47             1.00 4.00 0.00 154.3343
 0.00 3     1.000 100     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
1007350 'BaS2O3(aq)'          2.5990    2.3331            0.00 3.00 0.00 249.4572
 0.00 2     1.000 100     1.000 735
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     999.  999.  999.  999.  999.
     Krupka et al. 1988
1007320 'BaSO4(aq)'          0.0000      2.70             0.00 3.00 0.00 233.3906
 0.00 2     1.000 100     1.000 732
     1.10484e+3  -5.83257e+4  1.84304e-1  -4.03513e+2  3.28913e+6
     EQ3/6 version: mdas.3245
1004920 'BaNO3+1'            1.7050   -0.4962             1.00 4.00 0.00 199.3319
 0.00 2     1.000 100     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1001400 'BaCO3(aq)'           3.55      2.71             0.00 3.00 0.00 197.3362
 2.00 2     1.000 100     1.000 140
     1.13e-1  0.0000  8.721e-3  0.0000  0.0000
     Nordstrom et al. 1990
1001401 'BaHCO3+1'            1.999     11.31            1.00 4.00 0.00 198.3441
 1.00 3     1.000 100     1.000 140     1.000 330
     1.89679e+2  -1.03023e+4  5.69786e-2  -6.90466e+1  8.93037e+5
     Nordstrom et al. 1990
1001800 'BaCl+'              0.0000     -0.50             1.00 4.00 0.00 172.7930
 0.00 2     1.000 100     1.000 180
     9.27365e+2  -5.23771e+4  1.46668e-1  -3.36103e+2  3.17711e+6
     EQ3/6 version: mdas.3245
1002700 'BaF+'               0.0000     -0.18            1.00 4.00 0.00 156.3384
 0.00 2     1.000 100     1.000 270
     9.44371e+2  -5.37124e+4  1.47040e-1  -3.41609e+2  3.29298e+6
     EQ3/6 version: mdas.3245
0902700 'BF(OH)3-1'          1.8510   -0.4024          -1.00 4.00 0.00  80.8314
 0.00 2     1.000 090     1.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0902701 'BF2(OH)2-1'         0.0000    9.0575          -1.00 4.00 0.00  82.8225
 0.00 4     1.000 090     2.000 270    -1.000 002     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0902702 'BF3OH-1'           -6.8490   14.6531          -1.00 4.00 0.00  84.8135
 0.00 4     1.000 090     3.000 270    -2.000 002     2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0902703 'BF4-1'             -7.0640   20.0398          -1.00 4.00 0.00  86.8046
 0.00 4     1.000 090     4.000 270    -3.000 002     3.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0903301 'H2BO3-'             3.3750    -9.24           -1.00 4.00 1.00  42.8098
 0.00 2     1.000 090    -1.000 330
     -5.39813e+2  3.01537e+4  -8.31712e-2  1.92647e+2  -1.99636e+6
     Smith et al. 1986
0903302 'B4O7-2'             0.0000  -14.8158          -2.00 4.00 2.00 155.2398
 0.00 3     4.000 090    -2.000 330    -5.000 002
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0903304 'HB4O7-1'            0.0000   -0.7469          -1.00 4.00 1.00 156.2477
 0.00 3     4.000 090    -1.000 330    -5.000 002
     999.  999.  999.  999.  999.
     Krupka et al. 1988
0903305 'H2B4O7(aq)'         0.0000    5.3501           0.00 3.00 0.00 157.2557
 0.00 2     4.000 090    -5.000 002
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1503300 'CaOH+1'            14.7440   -12.60            1.00 4.00 0.00  57.0853
 0.00 3     1.000 150     1.000 002    -1.000 330
     2.97654e+3  -1.72892e+5  4.22128e-1  -1.07109e+3  1.02511e+7
     Reed and Spycher 1989: SOLVEQ database
1501400 'CaHCO3+1'           -0.871    11.44            1.00 4.00 0.00 101.0951
 1.00 3     1.000 150     1.000 140     1.000 330
     1.38502e+3  -4.38612e+4  3.54651e-1  -5.42041e+2  8.03206e+5
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     Nordstrom et al. 1990
1501401 'CaCO3(aq)'          3.545     3.224             0.00 3.00 0.00 100.0872
 2.00 2     1.000 150     1.000 140
     -1.228732e+3  3.551275e+4  -2.99444e-1  4.85818e+2  0.0000
     Nordstrom et al. 1990
1507320 'CaSO4(aq)'          1.65      2.11              0.00 3.00 0.00 136.1416
 0.00 2     1.000 150     1.000 732
     1.72726e+3  -9.53213e+4  2.67072e-1  -6.25751e+2  5.62661e+6
     EQ3/6 version: mdas.3245
1505800 'CaHPO4(aq)'        -0.2250   15.0819           0.00 3.00 0.00 136.0573
 0.00 3     1.000 150     1.000 580     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1505801 'CaPO4-1'            3.0450    6.4620           -1.00 4.00 0.00 135.0494
 0.00 2     1.000 150     1.000 580
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1505802 'CaH2PO4+1'         -1.1150   20.9531           1.00 4.00 0.00 137.0652
 0.00 3     1.000 150     1.000 580     2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1504920 'CaNO3+1'           -5.9650    0.7337           1.00 4.00 0.00 102.0829
 0.00 2     1.000 150     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1502700 'CaF+1'              4.12      0.68             1.00 4.00 0.00  59.0764
 0.00 2     1.000 150     1.000 270
     8.86755e+2  -5.04724e+4  1.41030e-1  -3.21003e+2  3.15200e+6
     EQ3/6 version: mdas.3245
1501800 'CaCl+'              0.0000    -0.70             1.00 4.00 0.00  75.5330
 0.00 2     1.000 150     1.000 180
     8.44845e+2  -4.80866e+4  1.34966e-1  -3.06548e+2  3.02475e+6
     EQ3/6 version: mdas.3245
1501801 'CaCl2(aq)'          0.0000    -0.64             0.00 3.00 0.00 110.9860
 0.00 2     1.000 150     2.000 180
     1.67741e+3  -9.43826e+4  2.67594e-1  -6.09292e+2  5.90016e+6
     EQ3/6 version: mdas.3245
1507350 'CaS2O3(aq)'         0.0000    1.8698            0.00 3.00 0.00 152.2082
 0.00 2     1.000 150     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1601800 'CdCl+1'             0.5880    2.7238            1.00 4.00 0.00 147.8637
 0.00 2     1.000 160     1.000 180
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1601801 'CdCl2(aq)'          1.2450    3.3673            0.00 3.00 0.00 183.3164
 0.00 2     1.000 160     2.000 180
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1601802 'CdCl3-1'            3.8870    2.7546           -1.00 4.00 0.00 218.7691
 0.00 2     1.000 160     3.000 180
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1601804 'CdCl4-2'            0.0000    1.6815           -2.00 4.00 0.00 254.2218
 0.00 2     1.000 160     4.000 180
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1602700 'CdF+1'              0.0000    1.0980            1.00 4.00 0.00 131.4094
 0.00 2     1.000 160     1.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
1602701 'CdF2(aq)'           0.0000    1.4997            0.00 3.00 0.00 150.4078
 0.00 2     1.000 160     2.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
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1603301 'Cd(OH)2(aq)'      21.3844  -20.8780           0.00 3.00 0.00 146.4257
 0.00 3     1.000 160     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Rai and Felmy 1991a
1603303 'Cd(OH)4-2'         0.0000  -47.4360          -2.00 4.00 0.00 180.4404
 0.00 3     1.000 160     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Rai and Felmy 1991a
1603304 'Cd2OH+3'          10.8970   -9.3859           3.00 5.00 0.00 241.8293
 0.00 3     2.000 160     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1603305 'Cd4(OH)4+4'        0.0000  -32.8524           4.00 5.00 0.00 517.6734
 0.00 3     4.000 160     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1601803 'CdOHCl(aq)'        0.0000   -7.4046           0.00 3.00 0.00 164.8710
 0.00 4     1.000 160     1.000 002    -1.000 330     1.000 180
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1604920 'CdNO3+1'          -5.2030    0.4984           1.00 4.00 0.00 174.4159
 0.00 2     1.000 160     1.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1604921 'Cd(NO3)2(aq)'      0.0000    0.1979           0.00 3.00 0.00 236.4209
 0.00 2     1.000 160     2.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607320 'CdSO4(aq)'         1.0820    2.4577           0.00 3.00 0.00 208.4746
 0.00 2     1.000 160     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607300 'CdHS+1'            0.0000    7.6208           1.00 4.00 0.00 145.4849
 0.00 2     1.000 160     1.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607301 'Cd(HS)2(aq)'       0.0000   14.6040           0.00 3.00 0.00 178.5589
 0.00 2     1.000 160     2.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607302 'Cd(HS)3-1'         0.0000   16.5002          -1.00 4.00 0.00 211.6328
 0.00 2     1.000 160     3.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607303 'Cd(HS)4-2'         0.0000   18.8949          -2.00 4.00 0.00 244.7068
 0.00 2     1.000 160     4.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1601300 'CdBr+1'           -0.8000    2.1667           1.00 4.00 0.00 192.3150
 0.00 2     1.000 160     1.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1601301 'CdBr2(aq)'         0.0000    2.9026           0.00 3.00 0.00 272.2190
 0.00 2     1.000 160     2.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1603800 'CdI+1'            -2.3680    2.1396           1.00 4.00 0.00 239.3155
 0.00 2     1.000 160     1.000 380
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1603801 'CdI2(aq)'          0.0000    3.5990           0.00 3.00 0.00 366.2199
 0.00 2     1.000 160     2.000 380
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1601400 'CdHCO3+1'          0.0000   12.4901           1.00 4.00 0.00 173.4281
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 1.00 3     1.000 160     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1601401 'CdCO3(aq)'          0.0000      4.71             0.00 3.00 0.00 172.4202
 2.00 2     1.000 160     1.000 140
      999.  999.  999.  999.  999.
      Rai and Felmy 1991b
1601402 'Cd(CO3)2-2'         0.0000      6.49            -2.00 4.00 0.00 292.4386
 4.00 2     1.000 160     3.000 140
      999.  999.  999.  999.  999.
      Rai and Felmy 1991b
1607321 'Cd(SO4)2-2'         0.0000    3.5007            -2.00 4.00 0.00 304.5382
 0.00 2     1.000 160     2.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607340 'CdSCN+1'           -0.7000    1.3304             1.00 4.00 0.00 170.4947
 0.00 2     1.000 160     1.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607341 'Cd(SCN)2(aq)'       0.0000    1.8808             0.00 3.00 0.00 228.5785
 0.00 2     1.000 160     2.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607342 'Cd(SCN)3-1'         0.0000    1.9124            -1.00 4.00 0.00 286.6622
 0.00 2     1.000 160     3.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607343 'Cd(SCN)4-2'         0.0000    2.9114            -2.00 4.00 0.00 344.7460
 0.00 2     1.000 160     4.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607350 'CdS2O3(aq)'         1.3010    3.8995             0.00 3.00 0.00 224.5412
 0.00 2     1.000 160     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607351 'Cd(S2O3)2-2'        0.0000    6.4429            -2.00 4.00 0.00 336.6714
 0.00 2     1.000 160     2.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607610 'Cd(SeO3)2-2'        0.0000  -11.1648            -2.00 4.00 0.00 366.3274
 0.00 3     2.000 761     1.000 160    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1607620 'CdSeO4(aq)'         0.0000    2.1843             0.00 3.00 0.00 255.3686
 0.00 2     1.000 762     1.000 160
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1702700 'CeF+2'              0.0000   -3.4770             2.00 5.00 0.00 159.1140
 0.00 2     1.000 170     1.000 270
      999.  999.  999.  999.  999.
      Peterson et al. 1986
1701800 'CeCl+2'           -24.9689    0.8040             2.00 5.00 0.00 175.5730
 0.00 2     1.000 170     1.000 180
      999.  999.  999.  999.  999.
      Peterson et al. 1986
1701810 'CeClO4+2'         -35.3227   12.4894             2.00 5.00 0.00 239.5710
 0.00 2     1.000 170     1.000 181
      999.  999.  999.  999.  999.
      Peterson et al. 1986
1701300 'CeBr+2'             0.0000   -0.6050             2.00 5.00 0.00 220.0240
 0.00 2     1.000 170     1.000 130
      999.  999.  999.  999.  999.
      Peterson et al. 1986
1707320 'CeSO4+'           -161.8738  -3.4460             1.00 4.00 0.00 236.1816
 0.00 2     1.000 170     1.000 732
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     999.  999.  999.  999.  999.
     Peterson et al. 1986
1707321 'Ce(SO4)2-1'      -325.6119  -5.0710          -1.00 4.00 0.00 332.2432
 0.00 2     1.000 170     2.000 732
     999.  999.  999.  999.  999.
     Peterson et al. 1986
1704920 'CeNO3+2'            0.0000  -1.0800           2.00 5.00 0.00 202.1249
 0.00 2     1.000 170     1.000 492
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003300 'CoOH+'              0.0000  -9.6681           1.00 4.00 0.00  75.9405
 0.00 3    -1.000 330     1.000 200     1.000 002
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003301 'Co(OH)2(aq)'        0.0000  -18.7571          0.00 3.00 0.00  92.9478
 0.00 3    -2.000 330     2.000 002     1.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003302 'Co(OH)3-'           0.0000  -32.2293         -1.00 4.00 0.00 109.9551
 0.00 3    -3.000 330     3.000 002     1.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003303 'Co(OH)4-2'          0.0000  -45.7822         -2.00 4.00 0.00 126.9624
 0.00 3    -4.000 330     4.000 002     1.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003304 'Co2OH+3'            0.0000  -11.2806          3.00 5.00 0.00 134.8737
 0.00 3    -1.000 330     1.000 002     2.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003305 'HCoO2-'             0.0000  -21.2419         -1.00 4.00 0.00  91.9399
 0.00 3    -3.000 330     2.000 002     1.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2003306 'Co4(OH)4+4'         0.0000  -30.3162          4.00 5.50 0.00 303.7620
 0.00 3    -4.000 330     4.000 002     4.000 200
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2002700 'CoF+'               0.0000    0.4105          1.00 4.00 0.00  77.9316
 0.00 2     1.000 200     1.000 270
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2001400 'CoCO3(aq)'          0.0000    3.1738          0.00 3.00 0.00 118.9424
 2.00 2     1.000 200     1.000 140
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2001401 'CoHCO3+'            0.0000   11.7204          1.00 4.00 0.00 119.9503
 1.00 3     1.000 200     1.000 140     1.000 330
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2007300 'CoHS+'              0.0000    6.5089          1.00 4.00 0.00  92.0011
 0.00 2     1.000 200     1.000 730
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2007301 'Co(HS)2(aq)'        0.0000    8.7665          0.00 3.00 0.00 125.0690
 0.00 2     1.000 200     2.000 730
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2007350 'CoS2O3(aq)'         0.0000  -16.8586          0.00 3.00 0.00 171.0514
 0.00 2     1.000 200     1.000 735
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2005800 'CoHPO4(aq)'         0.0000   14.5278          0.00 3.00 0.00 154.9125
 0.00 3     1.000 200     1.000 580     1.000 330
     999.  999.  999.  999.  999.
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     Peterson et al. 1986
2005801 'CoP2O7-2'          0.0000   26.8932          -2.00 4.00 0.00 232.8765
 0.00 4    -1.000 002     1.000 200     2.000 580     2.000 330
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2004900 'Co(NH3)+2'         11.0600   -7.2499           2.00 4.50 0.00  75.9636
 0.00 3    -1.000 330     1.000 200     1.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2004901 'Co(NH3)2+2'         0.0000  -15.0130           2.00 4.50 0.00  92.9940
 0.00 3    -2.000 330     1.000 200     2.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2004902 'Co(NH3)3+2'         0.0000  -23.4357           2.00 4.50 0.00 110.0244
 0.00 3    -3.000 330     1.000 200     3.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2004903 'Co(NH3)4+2'         0.0000  -32.0783           2.00 4.50 0.00 127.0548
 0.00 3    -4.000 330     1.000 200     4.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2004904 'Co(NH3)5+2'         0.0000  -41.2340           2.00 4.50 0.00 144.0852
 0.00 3    -5.000 330     1.000 200     5.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014907 'Co(NH3)6+3'        29.3100  -32.5562           3.00 5.00 0.00 161.1156
 0.00 3    -6.000 330     1.000 201     6.000 490
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014900 'Co(NH3)5(NO2)+2'   15.6600  -23.3272           2.00 4.50 0.00 190.0907
 0.00 4    -5.000 330     1.000 201     5.000 490     1.000 491
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014901 'Co(NH3)6(OH)+2'     0.0000  -43.6903           2.00 4.50 0.00 178.1229
 0.00 4    -7.000 330     1.000 201     6.000 490     1.000 002
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014902 'Co(NH3)5Cl+2'      27.0930  -18.0344           2.00 4.50 0.00 179.5382
 0.00 4    -5.000 330     1.000 201     5.000 490     1.000 180
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014903 'Co(NH3)6Cl+2'      24.9430  -34.0068           2.00 4.50 0.00 196.5686
 0.00 4    -6.000 330     1.000 201     6.000 490     1.000 180
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014904 'Co(NH3)6Br+2'      26.4490  -33.9980           2.00 4.50 0.00 241.0196
 0.00 4    -6.000 330     1.000 201     6.000 490     1.000 130
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014905 'Co(NH3)6I+2'       27.6090  -33.5912           2.00 4.50 0.00 288.0201
 0.00 4    -6.000 330     1.000 201     6.000 490     1.000 380
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2014906 'Co(NH3)6(SO4)+'    29.7300  -29.1625           1.00 4.00 0.00 257.1732
 0.00 4    -6.000 330     1.000 201     6.000 490     1.000 732
     999.  999.  999.  999.  999.
     Peterson et al. 1986
2113300 'Cr+3'               0.0000    3.5660           3.00 5.00 0.00  51.9961
 0.00 3     1.000 211     1.000 330    -1.000 002
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2113301 'Cr(OH)2+1'          0.0000   -6.2120           1.00 4.50 0.00  86.0108
 0.00 3     1.000 211    -1.000 330     1.000 002
     999.  999.  999.  999.  999.
     Krupka et al. 1988
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2110020 'Cr(OH)3(aq)'       0.0000  -12.5707            0.00 3.00 0.00 103.0181
 0.00 3     1.000 211     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2110021 'Cr(OH)4-1'         0.0000  -24.0602           -1.00 4.00 0.00 120.0255
 0.00 3     1.000 211     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2111300 'CrBr+2'            0.0000    2.7619            2.00 4.50 0.00 131.9001
 0.00 4     1.000 211     1.000 130     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2111800 'CrCl+2'            0.0000    3.6290            2.00 4.50 0.00  87.4488
 0.00 4     1.000 211     1.000 180     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2111801 'CrCl2+1'           0.0000    3.8753            1.00 4.00 0.00 122.9015
 0.00 4     1.000 211     2.000 180     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2111802 'CrOHCl2(aq)'       0.0000   -1.8090            0.00 3.00 0.00 139.9088
 0.00 2     1.000 211     2.000 180
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2112700 'CrF+2'             0.0000    9.2671            2.00 4.50 0.00  70.9945
 0.00 4     1.000 211     1.000 270     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2113800 'CrI+2'             0.0000    0.0872            2.00 4.50 0.00 178.9006
 0.00 4     1.000 211     1.000 380     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114900 'Cr(NH3)6+3'        0.0000  -37.2217            3.00 5.00 0.00 154.1795
 0.00 4     1.000 211     6.000 490    -5.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114901 'Cr(NH3)5(OH)+2'    0.0000  -34.9414            2.00 4.50 0.00 154.1562
 0.00 3     1.000 211     5.000 490    -5.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114902 'cisCrNH3)4OH'      0.0000  -34.5375            1.00 4.00 0.00 154.1330
 0.00 4     1.000 211     4.000 490    -5.000 330     1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114903 'transCrNH3)4'      0.0000  -35.2338            1.00 4.00 0.00 154.1330
 0.00 4     1.000 211     4.000 490    -5.000 330     1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114904 'Cr(NH3)6Cl+2'      0.0000  -35.7000            2.00 4.50 0.00 189.6322
 0.00 5     1.000 211     6.000 490     1.000 180    -1.000 002    -5.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114905 'Cr(NH3)6Br+2'      0.0000  -36.5232            2.00 4.50 0.00 234.0835
 0.00 5     1.000 211     6.000 490     1.000 130    -5.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114906 'Cr(NH3)6I+2'       0.0000  -36.5957            2.00 4.50 0.00 281.0839
 0.00 5     1.000 211     6.000 490     1.000 380    -5.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2114920 'CrNO3+2'           0.0000    3.8592            2.00 4.50 0.00 114.0010
 0.00 4     1.000 211     1.000 492     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2115800 'CrH2PO4+2'         0.0000   27.1204            2.00 4.50 0.00 148.9833
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 0.00 4     1.000 211     3.000 330     1.000 580    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2117320 'CrSO4+1'           0.0000    6.1776            1.00 4.00 0.00 148.0597
 0.00 4     1.000 211     1.000 732     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2117321 'CrOHSO4(aq)'       0.0000    3.4985            0.00 3.00 0.00 165.0670
 0.00 2     1.000 211     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2117322 '(CrOH)2(SO4)2'     0.0000    4.9740            0.00 3.00 0.00 330.1341
 0.00 2     2.000 211     2.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2117323 '(CrOH)2(SO4)+2'    0.0000    6.5844            2.00 4.50 0.00 234.0705
 0.00 2     2.000 211     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2123300 'HCrO4-1'           0.7000      6.49           -1.00 4.00 1.00 117.0016
 0.00 2     1.000 212     1.000 330
      9.95949e+2  -5.76582e+4  1.53532e-1  -3.57112e+2  3.71558e+6
      EQ3/6 database: version mdas.3245
2123301 'H2CrO4(aq)'        0.0000      5.18            0.00 3.00 0.00 118.0096
 0.00 2     1.000 212     2.000 330
      1.97477e+3  -9.60827e+4  3.80302e-1  -7.33671e+2  4.86318e+6
      EQ3/6 database: version mdas.3245
2123302 'Cr2O7-2'          -3.3050     14.52            -2.00 4.00 2.00 215.9880
 0.00 3     2.000 212     2.000 330    -1.000 002
      1.67402e+3  -9.42209e+4  2.60943e-1  -6.01663e+2  5.99851e+6
      EQ3/6 database: version mdas.3245
2121800 'CrO3Cl-1'          0.0000    7.9463            -1.00 4.00 0.00 135.4470
 0.00 4     1.000 212     1.000 180     2.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2125800 'CrO3H2PO4-'        0.0000   30.0084            -1.00 4.00 0.00 196.9815
 0.00 4     1.000 212     4.000 330     1.000 580    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2125801 'CrO3HPO4-2'        0.0000   27.3257            -2.00 4.00 0.00 195.9736
 0.00 4     1.000 212     3.000 330     1.000 580    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2127320 'CrO3SO4-2'         0.0000    9.6373            -2.00 4.00 0.00 196.0579
 0.00 4     1.000 212     1.000 732     2.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5002120 'NaCrO4-1'          0.0000    1.3289            -1.00 4.00 0.00 138.9835
 0.00 2     1.000 212     1.000 500
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4102120 'KCrO4-1'           0.0000    1.2952            -1.00 4.00 0.00 155.0920
 0.00 2     1.000 212     1.000 410
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2301802 'CuCl(aq)'          0.0000      4.21             0.00 3.00 0.00  98.9987
 0.00 2     1.000 230     1.000 180
      -2.26215e+3  1.41918e+5  -2.70518e-1  7.98465e+2  -9.31024e+6
      Reed and Spycher 1989: SOLVEQ database
2301800 'CuCl2-1'           0.0000      4.94            -1.00 4.00 0.00 134.4514
 0.00 2     1.000 230     2.000 180
      1.04189e+3  -5.45043e+4  1.76644e-1  -3.80743e+2  3.13976e+6
      EQ3/6 database: version mdas.3245
2301801 'CuCl3-2'           0.0000      5.14            -2.00 4.00 0.00 169.9041
 0.00 2     1.000 230     3.000 180
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     1.10569e+3  -5.76744e+4  1.90661e-1  -4.04655e+2  3.31933e+6
     EQ3/6 database: version mdas.3245
2301803 'Cu2Cl4-2'          0.0000   13.0222            -2.00 4.00 0.00 268.9028
 0.00 2     2.000 230     4.000 180
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2307300 'Cu(HS)2-'          0.0000     18.74            -1.00 4.00 0.00 129.6900
 0.00 2     1.000 230     2.000 730
     -3.24457e+3  2.04024e+5  -4.05548e-1  1.14987e+3  -1.29207e+7
     Reed and Spycher 1989: SOLVEQ database
2307301 'CuH(HS)3-'         0.0000     24.17            -1.00 4.00 0.00 163.7700
 0.00 3     1.000 230     1.000 330     3.000 730
     4.32938e+3  -2.41728e+5  6.25299e-1  -1.55651e+3  1.51651e+7
     Reed and Spycher 1989: SOLVEQ database
2311400 'CuCO3(aq)'         0.0000   -6.7640             0.00 3.00 0.00 123.5552
 2.00 2     1.000 231     1.000 140
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2311401 'Cu(CO3)2-2'        0.0000   -9.8498            -2.00 4.00 0.00 183.5644
 4.00 2     1.000 231     2.000 140
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2311800 'CuCl+1'            0.0000      0.10             1.00 4.00 0.00  98.9987
 0.00 2     1.000 231     1.000 180
     -4.74046e+2  3.11458e+4  -2.77565e-2  1.62463e+2  -2.14022e+6
     EQ3/6 database: version mdas.3245
2311801 'CuCl2(aq)'         0.0000     -0.69             0.00 3.00 0.00 134.4514
 0.00 2     1.000 231     2.000 180
     1.34508e+3  -7.73635e+4  2.14486e-1  -4.86091e+2  4.67105e+6
     EQ3/6 database: version mdas.3245
2311802 'CuCl3-1'           0.0000     -2.29            -1.00 4.00 0.00 169.9041
 0.00 2     1.000 231     3.000 180
     1.82525e+3  -1.05799e+5  2.83854e-1  -6.58524e+2  6.41145e+6
     EQ3/6 database: version mdas.3245
2311803 'CuCl4-2'           0.0000     -4.59            -2.00 4.00 0.00 205.3568
 0.00 2     1.000 231     4.000 180
     2.00790e+3  -1.14231e+5  3.20789e-1  -7.27527e+2  6.68483e+6
     EQ3/6 database: version mdas.3245
2312700 'CuF+1'             0.0000      1.20             1.00 4.00 0.00  82.5444
 0.00 2     1.000 231     1.000 270
     2.24360e+3  -1.25407e+5  3.39001e-1  -8.10787e+2  7.41045e+6
     EQ3/6 database: version mdas.3245
2313300 'CuOH+1'            8.7150     -6.09             1.00 4.00 0.00  80.5533
 0.00 3     1.000 231     1.000 002    -1.000 330
     2.68357e+2  -1.60329e+4  3.94791e-2  -9.67484e+1  6.18453e+5
     Reed and Spycher 1989: SOLVEQ database
2313301 'Cu(OH)2(aq)'       0.0000  -13.7273             0.00 3.00 0.00  97.5607
 0.00 3     1.000 231     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2313302 'Cu(OH)3-1'         0.0000  -27.3132            -1.00 4.00 0.00 114.5680
 0.00 3     1.000 231     3.000 002    -3.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2313303 'Cu(OH)4-2'         0.0000  -40.2614            -2.00 4.00 0.00 131.5754
 0.00 3     1.000 231     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2313304 'Cu2(OH)2+2'       17.9700  -10.4348             2.00 4.50 0.00 161.1067
 0.00 3     2.000 231     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2317320 'CuSO4(aq)'         0.0010      2.30             0.00 3.00 0.00 159.6096
 0.00 2     1.000 231     1.000 732
     5.66162e+2  -3.17754e+4  8.98382e-2  -2.04470e+2  1.94465e+6
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      Reed and Spycher 1989: SOLVEQ database
2317300 'CuS(HS)3-3'          0.0000     18.02            -3.00 4.00 0.00 163.7700
 0.00 3     1.000 231     4.000 730    -1.000 330
      999.  999.  999.  999.  999.
      Shea and Helz 1988
2317301 'CuS(HS)2-2'          0.0000     17.09            -2.00 4.00 0.00 130.6980
 0.00 3     1.000 231     3.000 730    -1.000 330
      999.  999.  999.  999.  999.
      Shea and Helz 1988
2311402 'CuHCO3+1'            0.0000   13.0266             1.00 4.00 0.00 124.5631
 1.00 3     1.000 231     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2307330 'CuSO3-1'             0.0000    7.8078            -1.00 4.00 0.00 143.6102
 0.00 2     1.000 733     1.000 230
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2307331 'Cu(SO3)2-3'          0.0000    8.6107            -3.00 4.00 0.00 223.6744
 0.00 2     1.000 230     2.000 733
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2307332 'Cu(SO3)3-5'          0.0000    9.3437            -5.00 5.00 0.00 303.7386
 0.00 2     1.000 230     3.000 733
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2307340 'Cu(SCN)4-3'        -11.7205    9.9363            -3.00 4.00 0.00 295.8810
 0.00 2     1.000 230     4.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2317340 'CuSCN+1'            -3.0000    2.3309             1.00 4.00 0.00 121.6297
 0.00 2     1.000 231     1.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2317341 'Cu(SCN)2(aq)'        0.0000    3.6803             0.00 3.00 0.00 179.7135
 0.00 2     1.000 231     2.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2311300 'CuBr+1'              0.0000    1.9534             1.00 4.00 0.00 143.4500
 0.00 2     1.000 231     1.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2317321 'Cu(SO4)2-2'          0.0000    1.0467            -2.00 4.00 0.00 255.6732
 0.00 2     1.000 231     2.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2317322 'CuHSO4+2'            0.0000    3.0456             1.00 4.50 0.00 160.6175
 0.00 3     1.000 231     1.000 330     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314920 'CuNO3+1'             0.0000    0.9030             1.00 4.00 0.00 125.5509
 0.00 2     1.000 231     1.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314921 'Cu(NO3)2(aq)'       -1.1280    0.4559             0.00 3.00 0.00 187.5559
 0.00 2     1.000 231     2.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314910 'CuNO2+1'             0.0000    2.8557             1.00 4.00 0.00 109.5515
 0.00 2     1.000 231     1.000 491
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314900 'CuNH3+2'             6.8910   -5.1705             2.00 4.50 0.00  80.5766
 0.00 3     1.000 231     1.000 490    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
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2314901 'Cu(NH3)2+2'        13.8620  -10.9874            2.00 4.50 0.00  97.6071
 0.00 3     1.000 231     2.000 490    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314902 'Cu(NH3)3+2'        20.8330  -17.3981            2.00 4.50 0.00 114.6377
 0.00 3     1.000 231     3.000 490    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314903 'Cu(NH3)4+2'        27.9040  -24.5931            2.00 4.50 0.00 131.6682
 0.00 3     1.000 231     4.000 490    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2314904 'Cu(NH3)5+2'         0.0000  -34.4122            2.00 4.50 0.00 148.6988
 0.00 3     1.000 231     5.000 490    -5.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2315800 'CuPO4-1'            0.0000    6.3674           -1.00 4.00 0.00 158.5174
 0.00 2     1.000 231     1.000 580
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2315801 'Cu(PO4)2-4'         0.0000    9.1418           -4.00 4.00 0.00 253.4887
 0.00 2     1.000 231     2.000 580
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2315802 'CuHPO4(aq)'         0.0000   15.5151            0.00 3.00 0.00 159.5253
 0.00 3     1.000 231     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2315803 'Cu(HPO4)2-2'        0.0000   27.4297           -2.00 4.00 0.00 255.5046
 0.00 3     1.000 231     2.000 580     2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2301301 'CuBr2-1'            0.0000    5.8800           -1.00 4.00 0.00 223.3540
 0.00 2     1.000 230     2.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2303801 'CuI2-1'             0.0000    8.9820           -1.00 4.00 0.00 317.3549
 0.00 2     1.000 230     2.000 380
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2304900 'CuNH3+1'            0.0000   -3.0859            1.00 4.00 0.00  80.5766
 0.00 3     1.000 230     1.000 490    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2304901 'Cu(NH3)2+1'         0.0000   -7.6201            1.00 4.00 0.00  97.6071
 0.00 3     1.000 230     2.000 490    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
1001431 'BaFe(CN)6-1'      -69.6800   55.4356           -1.00 4.00 0.00 349.2804
 0.00 3     1.000 100     1.000 281     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
1501434 'CaHFe(CN)6-'      -82.0000   52.7097           -2.00 4.00 0.00 253.0394
 0.00 5     1.000 150     1.000 330     1.000 280     6.000 143     1.000 001
      999.  999.  999.  999.  999.
      Sehmel (1989)
4101433 'KFe(CN)6-3'       -84.0000   48.1204           -3.00 4.00 0.00 251.0517
 0.00 3     1.000 410     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4101434 'K2Fe(CN)6-2'      -77.3000   48.9780           -2.00 4.00 0.00 290.1500
 0.00 3     2.000 410     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4101435 'KHFe(CN)6-'       -78.1000   51.4702           -2.00 4.00 0.00 252.0597
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 0.00 4     1.000 410     1.000 330     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4401432 'Li2Fe(CN)6-'     -83.4980   48.5338          -2.00 4.00 0.00 225.8354
 0.00 3     2.000 440     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4401433 'LiHFe(CN)6-2'    -80.9990   51.2188          -2.00 4.00 0.00 219.9024
 0.00 4     1.000 440     1.000 330     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4901431 'NH4Fe(CN)6-3'    -84.5000   48.0684          -3.00 4.00 0.00 314.0324
 0.00 3     1.000 490     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4901433 'NH4HFe(CN)6-'    -83.9000   51.4035          -2.00 4.00 0.00 315.0403
 0.00 4     1.000 490     1.000 330     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
5001431 'NaFe(CN)6-3'     -84.9000   47.9885          -3.00 4.00 0.00 234.9432
 0.00 3     1.000 500     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
5001432 'Na2Fe(CN)6-2'    -85.0000   48.7435          -2.00 4.00 0.00 257.9330
 0.00 3     2.000 500     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
5001433 'NaHFe(CN)6-2'    -85.6000   51.4335          -2.00 4.00 0.00 235.9512
 0.00 4     1.000 500     1.000 330     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
4901432 '(NH4)2Fe(CN)6-2' -83.0000   48.8666          -2.00 4.00 0.00 332.0709
 0.00 3     2.000 490     1.000 280     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
0201431 'Ag(CN)OH-'         0.0000   -0.5600          -1.00 4.00 0.00 150.8933
 0.00 4     1.000 143     1.000 020     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
0201432 'Ag(CN)2-'        -32.6750   20.3814          -1.00 4.00 0.00 159.9037
 0.00 2     2.000 143     1.000 020
      999.  999.  999.  999.  999.
      Sehmel (1989)
4101431 'K2H2Fe(CN)6(aq)' -85.8600   52.3058           0.00 3.00 0.00 292.1659
 0.00 4     6.000 143     2.000 410     2.000 330     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
1501431 'CaFe(CN)6-'      -69.5000   55.4730          -1.00 4.00 0.00 252.0314
 0.00 3     6.000 143     1.000 150     1.000 281
      999.  999.  999.  999.  999.
      Sehmel (1989)
1501432 'CaFe(CN)6-2'     -83.1000   49.6898          -2.00 0.00 0.00 252.0314
 0.00 3     6.000 143     1.000 150     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
1501433 'Ca2Fe(CN)6(aq)'  -83.7000   50.9952           0.00 3.00 0.00 292.1094
 0.00 3     6.000 143     2.000 150     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
1601431 'CdCN+'             0.0000    5.3200           1.00 4.00 0.00 138.4287
 0.00 2     1.000 143     1.000 160
      999.  999.  999.  999.  999.
      Sehmel (1989)
1601432 'Cd(CN)2O(aq)'    -13.0000   10.3703           0.00 3.00 0.00 164.4465
 0.00 2     2.000 143     1.000 160
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      999.  999.  999.  999.  999.
      Sehmel (1989)
1601433 'Cd(CN)3-'          -21.6000   14.8341            -1.00 4.00 0.00 190.4642
 0.00 2     3.000 143     1.000 160
      999.  999.  999.  999.  999.
      Sehmel (1989)
1601434 'Cd(CN)4-2'         -23.5600   18.2938            -2.00 4.00 0.00 216.4820
 0.00 2     4.000 143     1.000 160
      999.  999.  999.  999.  999.
      Sehmel (1989)
2301431 'Cu(CN)4-3'         -51.4000   30.3456            -3.00 4.00 0.00 167.6170
 0.00 2     4.000 143     1.000 230
      999.  999.  999.  999.  999.
      Sehmel (1989)
2301432 'Cu(CN)2-'          -29.1000   24.0272            -1.00 4.00 0.00 115.5815
 0.00 2     2.000 143     1.000 230
      999.  999.  999.  999.  999.
      Sehmel (1989)
2301433 'Cu(CN)3-2'         -40.2000   28.6524            -2.00 4.00 0.00 141.5992
 0.00 2     3.000 143     1.000 230
      999.  999.  999.  999.  999.
      Sehmel (1989)
2801431 'Fe(CN)6-4'         -85.8000   45.6063            -4.00 4.00 0.00 211.9534
 0.00 2     6.000 143     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
2801432 'HFe(CN)6-3'        -84.1600   49.9969            -3.00 4.00 0.00 212.9614
 0.00 3     6.000 143     1.000 280     1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
2801433 'H2Fe(CN)6-2'       -83.1000   52.4450            -2.00 0.00 0.00 213.9693
 0.00 3     6.000 143     2.000 330     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
2811431 'Fe(CN)6-3'         -70.1000   52.6283            -3.00 0.00 0.00 211.9534
 0.00 2     6.000 143     1.000 281
      999.  999.  999.  999.  999.
      Sehmel (1989)
3301431 'HCN(aq)'           -10.4000    9.2356             0.00 3.00 0.00  27.0257
 0.00 2     1.000 143     1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
3301441 'HOCN(aq)'           -2.0000    3.4450             0.00 3.00 0.00  43.0251
 0.00 2     1.000 144     1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611431 'HgCN+'             -33.8300   24.1738             1.00 4.00 0.00 226.6077
 0.00 4     1.000 143     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611432 'Hg(CN)2(aq)'       -57.2400   40.6513             0.00 3.00 0.00 252.6255
 0.00 4     2.000 143     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611433 'Hg(CN)3-'          -64.8300   44.4042            -1.00 4.00 0.00 278.6432
 0.00 4     3.000 143     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611434 'Hg(CN)4-2'         -69.9300   47.4094            -2.00 4.00 0.00 304.6610
 0.00 4     4.000 143     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611435 'Hg(CN)2Cl-'          0.0000   40.3735            -1.00 4.00 0.00 288.0782
 0.00 5     2.000 143     1.000 180     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
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      Sehmel (1989)
3611436 'Hg(CN)3Cl-2'       0.0000   43.8332          -2.00 4.00 0.00 314.0959
 0.00 5     3.000 143     1.000 180     1.000 361     2.000 330     -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3611437 'Hg(CN)3Br2-'       0.0000   44.9415          -2.00 4.00 0.00 358.5472
 0.00 5     3.000 143     1.000 130     1.000 361     2.000 330     -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3801432 'I2CN-'             0.0000  -11.8480          -1.00 4.00 0.00 279.8267
 0.00 3     1.000 143     2.000 380    -2.000 001
      999.  999.  999.  999.  999.
      Sehmel (1989)
3801433 'I(CN)2-'           0.0000  -11.4580          -1.00 4.00 0.00 178.9399
 0.00 3     2.000 143     1.000 380    -2.000 001
      999.  999.  999.  999.  999.
      Sehmel (1989)
4101432 'K3HFe(CN)6(aq)'  -85.9900   50.2241           0.00 3.00 0.00 330.2563
 0.00 4     6.000 143     3.000 410     1.000 330     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
4401431 'LiFe(CN)6-3'     -80.1490   47.6858          -3.00 4.00 0.00 218.8944
 0.00 3     6.000 143     1.000 440     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
4601431 'MgFe(CN)6-'      -69.3100   55.3916          -1.00 4.00 0.00 236.2584
 0.00 3     6.000 143     1.000 460     1.000 281
      999.  999.  999.  999.  999.
      Sehmel (1989)
4601432 'MgFe(CN)6-2'       0.0000   49.4251          -2.00 4.00 0.00 236.2584
 0.00 3     6.000 143     1.000 460     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
5401431 'Ni(CN)4-2'       -43.1900   30.1257          -2.00 4.00 0.00 162.7610
 0.00 2     4.000 143     1.000 540
      999.  999.  999.  999.  999.
      Sehmel (1989)
8001431 'SrFe(CN)6-'      -69.8300   55.6181          -1.00 4.00 0.00 299.5734
 0.00 3     1.000 800     1.000 281     6.000 143
      999.  999.  999.  999.  999.
      Sehmel (1989)
8701431 'Tl(CN)4-'          0.0000   -8.0189          -1.00 4.00 0.00 308.4543
 0.00 3     4.000 143     1.000 870    -2.000 001
      999.  999.  999.  999.  999.
      Sehmel (1989)
8701432 'TlFe(CN)6-3'     -84.8800   48.7508          -3.00 4.00 0.00 416.3367
 0.00 3     6.000 143     1.000 870     1.000 280
      999.  999.  999.  999.  999.
      Sehmel (1989)
9501431 'Zn(CN)4-2'       -25.5390   16.7150          -2.00 4.00 0.00 169.4610
 0.00 2     4.000 143     1.000 950
      999.  999.  999.  999.  999.
      Sehmel (1989)
9501432 'Zn(CN)3-'        -20.1990   16.0480          -1.00 4.00 0.00 143.4432
 0.00 2     3.000 143     1.000 950
      999.  999.  999.  999.  999.
      Sehmel (1989)
9501430 'Zn(CN)2(aq)'     -10.9990   11.0710           0.00 3.00 0.00 117.4255
 0.00 2     2.000 143     1.000 950
      999.  999.  999.  999.  999.
      Sehmel (1989)
5401436 'Ni(CN)3-'          0.0000   22.6346          -1.00 4.00 0.00 136.7432
 0.00 2     3.000 143     1.000 540
      999.  999.  999.  999.  999.
      Sehmel (1989)
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5401432 'NiH(CN)4-'          0.0000   36.7482          -1.00 4.00 0.00 163.7689
 0.00 3     4.000 143     1.000 540     1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
5401433 'NiH2(CN)4(aq)'      0.0000   41.4576           0.00 3.00 0.00 164.7768
 0.00 3     4.000 143     1.000 540     2.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
5401434 'NiH3(CN)4+'         0.0000   43.9498           1.00 4.00 0.00 165.7848
 0.00 3     4.000 143     1.000 540     3.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
5401435 'Ni(CN)2(aq)'        0.0000   14.5864           0.00 3.00 0.00 110.7255
 0.00 2     2.000 143     1.000 540
      999.  999.  999.  999.  999.
      Sehmel (1989)
2811432 'Fe2(CN)6(aq)'       0.0000   56.9822           0.00 3.00 0.00 267.8004
 0.00 2     6.000 143     2.000 281
      999.  999.  999.  999.  999.
      Sehmel (1989)
0201440 'Ag(OCN)2-'          0.0000    5.0034          -1.00 4.00 0.00 191.9025
 0.00 2     2.000 144     1.000 020
      999.  999.  999.  999.  999.
      Sehmel (1989)
0201433 'Ag(CN)3-2'        -33.4950   21.4002          -2.00 4.00 0.00 185.9214
 0.00 2     3.000 143     1.000 020
      999.  999.  999.  999.  999.
      Sehmel (1989)
1001430 'BaFe(CN)6-2'        0.0000   49.4032          -2.00 4.00 0.00 349.2804
 0.00 3     6.000 143     1.000 280     1.000 100
      999.  999.  999.  999.  999.
      Sehmel (1989)
1433300 'H-EDTA-3'           0.0000     10.72          -3.00 4.00 0.00 289.0000
 0.00 2     1.000 143     1.000 330
      999.  999.  999.  999.  999.
      Unknown
1433301 'H2-EDTA-2'          0.0000     17.25          -2.00 4.00 0.00 290.0000
 0.00 2     1.000 143     2.000 330
      999.  999.  999.  999.  999.
      Unknown
1433302 'H3-EDTA-1'          0.0000     20.22          -1.00 4.00 0.00 291.0000
 0.00 2     1.000 143     3.000 330
      999.  999.  999.  999.  999.
      Unknown
1433303 'H4-EDTA(aq)'        0.0000     22.39           0.00 3.00 0.00 292.0000
 0.00 2     1.000 143     4.000 330
      999.  999.  999.  999.  999.
      Unknown
2201300 'CsBr(aq)'           0.0000     -0.49           0.00 3.00 0.00 212.8090
 0.00 2     1.000 220     1.000 130
      7.62644e+2  -4.27392e+4  1.13568e-1  -2.75365e+2  2.46407e+6
      EQ6 database: version mdas.3245
2201800 'CsCl(aq)'           0.0000     -0.84           0.00 3.00 0.00 168.3580
 0.00 2     1.000 220     1.000 180
      7.86530e+2  -4.39528e+4  1.18449e-1  -2.84378e+2  2.52469e+6
      EQ6 database: version mdas.3245
2203800 'CsI(aq)'            0.0000     -0.10           0.00 3.00 0.00 259.8094
 0.00 2     1.000 220     1.000 380
      5.95978e+2  -3.24102e+4  9.26498e-2  -2.16392e+2  1.81741e+6
      EQ6 database: version mdas.3245
2803300 'FeOH+1'               13.2    -10.18           1.00 4.50 0.00  72.8543
 0.00 3     1.000 280     1.000 002    -1.000 330
      -7.04221e+1  2.23203e+3  -7.91998e-3  2.36559e+1  -3.03788e+5
      Reed and Spycher 1989: SOLVEQ database
2803302 'Fe(OH)2(aq)'       54.2850    -21.42           0.00 3.00 0.00  89.8617
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 0.00 3     1.000 280     2.000 002    -2.000 330
      -2.63306e+1  -3.86988e+3  -6.89352e-3  9.33506e+0  2.80216e+5
      Reed and Spycher 1989: SOLVEQ database
2803301 'Fe(OH)3-1'         67.6600    -34.22            -1.00 4.00 0.00 106.8690
 0.00 3     1.000 280     3.000 002    -3.000 330
      5.01543e+1  -1.16128e+4  7.16025e-4  -1.85882e+1  3.18024e+4
      Reed and Spycher 1989: SOLVEQ database
2801800 'FeCl+'               0.0000     -0.16             1.00 4.00 0.00  91.3000
 0.00 2     1.000 280     1.000 180
      9.41460e+2  -5.37141e+4  1.46834e-1  -3.40675e+2  3.35402e+6
      EQ3/6 database: version mdas.3245
2801801 'FeCl2(aq)'           0.0000     -2.55             0.00 3.00 0.00 126.7530
 0.00 2     1.000 280     2.000 180
      1.77032e+3  -1.00232e+5  2.79430e-1  -6.42446e+2  6.19418e+6
      EQ3/6 database: version mdas.3245
2801802 'FeCl4-2'             0.0000     -2.00            -2.00 4.00 0.00 162.2060
 0.00 2     1.000 280     4.000 180
      -3.88217e+2  1.87289e+4  -2.47579e-2  1.36306e+2  -5.72269e+5
      EQ3/6 database: version mdas.3245
2814920 'FeNO3+2'             0.0000    1.4513             2.00 4.50 0.00 117.8519
 0.00 2     1.000 281     1.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2807320 'FeSO4(aq)'             3.23      2.25             0.00 3.00 0.00 151.9106
 0.00 2     1.000 280     1.000 732
      3.96144e+3  -2.26022e+5  5.68925e-1  -1.42431e+3  1.36564e+7
      Reed and Spycher 1989: SOLVEQ database
2807321 'FeHSO4+'             0.0000      3.07             1.00 4.00 0.00 152.9166
 0.00 3     1.000 280     1.000 732     1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
2805800 'FeH2PO4+1'           0.0000   22.2439             1.00 4.00 0.00 152.8342
 0.00 3     1.000 280     1.000 580     2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2805801 'FeHPO4(aq)'          0.0000   15.9402             0.00 3.00 0.00 151.8263
 0.00 3     1.000 280     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2807300 'Fe(HS)2(aq)'         0.0000   11.2997             0.00 3.00 0.00 121.9949
 0.00 2     1.000 280     2.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2807301 'Fe(HS)3-1'           0.0000   13.3425            -1.00 4.00 0.00 155.0688
 0.00 2     1.000 280     3.000 730
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2801400 'FeCO3(aq)'           0.0000      4.38             0.00 3.00 0.00 115.8564
 2.00 2     1.000 280     1.000 140
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
2801401 'FeHCO3+'             0.0000     12.33             1.00 4.00 0.00 116.8644
 1.00 3     1.000 280     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
2802700 'FeF+'                0.0000      1.45             1.00 4.00 0.00  74.8450
 0.00 2     1.000 280     1.000 270
      3.10516e+3  -1.78430e+5  4.47162e-1  -1.11596e+3  1.09172e+7
      Reed and Spycher 1989: SOLVEQ database
2815800 'FeHPO4+1'           -8.0040   20.6445             1.00 4.00 0.00 151.8263
 0.00 3     1.000 281     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2817320 'FeSO4+1'               3.91      4.11             1.00 4.00 0.00 151.9106
 0.00 2     1.000 281     1.000 732
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     4.03611e+3  -2.25330e+5  6.11353e-1  -1.45832e+3  1.33311e+7
     EQ3/6 database: version mdas.3245
2817321 'Fe(SO4)2-1'          4.60       5.38            -1.00 4.00 0.00 247.9742
 0.00 2     1.000 281     2.000 732
     5.82271e+3  -3.25370e+5  8.49491e-1  -2.09864e+3  1.89866e+7
     EQ3/6 database: version mdas.3245
2817322 'FeHSO4+2'            0.00       4.47             2.00 4.50 0.00 152.9166
 0.00 3     1.000 281     1.000 732     1.000 330
     999.  999.  999.  999.  999.
     Nordstrom et al. 1990
2811800 'FeCl+2'              5.6        1.48             2.00 4.50 0.00  91.2997
 0.00 2     1.000 281     1.000 180
     2.82834e+3  -1.58407e+5  4.19490e-1  -1.02016e+3  9.21543e+6
     EQ3/6 database: version mdas.3245
2811801 'FeCl2+1'           0.0000       2.13             1.00 4.00 0.00 126.7524
 0.00 2     1.000 281     2.000 180
     3.71383e+3  -2.06737e+5  5.65615e-1  -1.34306e+3  1.21193e+7
     EQ3/6 database: version mdas.3245
2811802 'FeCl3(aq)'         0.0000       1.13             0.00 3.00 0.00 162.2051
 0.00 2     1.000 281     3.000 180
     7.31066e+2  -3.26020e+4  1.66711e-1  -2.77172e+2  1.38230e+6
     EQ3/6 database: version mdas.3245
2811803 'FeCl4-'            0.0000      -0.79            -1.00 4.00 0.00 197.6590
 0.00 2     1.000 281     4.000 180
     5.46927e+3  -3.05483e+5  8.25368e-1  -1.97716e+3  1.78449e+7
     EQ3/6 database: version mdas.3245
2813300 'FeOH+2'              10.4      -2.19             2.00 4.50 0.00  72.8543
 0.00 3     1.000 281     1.000 002    -1.000 330
     1.89655e+3  -1.07136e+5  2.72068e-1  -6.82492e+2  6.05783e+6
     EQ3/6 database: version mdas.3245
2813301 'Fe(OH)2+1'           17.1      -5.67             1.00 4.00 0.00  89.8617
 0.00 3     1.000 281     2.000 002    -2.000 330
     1.83990e+3  -1.04125e+5  2.67479e-1  -6.62920e+2  5.71165e+6
     EQ3/6 database: version mdas.3245
2813302 'Fe(OH)3(aq)'         24.8     -12.02             0.00 3.00 0.00 106.8690
 0.00 3     1.000 281     3.000 002    -3.000 330
     1.21577e+3  -6.54559e+4  2.25579e-1  -4.49231e+2  3.20761e+6
     EQ3/6 database: version mdas.3245
2813303 'Fe(OH)4-1'           31.9     -21.65            -1.00 4.00 0.00 123.8764
 0.00 3     1.000 281     4.000 002    -4.000 330
     1.68383e+3  -9.81284e+4  2.11264e-1  -6.03358e+2  4.76615e+6
     EQ3/6 database: version mdas.3245
2815801 'FeH2PO4+2'         0.0000    23.0194             2.00 4.50 0.00 152.8342
 0.00 3     1.000 281     1.000 580     2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
2812700 'FeF+2'               2.7        6.03             2.00 4.50 0.00  74.8454
 0.00 2     1.000 281     1.000 270
     3.02983e+3  -1.68497e+5  4.50084e-1  -1.09275e+3  9.87287e+6
     EQ3/6 database: version mdas.3245
2812701 'FeF2+1'              4.8       11.58             1.00 4.00 0.00  93.8438
 0.00 2     1.000 281     2.000 270
     4.28135e+3  -2.37695e+5  6.44184e-1  -1.54469e+3  1.40101e+7
     EQ3/6 database: version mdas.3245
2812702 'FeF3(aq)'            5.4       13.89             0.00 3.00 0.00 112.8422
 0.00 2     1.000 281     3.000 270
     2.62003e+3  -1.27431e+5  4.99498e-1  -9.71093e+2  6.68851e+6
     EQ3/6 database: version mdas.3245
2811400 'FeCO3+'            0.0000       9.70             1.00 4.00 0.00 115.8564
 2.00 2     1.000 281     1.000 140
     3.39290e+3  -1.83927e+5  5.35551e-1  -1.23342e+3  1.12017e+7
     EQ3/6 database: version mdas.3245
2813304 'Fe2(OH)2+4'          13.5      -2.95             4.00 5.50 0.00 145.7087
 0.00 3     2.000 281     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
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      Nordstrom et al. 1990
2813305 'Fe3(OH)4+5'          14.3      -6.3            5.00 6.00 0.00 235.5704
 0.00 3     3.000 281     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
2817340 'FeSCN+2'           -1.0880    2.9649           2.00 4.50 0.00 113.9307
 0.00 2     1.000 281     1.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2817341 'Fe(SCN)2+1'         0.0000    5.2965           1.00 4.00 0.00 172.0145
 0.00 2     1.000 281     2.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2817342 'Fe(SCN)3(aq)'       0.0000    6.1967           0.00 3.00 0.00 230.0982
 0.00 2     1.000 281     3.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2807340 'FeSCN+1'            0.0000    1.3120           1.00 4.00 0.00 113.9307
 0.00 2     1.000 280     1.000 734
      999.  999.  999.  999.  999.
      Krupka et al. 1988
2817350 'FeS2O3+1'           8.9000    2.1000           1.00 4.00 0.00 167.9772
 0.00 2     1.000 281     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3600000 'Hg(aq)'           -11.5915    6.5624           0.00 3.00 0.00 200.5900
 0.00 2     0.500 360     1.000 001
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613300 'Hg+2'             -10.8410    6.1409           2.00 4.50 0.00 200.5900
 0.00 3     1.000 361     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611301 'HgBr+'              0.0000   15.8427           1.00 4.00 0.00 280.4940
 0.00 4     1.000 361     1.000 130     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611302 'HgBr2(aq)'        -30.8130   23.6292           0.00 3.00 0.00 360.3980
 0.00 4     1.000 361     2.000 130     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611303 'HgBr3-1'            0.0000   25.8230          -1.00 4.00 0.00 440.3020
 0.00 4     1.000 361     2.000 330     3.000 130    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611304 'HgBr4-2'            0.0000   27.1153          -2.00 4.00 0.00 520.2060
 0.00 4     1.000 361     2.000 330     4.000 130    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611305 'HgBrCl(aq)'         0.0000   22.0335           0.00 3.00 0.00 315.9467
 0.00 5     1.000 361     1.000 130     1.000 180     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611306 'HgBrI(aq)'          0.0000   27.1923           0.00 3.00 0.00 407.3985
 0.00 5     1.000 361     1.000 130     1.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611307 'HgBrI3-2'           0.0000   34.4107          -2.00 4.00 0.00 661.2074
 0.00 5     1.000 361     1.000 130     3.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611308 'HgBrI2-2'           0.0000   32.5482          -2.00 4.00 0.00 614.2069
 0.00 5     1.000 361     2.000 130     2.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
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3611309 'HgBr3I-2'          0.0000   30.2532           -2.00 4.00 0.00 567.2065
 0.00 5     1.000 361     3.000 130     1.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613301 'HgBrOH(aq)'        0.0000   11.6171            0.00 3.00 0.00 297.5013
 0.00 4     1.000 361     1.000 130     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611800 'HgCl+1'          -16.2760   12.8983            1.00 4.00 0.00 236.0427
 0.00 4     1.000 361     1.000 180     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611801 'HgCl2(aq)'       -23.5280   19.3061            0.00 3.00 0.00 271.4954
 0.00 4     1.000 361     2.000 180     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611802 'HgCl3-1'         -24.7810   20.1248           -1.00 4.00 0.00 306.9481
 0.00 4     1.000 361     3.000 180     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611803 'HgCl4-2'         -24.3370   21.2602           -2.00 4.00 0.00 342.4008
 0.00 4     1.000 361     4.000 180     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611804 'HgClI(aq)'         0.0000   25.4206            0.00 3.00 0.00 362.9472
 0.00 5     1.000 361     1.000 180     1.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611805 'HgClOH(aq)'        0.0000   10.1313            0.00 3.00 0.00 253.0500
 0.00 4     1.000 361     1.000 180     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3612701 'HgF+1'           -10.0460    7.7198            1.00 4.00 0.00 219.5884
 0.00 4     1.000 361     1.000 270     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613801 'HgI+1'             0.0000   18.9513            1.00 4.00 0.00 327.4945
 0.00 4     1.000 361     1.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613802 'HgI2(aq)'        -45.3430   30.2275            0.00 3.00 0.00 454.3989
 0.00 4     1.000 361     2.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613803 'HgI3-1'          -49.1720   33.9760           -1.00 4.00 0.00 581.3034
 0.00 4     1.000 361     3.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613804 'HgI4-2'            0.0000   36.0313           -2.00 4.00 0.00 708.2079
 0.00 4     1.000 361     4.000 380     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614900 'HgNH3+2'           0.0000    5.6330            2.00 4.50 0.00 217.6206
 0.00 4     1.000 361     1.000 490     1.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614901 'Hg(NH3)2+2'        0.0000    5.0788            2.00 4.50 0.00 234.6511
 0.00 3     1.000 361     2.000 490    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614902 'Hg(NH3)3+2'        0.0000   -3.1790            2.00 4.50 0.00 251.6817
 0.00 4     1.000 361     3.000 490    -1.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614903 'Hg(NH3)4+2'        0.0000  -11.6347            2.00 4.50 0.00 268.7122
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 0.00 4     1.000 361     4.000 490    -2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614920 'HgNO3+1'           0.0000    6.8981            1.00 4.00 0.00 262.5949
 0.00 4     1.000 361     1.000 492     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3614921 'Hg(NO3)2(aq)'      0.0000    5.6814            0.00 3.00 0.00 324.5999
 0.00 4     1.000 361     2.000 492     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613302 'HgOH+1'           -3.6200    2.5625            1.00 4.00 0.00 217.5973
 0.00 3     1.000 361     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613303 'Hg(OH)3-1'         0.0000  -14.9558           -1.00 4.00 0.00 251.6120
 0.00 3     1.000 361     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613304 'Hg2OH+3'           0.0000    8.9915            3.00 5.00 0.00 418.1873
 0.00 3     2.000 361     3.000 330    -3.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3613305 'Hg3(OH)3+3'        0.0000   12.0415            3.00 5.00 0.00 652.7920
 0.00 3     3.000 361     3.000 330    -3.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3617300 'HgS2-2'            0.0000   31.8343           -2.00 4.00 0.00 264.7220
 0.00 3     1.000 361     2.000 730    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3617301 'Hg(HS)2(aq)'       0.0000   43.8515            0.00 3.00 0.00 266.7379
 0.00 4     1.000 361     2.000 730     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3617320 'HgSO4(aq)'         0.0000    7.5549            0.00 3.00 0.00 296.6536
 0.00 4     1.000 361     1.000 732     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611401 'HgCH3NH2+2'        0.0000   29.3817            2.00 4.50 0.00 231.6474
 0.02 6   1.000 361   1.000 140   1.000 490   6.000 001   9.000 330   -5.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
3611402 'Hg(CH3NH2)2+'    -87.7010   53.2007            2.00 4.50 0.00 262.7049
 0.02 6   1.000 361   2.000 140   2.000 490  12.000 001  16.000 330   -8.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4107320 'KSO4-1'              2.25      0.88           -1.00 4.00 0.00 135.1619
 0.00 2     1.000 410     1.000 732
      1.02908e+3  -5.87054e+4  1.55960e-1  -3.71254e+2  3.63008e+6
      EQ3/6 database: version mdas.3245
4107321 'KHSO4(aq)'         0.0000      0.26            0.00 3.00 0.00 136.1619
 0.00 3     1.000 410     1.000 732     1.000 330
      1.57859e+3  -9.17676e+4  2.42087e-1  -5.68384e+2  5.66278e+6
      EQ3/6 database: version mdas.3245
4103300 'KOH(aq)'           0.0000    -14.50            0.00 3.00 0.00  56.1056
 0.00 3     1.000 410     1.000 002    -1.000 330
      1.27418e+2  -1.00168e+4  1.50793e-2  -4.68937e+1  2.86152e+5
      EQ3/6 database: version mdas.3245
4101800 'KCl(aq)'           0.0000     -2.08            0.00 3.00 0.00  74.5510
 0.00 2     1.000 410     1.000 180
      6.97264e+2  -3.85213e+4  1.10199e-1  -2.53559e+2  2.17000e+6
      EQ3/6 database: version mdas.3245
4101300 'KBr(aq)'           0.0000     -1.74            0.00 3.00 0.00 119.0060
 0.00 2     1.000 410     1.000 130
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     6.90436e+2  -3.84860e+4  1.07816e-1  -2.50627e+2  2.21529e+6
     EQ3/6 database: version mdas.3245
4104920 'KNO3(aq)'          -2.9840    -0.1415             0.00 3.00 0.00 101.1032
 0.00 2     1.000 410     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4105800 'KHPO4-1'            0.0000    12.6323            -1.00 4.00 0.00 135.0776
 0.00 3     1.000 410     1.000 580     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4107350 'KS2O3-1'            0.0000     1.0020            -1.00 4.00 0.00 151.2285
 0.00 2     1.000 410     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4407320 'LiSO4-1'            0.0000     0.64              -1.00 4.00 0.00 103.0046
 0.00 2     1.000 440     1.000 732
     999.  999.  999.  999.  999.
     Nordstrom et al. 1990
4403300 'LiOH(aq)'           0.0000    -13.64              0.00 3.00 0.00  23.9464
 0.00 3     1.000 440     1.000 002    -1.000 330
     999.  999.  999.  999.  999.
     Nordstrom et al. 1990
4603300 'MgOH+1'            15.9350    -11.79              1.00 4.00 0.00  41.3123
 0.00 3     1.000 460     1.000 002    -1.000 330
     5.70148e+3  -3.41682e+5  7.45902e-1 -2.03167e+3  2.11095e+7
     EQ3/6 database: version mdas.3245
4601800 'MgCl+'              0.0000     -0.13              1.00 4.00 0.00  59.7650
 0.00 2     1.000 460     1.000 180
     9.89512e+2  -5.72979e+4  1.53374e-1  -3.57489e+2  3.67899e+6
     EQ3/6 database: version mdas.3245
4602700 'MgF+1'                3.2      1.35              1.00 4.00 0.00  43.3034
 0.00 2     1.000 460     1.000 270
     9.97654e+2  -5.72281e+4  1.52875e-1 -3.59692e+2  3.56374e+6
     EQ3/6 database: version mdas.3245
4601400 'MgCO3(aq)'          2.713      2.98              0.00 3.00 0.00  84.3142
 2.00 2     1.000 460     1.000 140
     9.910e-1  0.0000  6.67e-3  0.0000  0.0000
     Nordstrom et al. 1990.
4601401 'MgHCO3+1'          -2.771     11.40              1.00 4.00 0.00  85.3221
 1.00 3     1.000 460     1.000 140     1.000 330
     8.95566e+1  -5.28234e+3  3.71053e-2  -3.22917e+1  7.46383e+5
     Nordstrom et al. 1990.
4607320 'MgSO4(aq)'          4.55      2.41              0.00 3.00 0.00 120.3686
 0.00 2     1.000 460     1.000 732
     1.30648e+3  -6.73089e+4  2.29421e-1  -4.80032e+2  3.65366e+6
     EQ3/6 database: version mdas.3245
4605800 'MgPO4-1'            3.0960     6.5859            -1.00 4.00 0.00 119.2764
 0.00 2     1.000 460     1.000 580
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4605801 'MgH2PO4+1'         -1.1140    21.0623             1.00 4.00 0.00 121.2922
 0.00 3     1.000 460     1.000 580     2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4605802 'MgHPO4(aq)'        -0.5140    15.2644             0.00 3.00 0.00 120.2843
 0.00 3     1.000 460     1.000 580     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4607350 'MgS2O3(aq)'         0.0000     1.8105             0.00 3.00 0.00 136.4352
 0.00 2     1.000 460     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
4701800 'MnCl+1'             0.0000      0.61              1.00 4.00 0.00  90.3908
 0.00 2     1.000 470     1.000 180
     999.  999.  999.  999.  999.
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      Nordstrom et al. 1990
4701801 'MnCl2(aq)'          0.0000      0.25              0.00 3.00 0.00 125.8435
 0.00 2     1.000 470     2.000 180
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
4701802 'MnCl3-1'            0.0000     -0.31             -1.00 4.00 0.00 161.2962
 0.00 2     1.000 470     3.000 180
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
4703300 'MnOH+1'              14.4    -10.58              1.00 5.00 0.00  71.9454
 0.00 3     1.000 470     1.000 002    -1.000 330
      1.38960e+3 -8.26872e+4  1.95039e-1 -4.99435e+2  4.87370e+6
      Reed and Spycher 1989: SOLVEQ database
4703301 'Mn(OH)3-1'          0.0000  -34.2099            -1.00 4.00 0.00 105.9601
 0.00 3     1.000 470     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4703302 'Mn(OH)2(aq)'        0.0000  -24.6774             0.00 3.00 0.00  88.9527
 0.00 3     1.000 470     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4703303 'Mn(OH)4-1'          0.0000  -48.3161            -2.00 4.00 0.00 122.9674
 0.00 3     1.000 470     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4703304 'Mn2(OH)3+1'         0.0000  -23.8652             1.00 4.00 0.00 160.8981
 0.00 3     2.000 470     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4702700 'MnF+1'              0.0000      1.34             1.00 4.00 0.00  73.9365
 0.00 2     1.000 470     1.000 270
      -2.57232e+3  1.49811e+5 -3.34952e-1  9.18953e+2 -9.13362e+6
      EQ3/6 database: version mdas.3245
4707320 'MnSO4(aq)'          3.3720      2.35             0.00 3.00 0.00 151.0017
 0.00 2     1.000 470     1.000 732
      1.88762e+3 -1.05038e+5  2.87564e-1 -6.82473e+2  6.22415e+6
      EQ3/6 database: version mdas.3245
4704920 'Mn(NO3)2(aq)'       0.0000    0.6032             0.00 3.00 0.00 178.9479
 0.00 2     1.000 470     2.000 492
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4701400 'MnCO3(aq)'          0.0000      4.90             0.00 3.00 0.00 114.9474
 2.00 2     1.000 470     1.000 140
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
4701401 'MnHCO3+1'           0.0000     12.28             1.00 4.00 0.00 115.9552
 1.00 3     1.000 470     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990
4707340 'MnSCN+1'            0.0000    1.0526             1.00 4.00 0.00 113.0218
 0.00 2     1.000 734     1.000 470
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4707341 'Mn(SCN)2(aq)'       0.0000    1.3172             0.00 3.00 0.00 171.1055
 0.00 2     2.000 734     1.000 470
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4707350 'MnS2O3(aq)'         0.0000    1.9519             0.00 3.00 0.00 167.0682
 0.00 2     1.000 470     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4707600 'MnSe(aq)'           0.0000   -6.7413             0.00 3.00 0.00 133.8981
 0.00 3     1.000 760     1.000 470    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
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4707620 'MnSeO4(aq)'          3.4510    2.4284              0.00 3.00 0.00 197.8957
 0.00 2     1.000 762     1.000 470
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803300 'MoO2+2'              0.0000    8.6052              2.00 4.50 0.00 127.9388
 0.00 3     1.000 480     4.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803301 'MoO2(OH)+1'          0.0000    8.1618              1.00 4.00 0.00 144.9461
 0.00 3     1.000 480     3.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803302 'H2MoO4(aq)'          0.0000    8.2241              0.00 3.00 0.00 161.9535
 0.00 2     1.000 480     2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803303 'HMoO4-1'             0.0000    4.2660             -1.00 4.00 0.00 160.9455
 0.00 2     1.000 480     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803304 'Mo7O24-6'            0.0000   58.6461             -6.00 5.00 0.00 1055.566
 0.00 3     7.000 480     8.000 330    -4.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803305 'Mo7O23OH-5'          0.0000   63.0953             -5.00 5.00 0.00 1056.574
 0.00 3     7.000 480     9.000 330    -4.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803306 'Mo7O22(OH)2-4'       0.0000   66.6796             -4.00 5.00 0.00 1057.582
 0.00 3     7.000 480    10.000 330    -4.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803307 'Mo7O21(OH)3-3'       0.0000   69.2670             -3.00 4.00 0.00 1058.589
 0.00 3     7.000 480    11.000 330    -4.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
4803308 'Mo19O59-4'           0.0000  199.1262             -4.00 5.00 0.00 2766.825
 0.00 3    19.000 480    34.000 330   -17.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5001400 'NaCO3-1'               8.91      1.27             -1.00 4.00 0.00  82.9990
 2.00 2     1.000 500     1.000 140
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990 (logK), Krupka et al. 1988 (del H)
5001401 'NaHCO3(aq)'          -6.3700     10.08              0.00 3.00 0.00  84.0069
 1.00 3     1.000 500     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Nordstrom et al. 1990 (logK), Krupka et al. 1988 (del H)
5007320 'NaSO4-1'             1.1210     0.72             -1.00 4.00 0.00 119.0534
 0.00 2     1.000 500     1.000 732
      1.57827e+3  -8.98364e+4  2.28583e-1  -5.68036e+2  5.43918e+6
      Reed and Spycher 1989: SOLVEQ database
5005800 'NaHPO4-1'            0.0000   12.6352             -1.00 4.00 0.00 118.9691
 0.00 3     1.000 500     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5002700 'NaF(aq)'             0.0000     -1.00              0.00 3.00 0.00  41.9882
 0.00 2     1.000 500     1.000 270
      9.04051e+2  -5.09302e+4  1.37420e-1  -3.27126e+2  3.04423e+6
      EQ3/6 database: version mdas.3245
5007350 'NaS2O3-1'            0.0000    0.5813             -1.00 4.00 0.00 135.1200
 0.00 2     1.000 500     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5003300 'NaOH(aq)'            0.0000    -14.18              0.00 3.00 0.00  39.9971
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 0.00 3     1.000 500     1.000 002    -1.000 330
      -5.60875e+2  2.28780e+4  -1.13443e-1  2.09515e+2  -1.30187e+6
      EQ3/6 database: version mdas.3245
5001800 'NaCl(aq)'           0.0000     -0.78             0.00 3.00 0.00  58.4428
 0.00 2     1.000 500     1.000 180
      9.18777e+2  -5.18562e+4  1.39050e-1  -3.32268e+2  3.11852e+6
      EQ3/6 database: version mdas.3245
5007300 'NaHS(aq)'           0.0000     -1.10             0.00 3.00 0.00  56.0618
 0.00 2     1.000 500     1.000 730
      1.24269e+3  -6.98905e+4  1.83456e-1  -4.48614e+2  4.08975e+6
      Reed and Spycher 1989: SOLVEQ database
5401300 'NiBr+1'             0.0000     0.5006            1.00 4.00 0.00 138.5940
 0.00 2     1.000 540     1.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5401800 'NiCl+1'             0.0000     0.4002            1.00 4.00 0.00  94.1427
 0.00 2     1.000 540     1.000 180
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5402700 'NiF+1'              0.0000     1.3032            1.00 4.00 0.00  77.6884
 0.00 2     1.000 540     1.000 270
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403300 'NiOH+1'            12.4150    -9.6585            1.00 0.00 0.00  75.6973
 0.00 3     1.000 540     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403301 'Ni(OH)2(aq)'        0.0000   -18.9843            0.00 3.00 0.00  92.7047
 0.00 3     1.000 540     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403302 'Ni(OH)3-1'          0.0000   -29.9754           -1.00 4.00 0.00 109.7120
 0.00 3     1.000 540     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403303 'Ni(OH)4-2'          0.0000   -43.9791           -2.00 4.00 0.00 126.7194
 0.00 3     1.000 540     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403304 'Ni2OH+3'            0.0000   -10.6979            3.00 5.00 0.00 134.3873
 0.00 3     2.000 540     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5403305 'Ni4(OH)4+4'         0.0000   -27.7361            4.00 5.50 0.00 302.7894
 0.00 3     4.000 540     4.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5407320 'NiSO4(aq)'          3.3410     2.3038            0.00 3.00 0.00 154.7536
 0.00 2     1.000 540     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5401801 'NiCl2(aq)'          0.0000     0.9617            0.00 3.00 0.00 129.5954
 0.00 2     1.000 540     2.000 180
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5401400 'NiHCO3+1'           0.0000    11.9476            1.00 4.00 0.00 119.7071
 1.00 3     1.000 540     1.000 140     1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5401401 'NiCO3(aq)'          0.0000     5.1969            0.00 3.00 0.00 118.6992
 2.00 2     1.000 540     1.000 140
      999.  999.  999.  999.  999.
      Krupka et al. 1988
5401402 'Ni(CO3)2-2'         0.0000    10.1079           -2.00 4.00 0.00 178.7084
 4.00 2     1.000 540     2.000 140
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     999.  999.  999.  999.  999.
     Krupka et al. 1988
5407321 'Ni(SO4)2-2'          0.0000    1.0232            -2.00 4.00 0.00 250.8172
 0.00 2     1.000 540     2.000 732
     999.  999.  999.  999.  999.
     Krupka et al. 1988
5407340 'NiSCN+1'            13.1390    1.6470             1.00 4.00 0.00 116.7737
 0.00 2     1.000 734     1.000 540
     999.  999.  999.  999.  999.
     Krupka et al. 1988
5407350 'NiS2O3(aq)'          0.0000    2.0597             0.00 3.00 0.00 170.8202
 0.00 2     1.000 540     1.000 735
     999.  999.  999.  999.  999.
     Krupka et al. 1988
5407620 'NiSeO4(aq)'          3.5000    2.6607             0.00 3.00 0.00 201.6476
 0.00 2     1.000 762     1.000 540
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6001800 'PbCl+1'              4.3780      1.44             1.00 4.00 0.00 242.6527
 0.00 2     1.000 600     1.000 180
     9.98508e+2  -5.62014e+4  1.55257e-1  -3.61076e+2  3.43086e+6
     EQ3/6 database: version mdas.3245
6001801 'PbCl2(aq)'           1.0800      2.00             0.00 3.00 0.00 278.1054
 0.00 2     1.000 600     2.000 180
     1.65699e+3  -9.23435e+4  2.60093e-1  -6.00284e+2  5.55945e+6
     EQ3/6 database: version mdas.3245
6001802 'PbCl3-1'             2.1720      1.69            -1.00 4.00 0.00 313.5581
 0.00 2     1.000 600     3.000 180
     1.99277e+3  -1.11718e+5  3.11394e-1  -7.21697e+2  6.80568e+6
     EQ3/6 database: version mdas.3245
6001803 'PbCl4-2'             3.5340      1.49            -2.00 4.00 0.00 349.0108
 0.00 2     1.000 600     4.000 180
     1.99771e+3  -1.13651e+5  3.13747e-1  -7.23210e+2  7.19506e+6
     EQ3/6 database: version mdas.3245
6001400 'PbCO3(aq)'           0.0000      9.98             0.00 3.00 0.00 267.2092
 2.00 2     1.000 600     1.000 140
     -6.88193e+3  4.02048e+5  -9.24593e-1  2.46376e+3  -2.46510e+7
     Reed and Spycher 1989: SOLVEQ database
6001401 'Pb(CO3)2-2'          0.0000    9.7934            -2.00 4.00 0.00 327.2184
 4.00 2     1.000 600     2.000 140
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6001402 'PbHCO3+1'            0.0000   13.2311             1.00 4.00 0.00 268.2171
 1.00 3     1.000 600     1.000 140     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6002700 'PbF+1'               0.0000      2.09             1.00 4.00 0.00 226.1984
 0.00 2     1.000 600     1.000 270
     2.92993e+3  -1.67357e+5  4.24550e-1  -1.05387e+3  1.01911e+7
     Reed and Spycher 1989: SOLVEQ database
6002701 'PbF2(aq)'            0.0000    2.5559             0.00 3.00 0.00 245.1968
 0.00 2     1.000 600     2.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6002702 'PbF3-1'              0.0000    3.4194            -1.00 4.00 0.00 264.1952
 0.00 2     1.000 600     3.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6002703 'PbF4-2'              0.0000    3.1027            -2.00 4.00 0.00 283.1936
 0.00 2     1.000 600     4.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003300 'PbOH+1'              0.0000     -7.60             1.00 4.00 0.00 224.2073
 0.00 3     1.000 600     1.000 002    -1.000 330
     2.18189e+2  -1.47019e+4  3.23247e-2  -7.81219e+1  6.39475e+5
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     EQ3/6 database: version mdas.3245
6003301 'Pb(OH)2(aq)'        0.0000  -17.1489            0.00 3.00 0.00 241.2147
 0.00 3     1.000 600     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003302 'Pb(OH)3-1'          0.0000  -28.0689           -1.00 4.00 0.00 258.2220
 0.00 3     1.000 600     3.000 002    -3.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003303 'Pb2OH+3'            0.0000   -6.3425            3.00 5.00 0.00 431.4073
 0.00 3     2.000 600     1.000 002    -1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003304 'Pb3(OH)4+2'        26.4880  -23.3360            2.00 4.50 0.00 689.6294
 0.00 3     3.000 600     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003305 'Pb(OH)4-2'          0.0000  -39.6977           -2.00 4.00 0.00 275.2294
 0.00 3     1.000 600     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003306 'Pb4(OH)4+4'        20.0840  -19.2599            4.00 5.50 0.00 896.8294
 0.00 3     4.000 600     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6004920 'PbNO3+1'            0.0000    1.5107            1.00 4.00 0.00 269.2049
 0.00 2     1.000 600     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6007320 'PbSO4(aq)'          0.0000    2.7516            0.00 3.00 0.00 303.2636
 0.00 2     1.000 600     1.000 732
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6007321 'Pb(SO4)2-2'         0.0000    1.9549           -2.00 4.00 0.00 399.3272
 0.00 2     1.000 600     2.000 732
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6007300 'Pb(HS)2(aq)'        0.0000     13.84            0.00 3.00 0.00 273.3479
 0.00 2     1.000 600     2.000 730
     6.11091e+3  -3.70987e+5  7.59448e-1  -2.16058e+3  2.37377e+7
     Reed and Spycher 1989: SOLVEQ database
6007301 'Pb(HS)3-1'          0.0000     15.92           -1.00 4.00 0.00 306.4218
 0.00 2     1.000 600     3.000 730
     1.77048e+3  -9.80861e+4  2.51791e-1  -6.35288e+2  6.34102e+6
     Reed and Spycher 1989: SOLVEQ database
6007302 'PbH(HS)3(aq)'       0.0000     23.08            0.00 3.00 0.00 307.4140
 0.00 3     1.000 600     3.000 730     1.000 330
     6.73695e+3  -3.81214e+5  9.70070e-1  -2.42117e+3  2.36950e+7
     Reed and Spycher 1989: SOLVEQ database
6001300 'PbBr+1'             0.0000    1.1053            1.00 4.00 0.00 287.1040
 0.00 2     1.000 600     1.000 130
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6001301 'PbBr2(aq)'          0.0000    1.4454            0.00 3.00 0.00 367.0080
 0.00 2     1.000 600     2.000 130
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003800 'PbI+1'              0.0000    1.9263            1.00 4.00 0.00 334.1045
 0.00 2     1.000 600     1.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
6003801 'PbI2(aq)'           0.0000    3.0705            0.00 3.00 0.00 461.0089
 0.00 2     1.000 600     2.000 380
     999.  999.  999.  999.  999.
     Krupka et al. 1988
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6005800 'PbHPO4(aq)'          0.0000   15.4557            0.00 3.00 0.00 303.1793
 0.00 3     1.000 600     1.000 330     1.000 580
      999.  999.  999.  999.  999.
      Krupka et al. 1988
6005801 'PbH2PO4+1'           0.0000   21.0264            1.00 4.00 0.00 304.1872
 0.00 3     1.000 600     2.000 330     1.000 580
      999.  999.  999.  999.  999.
      Krupka et al. 1988
6007340 'PbSCN+1'             0.2960    0.8898            1.00 4.00 0.00 265.2837
 0.00 2     1.000 734     1.000 600
      999.  999.  999.  999.  999.
      Krupka et al. 1988
7403300 'SbO+1'               0.0000    1.1803            1.00 4.00 0.00 137.7494
 0.00 3     1.000 740     1.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
7403301 'SbO2-1'              0.0000  -11.8030           -1.00 4.00 0.00 153.7488
 0.00 3     1.000 740    -1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Sehmel (1989)
7402700 'SbOF(aq)'            0.0000    6.684             0.00 3.00 0.00 156.7478
 0.00 4     1.000 330     1.000 740     1.000 270    -2.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
7402702 'Sb(OH)2F(aq)'        0.0000    6.695             0.00 3.00 0.00 174.7630
 0.00 4     1.000 740     1.000 270     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
7407300 'Sb2S4-2'           -75.6801   49.2867            -2.00 4.00 0.00 371.7400
 0.00 4     2.000 740     4.000 730     2.000 330    -6.000 002
      999.  999.  999.  999.  999.
      Sehmel (1989)
3307601 'Se-2'                0.0000   -14.96             -1.00 4.00 2.00  79.9600
 0.00 2     1.000 760    -1.000 330
      8.93176e+2  -6.45447e+4  9.75464e-2  -3.11918e+2  4.54110e+6
      EQ3/6 database: version mdas.3245
3307600 'H2Se(aq)'            0.7890    3.80              0.00 3.00 0.00  80.9759
 0.00 2     1.000 760     2.000 330
      2.95859e+3  -1.63538e+5  4.77155e-1  -1.07513e+3  9.93768e+6
      EQ3/6 database: version mdas.3245
3307611 'SeO3-2'              1.2800    -7.29             -2.00 4.00 2.00 126.9582
 0.00 2     1.000 761    -1.000 330
      -8.1811e+2  4.64456e+4  -1.29542e-1  2.93997e+2  -3.00537e+6
      EQ3/6 database: version mdas.3245
3307610 'H2SeO3(aq)'          1.6900    2.57              0.00 3.00 0.00 128.9741
 0.00 2     1.000 761     1.000 330
      2.61100e+3  -1.34917e+5  4.31854e-1  -9.56554e+2  7.31215e+6
      EQ3/6 database: version mdas.3245
3307620 'HSeO4-1'             4.0900    1.91              -1.00 4.00 1.00 143.9655
 0.00 2     1.000 762     1.000 330
      7.62796e+2  -4.22713e+4  1.18805e-1  -2.75519e+2  2.41934e+6
      EQ3/6 database: version mdas.3245
2817610 'FeHSeO3+2'           0.0000    1.8610            2.00 4.50 0.00 183.8131
 0.00 2     1.000 761     1.000 281
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507620 'ZnSeO4(aq)'          0.0000    2.2591            0.00 3.00 0.00 208.3476
 0.00 2     1.000 762     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507621 'Zn(SeO4)2-2'         0.0000    0.0088           -2.00 4.00 0.00 351.3052
 0.00 2     2.000 762     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
6703300 'RaOH+'               0.0000   -13.49             1.00 4.00 0.00 243.0574
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 0.00 3     1.000 670     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
     Nordstrom et al. 1990
6701400 'RaCO3(aq)'           1.07       2.5             0.00 3.00 0.00 326.0594
 2.00 2     1.000 670     1.000 140
      999.  999.  999.  999.  999.
     Nordstrom et al. 1990
6707320 'RaSO4(aq)'           1.3        2.75            0.00 3.00 0.00 362.1116
 0.00 2     1.000 670     1.000 732
      999.  999.  999.  999.  999.
     Nordstrom et al. 1990
3307700 'H3SiO4-1'            6.12      -9.83           -1.00 4.00 1.00  95.1069
 0.00 2     1.000 770    -1.000 330
     -3.023724e+2  1.566969e+4  -5.0698e-2  1.0818466e+2  -1.119669e+6
     Nordstrom et al. 1990
3307701 'H2SiO4-2'            17.6      -23.0           -2.00 4.00 2.00  94.0990
 0.00 2     1.000 770    -2.000 330
     -2.940184e+2  1.120449e+4  -7.02650e-2  1.0818466e+2  -1.119669e+6
     Nordstrom et al. 1990
3307702 'Si4O6(OH)6-2'        0.0000   -13.3257          -2.00 4.00 2.00 310.3824
 0.00 3     4.000 770    -2.000 330    -4.000 002
      999.  999.  999.  999.  999.
     Krupka et al. 1988
7702700 'SiF6-2'             -16.26      26.27           -2.00 4.00 0.00 142.0759
 0.00 4     1.000 770     6.000 270     4.000 330    -4.000 002
     3.78324e+3  -2.15440e+5  5.57602e-1 -1.35657e+3  1.38766e+7
     EQ3/6 database: version mdas.3245
8003300 'SrOH+1'            14.4950    -13.18            1.00 4.00 0.00 104.6273
 0.00 3     1.000 800     1.000 002    -1.000 330
     1.04013e+3  -6.23874e+4  1.42215e-1  -3.74204e+2  3.50919e+6
     Reed and Spycher 1989: SOLVEQ database
8007320 'SrSO4(aq)'           2.08       2.30            0.00 3.00 0.00 183.6836
 0.00 2     1.000 800     1.000 732
     6.64796e+2  -3.15405e+4  1.31700e-1  -2.47918e+2  1.55401e+6
     EQ3/6 database: version mdas.3245
8001400 'SrHCO3+1'            2.489      11.51           1.00 4.00 0.00 148.6371
 1.00 3     1.000 800     1.000 140     1.000 330
     1.56841e+2  -8.51454e+3  5.34418e-2  -5.72342e+1  7.92311e+5
     Nordstrom et al. 1990
8001401 'SrCO3(aq)'           5.22       2.81            0.00 3.00 0.00 147.6292
 2.00 2     1.000 800     1.000 140
     -1.019e+0  0.0000  1.2826e-2  0.0000  0.0000
     Nordstrom et al. 1990
8001800 'SrCl+'               0.0000     -0.25           1.00 4.00 0.00 123.0730
 0.00 2     1.000 800     1.000 180
     8.71526e+2  -4.92651e+4  1.38376e-1  -3.15935e+2  3.01891e+6
     EQ3/6 database: version mdas.3245
8002700 'SrF+'                0.0000     0.14            1.00 4.00 0.00 106.6184
 0.00 2     1.000 800     1.000 270
     9.10754e+2  -5.19130e+4  1.41686e-1  -3.29365e+2  3.22211e+6
     EQ3/6 database: version mdas.3245
8007350 'SrS2O3(aq)'          0.0000     2.0384          0.00 3.00 0.00 199.7502
 0.00 2     1.000 800     1.000 735
      999.  999.  999.  999.  999.
     Krupka et al. 1988
8503300 'Th(OH)+3'            0.000      -3.20           3.00 5.00 0.00 249.0454
 0.00 3    -1.000 330     1.000 850     1.000 002
      999.  999.  999.  999.  999.
     Langmuir and Herman (1980)
8503301 'Th(OH)2 +2'          0.000      -6.93           2.00 4.50 0.00 266.0527
 0.00 3    -2.000 330     1.000 850     2.000 002
      999.  999.  999.  999.  999.
     Langmuir and Herman (1980)
28503302 'Th2(OH)2+6'         0.0000     -6.14           6.00 5.50 0.00 498.0907
 0.00 3    -2.000 330     2.000 850     2.000 002
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      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8502700 'ThF+3'              0.0000      8.03              3.00 5.00 0.00 251.0364
 0.00 2     1.000 850     1.000 270
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8502701 'ThF2+2'             0.0000     14.25              2.00 4.50 0.00 270.0348
 0.00 2     1.000 850     2.000 270
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8502702 'ThF3+1'             0.0000     18.93              1.00 4.00 0.00 289.0332
 0.00 2     1.000 850     3.000 270
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8502703 'ThF4(aq)'           0.0000     22.31              0.00 3.00 0.00 308.0316
 0.00 2     1.000 850     4.000 270
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8501800 'ThCl+3'             0.0000      1.09              3.00 5.00 0.00 267.4910
 0.00 2     1.000 850     1.000 180
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8501801 'ThCl2+2'            0.0000      0.80              2.00 4.50 0.00 302.9440
 0.00 2     1.000 850     2.000 180
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8501802 'ThCl3+1'            0.0000      1.65              1.00 4.00 0.00 338.3970
 0.00 2     1.000 850     3.000 180
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8507320 'ThSO4+2'            0.0000      5.45              2.00 4.50 0.00 328.0996
 0.00 2     1.000 850     1.000 732
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8507321 'Th(SO4)(aq)'        0.0000      9.73              0.00 3.00 0.00 424.0996
 0.00 2     1.000 850     2.000 732
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8507322 'Th(SO4)3-2'         0.0000     10.50             -2.00 4.00 0.00 520.2228
 0.00 2     1.000 850     3.000 732
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8507322 'Th(SO4)4-4'         0.0000      8.48             -4.00 4.00 0.00 616.2854
 0.00 2     1.000 850     4.000 732
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8504920 'ThNO3+3'            0.0000      0.94              3.00 5.00 0.00 294.0429
 0.00 2     1.000 850     1.000 492
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8504921 'Th(NO3)2+2'         0.0000      1.97              2.00 4.50 0.00 356.0478
 0.00 2     1.000 850     2.000 492
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8505800 'ThH2PO4+3'          0.0000     24.07              3.00 5.00 0.00 329.0271
 0.00 3     1.000 850     1.000 580     2.000 330
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8505801 'Th(H2PO4)2+2'       0.0000     47.98              2.00 4.50 0.00 426.0127
 0.00 3     1.000 850     2.000 580     4.000 330
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8505802 'ThH3PO4+4'          0.0000     23.61              4.00 5.00 0.00 330.0334
 0.00 3     1.000 850     1.000 580     3.000 330
      999.  999.  999.  999.  999.
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      Langmuir and Herman (1980)
8505803 'ThHPO4+2'          0.0000     23.14            2.00 4.50 0.00 328.0174
 0.00 3     1.000 850     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8505804 'Th(HPO4)2(aq)'     0.0000     47.49            0.00 3.00 0.00 423.9968
 0.00 3     1.000 850     2.000 580     2.000 330
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8505805 'Th(HPO4)3-2        0.0000     68.33           -2.00 4.00 0.00 519.9762
 0.00 3     1.000 850     3.000 580     3.000 330
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8503303 'Th(OH)3+1'         0.0000    -11.70            1.00 4.00 0.00 283.0601
 0.00 3    -3.000 330     1.000 850     3.000 002
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8503304 'Th(OH)4(aq)'       0.0000    -15.90            0.00 3.00 0.00 300.0675
 0.00 3    -4.000 330     1.000 850     4.000 002
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8503305 'Th4(OH)8+8'        0.0000    -21.10            8.00 5.50 0.00 1064.211
 0.00 3    -8.000 330     4.000 850     8.000 002
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8503306 'Th6(OH)15+9'       0.0000    -36.76            9.00 5.50 0.00 1647.339
 0.00 3   -15.000 330     6.000 850     15.000 002
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8501803 'ThCl4(aq)'         0.0000      1.16            0.00 3.00 0.00 338.3970
 0.00 2     1.000 850     4.000 180
      999.  999.  999.  999.  999.
      Langmuir and Herman (1980)
8703300 'TlOH(aq)'         13.9350   -13.1717           0.00 3.00 0.00 221.3773
 0.00 3     1.000 870     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8702700 'TlF(aq)'           0.0000    -0.4251           0.00 3.00 0.00 223.3684
 0.00 2     1.000 870     1.000 270
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8701800 'TlCl(aq)'         -1.1470     0.6824           0.00 3.00 0.00 239.8230
 0.00 2     1.000 870     1.000 180
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8701801 'TlCl2-1'           0.0000     0.2434          -1.00 4.00 0.00 275.2760
 0.00 2     1.000 870     2.000 180
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8701300 'TlBr(aq)'         -2.4610     0.9477           0.00 3.00 0.00 284.2740
 0.00 2     1.000 870     1.000 130
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8701301 'TlBr2-1'           2.9980     0.9719          -1.00 4.00 0.00 364.1780
 0.00 2     1.000 870     2.000 130
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8701302 'TlBrCl-1'          0.0000     0.8165          -1.00 4.00 0.00 319.7270
 0.00 3     1.000 870     1.000 130     1.000 180
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8703800 'TlI(aq)'           0.0000     1.4279           0.00 3.00 0.00 331.2745
 0.00 2     1.000 870     1.000 380
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
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8703801 'TlI2-1'            0.0000    1.8588            -1.00 4.00 0.00 458.1790
 0.00 2     1.000 870     2.000 380
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8703802 'TlIBr-1'           0.0000    2.1850            -1.00 4.00 0.00 411.1785
 0.00 3     1.000 870     1.000 380     1.000 130
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8707320 'TlSO4-1'           -0.2200   1.3853            -1.00 4.00 0.00 300.4276
 0.00 2     1.000 870     1.000 732
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8704920 'TlNO3(aq)'         -0.6500   0.3665             0.00 3.00 0.00 266.3749
 0.00 2     1.000 870     1.000 492
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8704910 'TlNO2(aq)'         0.0000    0.9969             0.00 3.00 0.00 250.3755
 0.00 2     1.000 870     1.000 491
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8707300 'TlHS(aq)'          0.0000    1.8178             0.00 3.00 0.00 237.4379
 0.00 2     1.000 870     1.000 730
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8707301 'Tl2HS+1'           0.0000    7.6979             1.00 4.00 0.00 441.8079
 0.00 2     2.000 870     1.000 730
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8707302 'Tl2OH(HS)3-'       0.0000    1.0044            -2.00 4.00 0.00 524.9510
 0.00 4     2.000 870     3.000 730     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8707303 'Tl2(OH)2(HS)2-2'   0.0000  -11.0681            -2.00 4.00 0.00 508.8904
 0.00 4     2.000 870     2.000 730     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8713300 'Tl+3'              0.0000    4.7424             3.00 5.00 0.00 204.3700
 0.00 3     1.000 871     3.000 330    -3.000 002
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8713301 'TlOH+2'            0.0000    3.5770             2.00 4.50 0.00 221.3773
 0.00 3     1.000 871     2.000 330    -2.000 002
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8713302 'Tl(OH)2+1'         0.0000    2.1183             1.00 4.00 0.00 238.3846
 0.00 3     1.000 871     1.000 330    -1.000 002
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711800 'TlCl+2'            0.0000   12.2342             2.00 4.00 0.00 239.8230
 0.00 4     1.000 871     1.000 180     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711801 'TlCl2+1'           0.0000   18.0402             1.00 4.00 0.00 275.2760
 0.00 4     1.000 871     2.000 180     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
711802 'TlCl3(aq)'          0.0000   21.4273               0.00 3.00 0.00 310.7290
 0.00 4     1.000 871     3.000 180     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711803 'TlCl4-1'           0.0000   24.2281            -1.00 4.00 0.00 346.1820
 0.00 4     1.000 871     4.000 180     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711300 'TlBr+2'            0.0000   14.2221             2.00 4.50 0.00 284.2740
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 0.00 4     1.000 871     1.000 130     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711301 'TlBr2+1'            0.0000   21.5761           1.00 4.00 0.00 364.1780
 0.00 4     1.000 871     2.000 130     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711302 'TlBr3(aq)'          0.0000   27.0244           0.00 3.00 0.00 444.0820
 0.00 4     1.000 871     3.000 130     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711303 'TlBr4-1'            0.0000   31.1533          -1.00 4.00 0.00 523.9860
 0.00 4     1.000 871     4.000 130     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8713800 'TlI4-1'             0.0000   34.7596          -1.00 4.00 0.00 711.9880
 0.00 4     1.000 871     4.000 380     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8714920 'TlNO3+2'            0.0000    7.0073           2.00 4.50 0.00 266.3749
 0.00 4     1.000 871     1.000 492     3.000 330    -3.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8713303 'Tl(OH)4-1'          0.0000  -10.2545          -1.00 4.00 0.00 272.3992
 0.00 3     1.000 871     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8711804 'TlOHCl+1'           0.0000   10.6290           1.00 4.00 0.00 256.8303
 0.00 4     1.000 871     1.000 180     2.000 330    -2.000   2
      999.  999.  999.  999.  999.
      Deutsch and Krupka (1985)
8913300 'UOH+3'                11.715     -0.66           3.00 5.00 0.00 255.0364
 0.00 3     1.000 891     1.000 002    -1.000 330
      -7.7213e+3  -1.4536e+1  8.9328e-3  2.4202e+5  1.0269e+2
      NEA (1989), EQ3/6 database: version mdas.3245
8913301 'U(OH)2+2'             17.730     -2.25           2.00 4.50 0.00 272.0437
 0.00 3    -2.000 330     1.000 891     2.000   2
      -9.1223e+3  -1.7463e+1  1.2796e-2  1.7625e+5  1.2205e+2
      NEA (1989), EQ3/6 database: version mdas.3245
8913302 'U(OH)3+1'             22.645     -4.88           1.00 4.00 0.00 289.0511
 0.00 3     1.000 891     3.000 002    -3.000 330
      -7.1444e+3  -1.2193e+1  1.0960e-2  -6.6363e+4  8.6037e+1
      NEA (1989), EQ3/6 database: version mdas.3245
8913303 'U(OH)4(aq)'           24.760     -8.53           0.00 3.00 0.00 306.0586
 0.00 3     1.000 891     4.000   2    -4.000 330
      -1.5817e+5  -4.5755e+2  4.7482e-1  8.7252e+6  2.8892e+3
      NEA (1989), EQ3/6 database: version mdas.3245
8913304 'U(OH)5-1'             27.575    -16.50          -1.00 4.00 0.00 323.0659
 0.00 3     1.000 891     5.000 002    -5.000 330
      2.8116e+3  1.9646e+1  -4.5239e-2  -1.1922e+6  -1.1095e+2
      EQ3/6 database: version mdas.3245
8912700 'UF+3'                 5.050      8.63           3.00 5.00 0.00 257.0274
 0.00 2     1.000 891     1.000 270
      -7.0038e+4  -1.9478e+2  1.8768e-1  4.1074e+6  1.2511e+3
      NEA (1989), EQ3/6 database: version mdas.3245
8912701 'UF2+2'                7.200     14.48           2.00 4.50 0.00 276.0258
 0.00 2     1.000 891     2.000 270
      -1.3599e+5  -3.8224e+2  3.7385e-1  7.9989e+6  2.4470e+3
      NEA (1989), EQ3/6 database: version mdas.3245
8912702 'UF3+1'                7.150     19.15           1.00 4.00 0.00 295.0242
 0.00 2     1.000 891     3.000 270
      -2.0755e+5  -5.8533e+2  5.7485e-1  1.2305e+7  3.7404e+3
      NEA (1989), EQ3/6 database: version mdas.3245
8912703 'UF4(aq)'              4.600     23.68           0.00 3.00 0.00 314.0226
 0.00 2     1.000 891     4.000 270
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     -2.9047e+5  -9.0590e+2  9.9490e-1 1.6066e+7  5.6820e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8912704 'UF5-1'              4.850     25.28           -1.00 4.00 0.00 333.0210
 0.00 2     1.000 891     5.000 270
     -3.2573e+5  -9.2198e+2  8.9183e-1  1.9231e+7  5.8885e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8912705 'UF6-2'              3.300     27.75           -2.00 4.00 0.00 352.0194
 0.00 2     1.000 891     6.000 270
     -3.9402e+5  -1.1190e+3  1.0924e+0  2.3358e+7  7.1364e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8911800 'UCl+3'              9.933     1.33             3.00 5.00 0.00 273.4820
 0.00 2     1.000 891     1.000 180
     -5.8147e+4  -1.5897e+2  1.5562e-1  3.3375e+6  1.0181e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8917320 'USO4+2'             3.700     5.46             2.00 4.50 0.00 334.0906
 0.00 2     1.000 891     1.000 732
     -1.1580e+5  -3.2819e+2  3.3136e-1  6.9608e+6  2.0866e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8917321 'U(SO4)2(aq)'        7.600     9.75             0.00 3.00 0.00 430.1522
 0.00 2     1.000 891     2.000 732
     -2.5921e+5  -7.6796e+2  7.9007e-1  1.4746e+7  4.8532e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8915800 'UHPO4+2'            7.500     24.30            2.00 4.50 0.00 334.0084
 0.00 3     1.000 891     1.000 580     1.000 330
     -5.7210e+4  -1.4810e+2  1.5969e-1  3.8064e+6  9.6954e+2
     NEA (1989), EQ3/6 database: version mdas.3245
8915801 'U(HPO4)2(aq)'       1.700     46.62            0.00 3.00 0.00 429.9877
 0.00 3     1.000 891     2.000 580     2.000 330
     -3.9768e+5  -1.1902e+3  1.26630e+0  2.3077e+7  7.5248e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8915802 'U(HPO4)3-2'        -7.800     67.55           -2.00 0.00 0.00 525.9671
 0.00 3     1.000 891     3.000 580     3.000 330
     -1.3118e+5  -3.6456e+2  4.2390e-1  9.1823e+6  2.3549e+3
     NEA (1989), EQ3/6 database: version mdas.3245
8915803 'U(HPO4)4-4'        -26.500     87.90           -4.00 4.00 0.00 621.9465
 0.00 3     1.000 891     4.000 580     4.000 330
     -1.8094e+5  -5.0753e+2  5.8319e-1  1.2948e+7  3.2669e+3
     EQ3/6 database: version mdas.3245
8933300 'UO2OH+1'            0.0000     -5.2             1.00 4.00 0.00 287.0352
 0.00 3     1.000 893     1.000 002    -1.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933301 'UO2(OH)2(aq)'       0.0000     -12.0            0.00 3.00 0.00 304.0420
 0.00 3     1.000 893     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933302 'UO2(OH)3-1'         0.0000     -20.0           -1.00 4.00 0.00 321.0500
 0.00 3     1.000 893     3.000 002    -3.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933303 'UO2(OH)4-2'        0.00000     -33.0           -2.00 4.00 0.00 338.0570
 0.00 3     1.000 893     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933304 '(UO2)2(OH)+3'       0.0000     -2.8             3.00 5.00 0.00 574.0703
 0.00 3     2.000 893     1.000 002    -1.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933305 '(UO2)2(OH)2+2'      0.0000     -5.63            2.00 4.50 0.00 574.0703
 0.00 3     2.000 893     2.000 002    -2.000 330
     999.  999.  999.  999.  999.
     NEA 1989
8933306 '(UO2)3(OH)4+2'      0.0000     -11.9            2.00 4.50 0.00 878.1130
 0.00 3     3.000 893     4.000 002    -4.000 330
     999.  999.  999.  999.  999.
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      NEA 1989
8933307 '(UO2)3(OH)5+1'      0.0000    -15.56            1.00 4.00 0.00 895.1203
 0.00 3     3.000 893     5.000 002    -5.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8933308 '(UO2)3(OH)7-1'      0.0000     -31.            -1.00 4.00 0.00 929.1350
 0.00 3     3.000 893     7.000 002    -7.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8933309 '(UO2)4(OH)7+1'      0.0000     -21.9           1.00 4.00 0.00 1199.1620
 0.00 3     4.000 893     7.000 002    -7.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8931400 'UO2CO3(aq)'         0.0000      9.65            0.00 3.00 0.00 330.0372
 2.00 2     1.000 893     1.000 140
     -1.2933e+5  -3.4370e+2  3.2122e-1  8.2635e+6  2.2130e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8931401 'UO2(CO3)2-2'        0.0000     17.07           -2.00 4.00 0.00 390.0465
 4.00 2     1.000 893     2.000 140
     -3.2424e+5  -8.5855e+2  7.8720e-1  2.0589e+7  5.5299e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8931402 'UO2(CO3)3-4'        0.0000     21.69           -4.00 4.00 0.00 450.0559
 6.00 2     1.000 893     3.000 140
     -4.5908e+5  -1.2263e+3  1.1298e+0  2.9336e+7  7.8817e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8932700 'UO2F+1'           -0.450          5.08            1.00 4.00 0.00 289.0262
 0.00 2     1.000 893     1.000 270
     -6.3929e+4  -1.8474e+2  1.8649e-1  3.8003e+6  1.1737e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8932701 'UO2F2(aq)'        -0.900          8.84            0.00 3.00 0.00 308.0246
 0.00 2     1.000 893     2.000 270
     -6.3066e+4  -2.1037e+2  2.4658e-1  3.3397e+6  1.3079e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8932702 'UO2F3-1'          -0.850          11.24           -1.00 4.00 0.00 327.0230
 0.00 2     1.000 893     3.000 270
     -1.8293e+5  -5.2137e+2  4.9492e-1  1.0674e+7  3.3277e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8932703 'UO2F4-2'          -1.100         12.43           -2.00 4.00 0.00 346.0214
 0.00 2     1.000 893     4.000 270
     -2.5208e+5  -7.2128e+2  7.0262e-1  1.4852e+7  4.5909e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8931800 'UO2Cl+1'           1.233          0.23            1.00 4.00 0.00 305.4808
 0.00 2     1.000 893     1.000 180
     -5.5368e+4  -1.5774e+2  1.6056e-1  3.3291e+6  9.9935e+2
      NEA 1989, EQ3/6 database: version mdas.3245
8937320 'UO2SO4(aq)'        5.100          2.75            0.00 3.00 0.00 366.0894
 0.00 2     1.000 893     1.000 732
     -6.5580e+4  -2.0327e+2  2.2541e-1  3.5631e+6  1.2736e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8937321 'UO2(SO4)2-2'         6.100      4.25           -2.00 4.00 0.00 462.1510
 0.00 2     1.000 893     2.000 732
     -2.2978e+5  -6.4871e+2  6.3610e-1  1.3647e+7  4.1278e+3
      NEA 1989, EQ3/6 database: version mdas.3245
8935800 'UO2HPO4(aq)'        -2.100     20.81            0.00 3.00 0.00 366.0072
 0.00 3     1.000 893     1.000 580     1.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8935801 'UO2(HPO4)2-2'      -11.399     42.99           -2.00 4.00 0.00 461.9865
 0.00 3     1.000 893     2.000 580     2.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8935802 'UO2H2PO4+1'         -3.700    22.643            1.00 4.00 0.00 367.0151
 0.00 3     1.000 893     1.000 580     2.000 330
      999.  999.  999.  999.  999.
      NEA 1989
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8935803 'UO2(H2PO4)2(aq)'    -16.5     44.70          0.00 3.00 0.00 464.0020
 0.00 3     1.000 893     2.000 580     4.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8935804 'UO2(H2PO4)3-1'      -28.6     66.25         -1.00 4.00 0.00 560.9890
 0.00 3     1.000 893     3.000 580     6.000 330
      999.  999.  999.  999.  999.
      NEA 1989
8937700 'UO2H3SiO4+1'         0.0000    -2.4          1.00 4.00 0.00 365.1350
 0.00 3     1.000 893     1.000 770    -1.000 330
      999.  999.  999.  999.  999.
      NEA 1989
9003300 'VOH+1'               0.0000   -5.6257        1.00 4.00 0.00  67.9488
 0.00 3     1.000 900     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9013300 'VOH+2'               0.0000   -2.2466        2.00 4.50 0.00  67.9488
 0.00 3     1.000 901     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9013301 'V(OH)2+1'            0.0000   -5.8272         1.00 4.00 0.00  84.9562
 0.00 3     1.000 901     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9013302 'V(OH)3(aq)'          0.0000  -10.9398        0.00 3.00 0.00 101.9635
 0.00 3     1.000 901     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9017320 'VSO4+1'              0.0000    1.4315        1.00 4.00 0.00 147.0051
 0.00 2     1.000 901     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9013303 'V2(OH)3+3'           0.0000   -7.5094        3.00 5.00 0.00 152.9050
 0.00 3     2.000 901     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9013304 'V2(OH)2+4'           0.0000   -3.7749        4.00 5.50 0.00 135.8977
 0.00 3     2.000 901     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9023300 'V(OH)3+1'            0.0000   -5.6440        1.00 4.00 0.00 101.9635
 0.00 3     1.000 902     2.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9023301 'H2V2O4+2'            0.0000   -6.3990        2.00 4.50 0.00 167.8965
 0.00 3     2.000 902     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9022700 'VOF+1'               1.9000    3.8687        1.00 4.00 0.00  85.9393
 0.00 2     1.000 902     1.000 270
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9022701 'VOF2(aq)'            3.5000    6.7845        0.00 3.00 0.00 104.9377
 0.00 2     1.000 902     2.000 270
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9022702 'VOF3-1'              4.9000    8.8501       -1.00 4.00 0.00 123.9361
 0.00 2     1.000 902     3.000 270
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9022703 'VOF4-2'              6.4000   10.1826       -2.00 4.00 0.00 142.9345
 0.00 2     1.000 902     4.000 270
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9027320 'VOSO4(aq)'           4.1210    2.4650        0.00 3.00 0.00 163.0045
```

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 0.00 2     1.000 902     1.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9021800 'VOCl+1'            0.0000    0.0337            1.00 4.00 0.00 102.3936
 0.00 2     1.000 902     1.000 180
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033305 'H4VO4+1'           0.0400    0.0147            1.00 4.00 0.00 118.9709
 0.00 2     1.000 903     2.000 002
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033300 'H3VO4(aq)'        10.6202   -3.2618            0.00 3.00 0.00 117.9629
 0.00 3     1.000 903     2.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033301 'H2VO4-1'          11.3470   -7.0902           -1.00 3.00 1.00 116.9550
 0.00 3     1.000 903     2.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033302 'HVO4-2'           14.9300  -15.1508           -2.00 4.00 2.00 115.9470
 0.00 3     1.000 903     2.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033303 'VO4-3'             0.0000  -28.4251           -3.00 4.00 3.00 114.9391
 0.00 3     1.000 903     2.000 002    -4.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9023302 'VOOH+1'            0.0000   -5.6550            1.00 4.00 0.00  83.9482
 0.00 3     1.000 902     1.000 002    -1.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9033304 'VO3-1'            11.3150   -7.1063           -1.00 4.00 0.00  98.9397
 0.00 3     1.000 903     1.000 002    -2.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030020 'V2O7-4'            0.0000  -29.0445           -4.00 4.00 4.00 213.8788
 0.00 3     2.000 903     3.000 002    -6.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030021 'HV2O7-3'           0.0000  -16.3302           -3.00 4.00 3.00 214.8867
 0.00 3     2.000 903     3.000 002    -5.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030022 'H3V2O7-1'          0.0000   -3.7866           -1.00 0.00 1.00 216.9026
 0.00 3     2.000 903     3.000 002    -3.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030023 'V3O9-3'            0.0000  -15.8508           -3.00 4.00 0.00 296.8191
 0.00 3     3.000 903     3.000 002    -6.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030024 'V4O12-4'           0.0000  -20.7435           -4.00 4.00 0.00 395.7588
 0.00 3     4.000 903     4.000 002    -8.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030025 'V10O28-6'          0.0000  -17.4450           -6.00 4.00 0.00 957.3982
 0.00 3    10.000 903     8.000 002   -16.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030026 'HV10O28-5'        21.7200  -11.4346           -5.00 4.00 0.00 958.4061
 0.00 3    10.000 903     8.000 002   -15.000 330
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9030027 'H2V10O28-4'        0.0000   -7.7696           -4.00 4.00 0.00 959.4141
 0.00 3    10.000 903     8.000 002   -14.000 330
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     999.  999.  999.  999.  999.
     Krupka et al. 1988
9032700 'VO2F(aq)'          0.0000    3.6415            0.00 3.00 0.00 101.9387
 0.00 2     1.000 903     1.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9032701 'VO2F2-1'           0.0000    6.7112           -1.00 4.00 0.00 120.9371
 0.00 2     1.000 903     2.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9032702 'VO2F3-2'           0.0000    8.5275           -2.00 4.00 0.00 139.9355
 0.00 2     1.000 903     3.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9032703 'VO2F4-3'           0.0000    9.1491           -3.00 4.00 0.00 158.9339
 0.00 2     1.000 903     4.000 270
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9037320 'VO2SO4-1'          0.0000    1.7247           -1.00 4.00 0.00 179.0039
 0.00 2     1.000 903     1.000 732
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9034920 'VO2NO3(aq)'        0.0000    0.0293            0.00 3.00 0.00 144.9452
 0.00 2     1.000 903     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9504920 'ZnNO3+1'           0.0000    0.3973            1.00 4.00 0.00 127.3949
 0.00 2     1.000 950     1.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9504921 'Zn(NO3)2(aq)'      0.0000   -0.2991            0.00 3.00 0.00 189.3999
 0.00 2     1.000 950     2.000 492
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9505800 'ZnHPO4(aq)'        0.0000   14.7161            0.00 3.00 0.00 161.3693
 0.00 3     1.000 950     1.000 580     1.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9505801 'ZnH2PO4+1'         0.0000   20.7266            1.00 4.00 0.00 162.3772
 0.00 3     1.000 950     1.000 580     2.000 330
     999.  999.  999.  999.  999.
     Krupka et al. 1988
9501800 'ZnCl+1'            7.7930      0.46            1.00 4.00 0.00 100.8427
 0.00 2     1.000 950     1.000 180
     -1.44418e+2  1.03861e+4  1.98468e-2  4.42372e+1  -4.74379e+5
     Bourcier and Barnes, 1983
9501801 'ZnCl2(aq)'         8.5000      0.48            0.00 3.00 0.00 136.2954
 0.00 2     1.000 950     2.000 180
     2.82381e+3  -1.69427e+5  4.02199e-1  -1.00962e+3  1.09580e+7
     Bourcier and Barnes, 1983
9501802 'ZnCl3-1'           9.5570      0.33           -1.00 4.00 0.00 171.7481
 0.00 2     1.000 950     3.000 180
     -1.24165e+3  7.50921e+4  -1.27076e-1  4.37294e+2  -4.80474e+6
     Bourcier and Barnes, 1983
9501803 'ZnCl4-2'          10.9590      0.11           -2.00 4.00 0.00 207.2008
 0.00 2     1.000 950     4.000 180
     -7.80601e+3  4.73376e+5  -9.57839e-1  2.76557e+3  -3.01579e+7
     Bourcier and Barnes, 1983
9502700 'ZnF+1'             1.9810      1.15            1.00 4.00 0.00  84.3884
 0.00 2     1.000 950     1.000 270
     2.75343e+3  -1.54068e+5  4.09645e-1  -9.94052e+2  9.07207e+6
     Reed and Spycher 1989: SOLVEQ database
9503300 'ZnOH+1'           13.3960     -8.96            1.00 4.00 0.00  82.3973
 0.00 3     1.000 950     1.000 002    -1.000 330
     6.27653e+0  -3.28558e+3  6.35388e-4  -1.89907e+0  2.60831e+4
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      Bourcier and Barnes, 1983
9503301 'Zn(OH)2(aq)'        0.0000    -18.42             0.00 3.00 0.00  99.4047
 0.00 3     1.000 950     2.000 002    -2.000 330
    -1.10576e+1 -3.08326e+3 -5.85311e-4 1.33963e+0 -1.42589e+4
      Bourcier and Barnes, 1983
9503302 'Zn(OH)3-1'          0.0000    -29.90            -1.00 4.00 0.00 116.4120
 0.00 3     1.000 950     3.000 002    -3.000 330
      -8.79825e+1 -2.46464e+3 -2.68683e-2 3.20056e+1 -4.29809e+5
      Bourcier and Barnes 1983
9503303 'Zn(OH)4-2'          0.0000    -42.71            -2.00 4.00 0.00 133.4194
 0.00 3     1.000 950     4.000 002    -4.000 330
      -1.83528e+1 -1.02956e+4 -3.56461e-2 8.97994e+0 -1.25943e+5
      Bourcier and Barnes, 1983
9507300 'Zn(HS)2(aq)'        0.0000     13.13             0.00 3.00 0.00 131.5379
 0.00 2     1.000 950     2.000 730
      4.66631e+4  -2.87488e+6  5.91673e+0  -1.65320e+4  1.89854e+8
      Hayashi et al. 1990
9507301 'Zn(HS)3-1'          0.0000     15.13            -1.00 4.00 0.00 164.5860
 0.00 2     1.000 950     3.000 730
      -1.68590e+4  1.07843e+6  -1.98413e+0  5.92792e+3  -7.28580e+7
      Hayashi et al. 1990
9507302 'Zn(HS)4-2'          0.0000     15.03            -2.00 4.00 0.00 197.6580
 0.00 2     1.000 950     4.000 730
      2.82817e+3  -1.70536e+5  3.83553e-1  -1.00470e+3  1.16046e+7
      Hayashi et al. 1990
9507303 'ZnOH(HS)2-1'        0.0000      7.04            -1.00 4.00 0.00 148.5453
 0.00 4     1.000 950     1.000 002     2.000 730    -1.000 330
      -3.38370e+4  2.11611e+6  -4.19013e+0  1.19566e+4  -1.41328e+8
      Hayashi et al. 1990
9507304 'ZnOH(HS)3-2'        0.0000      6.54            -2.00 4.00 0.00 181.5933
 0.00 4     1.000 950     1.000 002     3.000 730    -1.000 330
      6.54000e+0  5.37000e+0  4.83000e+0  5.61435e-1  1.23118e+5
      Hayashi et al. 1990
9507320 'ZnSO4(aq)'          3.6920      2.32             0.00 3.00 0.00 161.4536
 0.00 2     1.000 950     1.000 732
      6.19723e+2  -3.51627e+4  9.76016e-2  -2.23554e+2  2.18714e+6
      Reed and Spycher 1989: SOLVEQ database
9507321 'Zn(SO4)2-2'         0.0000     3.2823           -2.00 4.00 0.00 257.5172
 0.00 2     1.000 950     2.000 732
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9501300 'ZnBr+1'             0.0000    -0.5813            1.00 4.00 0.00 145.2940
 0.00 2     1.000 950     1.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9501301 'ZnBr2(aq)'          0.0000    -0.9771            0.00 3.00 0.00 225.1980
 0.00 2     1.000 950     2.000 130
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9503800 'ZnI+1'              0.0000    -2.9136            1.00 4.00 0.00 192.2945
 0.00 2     1.000 950     1.000 380
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9503801 'ZnI2(aq)'           0.0000    -1.6822            0.00 4.00 0.00 319.1989
 0.00 2     1.000 950     2.000 380
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9501400 'ZnHCO3+1'           0.0000     11.75             1.00 4.00 0.00 126.4071
 1.00 3     1.000 950     1.000 140     1.000 330
      2.92030e+3  -1.65531e+5  4.41600e-1  -1.05124e+3  1.03308e+7
      Reed and Spycher 1989: SOLVEQ database
9501401 'ZnCO3(aq)'          0.0000     4.7659            0.00 3.00 0.00 125.3992
 2.00 2     1.000 950     1.000 140
      999.  999.  999.  999.  999.
      Krupka et al. 1988
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9501402 'Zn(CO3)2-2'          0.0000    9.6329          -2.00 4.00 0.00 185.4084
 4.00 2     1.000 950     2.000 140
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507340 'ZnSCN+1'             0.2210    1.5026           1.00 4.00 0.00 123.4737
 0.00 2     1.000 734     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507341 'Zn(SCN)2(aq)'        0.0000    0.9214           0.00 3.00 0.00 181.5575
 0.00 2     2.000 734     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507342 'Zn(SCN)3-1'          0.0000    1.9981          -1.00 4.00 0.00 239.6412
 0.00 2     3.000 734     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507343 'Zn(SCN)4-2'          0.0000    1.2923          -2.00 4.00 0.00 297.7250
 0.00 2     4.000 734     1.000 950
      999.  999.  999.  999.  999.
      Krupka et al. 1988
9507350 'ZnS2O3(aq)'          3.1010    2.2884           0.00 3.00 0.00 177.5202
 0.00 2     1.000 950     1.000 735
      999.  999.  999.  999.  999.
      Krupka et al. 1988
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0000000
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APPENDIX E

COMPLETE LISTING OF THE SOLIDS.DAT(4.00) DATA FILE

APPENDIX E

COMPLETE LISTING OF THE SOLIDS.DAT(4.00) DATA FILE

```
SOLIDS.DAT:  Thermochemical data for Solid Species
File History:
Date       Version   Person   Action
9-20-91     4.00     T. Eary  A four-line database created for use by both
                              the GM and MINTEQ geochemical models. Data
                              included are as follows.
                              Line 1: ID#, name, del H(rxn), logK(25C), charge,
                                      ion size (angstroms), noncarbonate
                                      alkalinity factor, and molecular wt.
                              Line 2: carbonate alkalinity factor, number of
                                      reactants in formation reaction,
                                      reaction stoichiometry and species ID
                                      number (same as in old GM and MINTEQ)
                              Line 3: Coefficients for temperature dependence
                                      of the log K i.e., log K = a0 + a1/T +
                                      a2*T + a3*log(T) + a4/T**2 where T is
                                      in degrees K.  Values of 999. indicate
                                      no temperature data available.  In such
                                      cases, the enthalpy of reaction, if
                                      available, will be used to calculate
                                      log K values for temperatures other than
                                      25 C using the Van't Hoff equation.  If
                                      the enthalpy of reaction is absent, then
                                      the codes will default to the 25C-logK
                                      value.
                               Line 4: Reference for source of data.  Full
                                       citations are given at the bottom of
                                       the file.

                               Note:   All data is read in FREE FORMAT with all
                                       names as 18 character length strings.
STOP.
Version 4.00
0073000 'Sulfur'            4.2070    2.1161                          32.0660
  3     1.000 730    -1.000 330    -2.000 001
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    S(rhombic)
0002000 'Ag(metal)'        -25.2750   13.5060                         107.8682
  2     1.000 020     1.000 001
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag(metal)
4002000 'Bromyrite'        -20.2130   12.2694                         187.7722
  2     1.000 020     1.000 130
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgBr
4102000 'Cerargyrite'      -15.6930    9.7502                         143.3209
  2     1.000 020     1.000 180
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgCl
5002000 'Ag2CO3'            -9.6000   11.0695                         275.7456
  2     2.000 020     1.000 140
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2CO3
4202000 'AgF:4H2O'          -4.3250   -0.5615                         198.9277
  3     1.000 020     1.000 270     4.000 002
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgF:4H2O
4302000 'Iodyrite'         -26.8640   16.0670                         234.7727
  2     1.000 020     1.000 380
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  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgI
2002000 'Ag2O'            10.3440  -12.5678                          231.7358
  3    -2.000 330     2.000 020     1.000 002
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2O
2002001 'AgO'             40.1370  -30.4533                          123.8676
  4    -2.000 330     1.000 020     1.000 002    -1.000 001
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgO
7002000 'Ag3PO4'           0.0000   17.5425                          418.5760
  2     3.000 020     1.000 580
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag3PO4
1002000 'Acanthite'       -54.1320    36.04                           247.8024
  3    -1.000 330     2.000 020     1.000 730
  8.80098e+2  -3.62311e+4  1.38745e-1  -3.21458e+2  2.80159e+6
  EQ3/6 database: version mdas.3245     Ag2S
1002001 'Proustite'        0.0000    78.76                           494.7176
  4     3.000 020     3.000 730     1.000 060    -3.000 002
  4.40861e+3  -2.31349e+5  6.37660e-1  -1.58609e+3  1.60623e+7
  Reed and Spycher 1989: SOLVEQ database  Ag3AsS3
6002000 'Ag2SO4'           -4.3290    4.9147                          311.8000
  2     2.000 020     1.000 732
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2SO4
1002002 'Ag2SO3'          -15.9640   13.8175                          295.8006
  2     2.000 020     1.000 733
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2SO3
1002001 'AgSCN'           -22.5350   11.9850                          165.9519
  2     1.000 020     1.000 734
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    AgSCN
1202000 'Naumannite'      -64.9500   43.6654                          294.6964
  3     1.000 760     2.000 020    -1.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2Se(alpha)
6102000 'Ag2SeO3'          -9.4700    8.2175                          342.6946
  3     1.000 761     2.000 020    -1.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2SeO3
6102001 'Ag2SeO4'         -10.4600    8.9292                          358.6940
  2     1.000 762     2.000 020
  999. 999. 999. 999. 999.
  Krupka et al. 1988                    Ag2SeO4
2003001 'Boehmite'         26.1940    -8.43                            59.9883
  3    -3.000 330     1.000 030     2.000 002
  5.90327e+2  -3.76085e+4  8.99270e-2  -2.10225e+2  1.84488e+6
  EQ3/6 database: version mdas.3245     AlOOH
2003002 'Diaspore'         24.3940    -7.59                            59.9883
  3    -3.000 330     1.000 030     2.000 002
  5.81978e+2  -3.67364e+4  8.87944e-2  -2.07448e+2  1.82092e+6
  EQ3/6 database: version mdas.3245     AlOOH
2003003 'Gibbsite(c)'        22.8     -8.11                            78.0036
  3    -3.000 330     1.000 030     3.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990 (crystalline)   Al(OH)3
2003005 'Gibbsite(uc)'       24.5     -9.35                            78.0036
  3    -3.000 330     1.000 030     3.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al.1990(microcrystalline)  Al(OH)3
2003000 'Al(OH)3(am)'        26.5     -10.8                            78.0036
  3    -3.000 330     1.000 030     3.000 002
  999.  999.  999.  999.  999.
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  Nordstrom et al. 1990                    Al(OH)3
6003001 'Alunite'            50.25       1.4                                414.2142
  5     1.000 410     3.000 030     2.000 732     6.000 002    -6.000 330
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                    KAl3(SO4)2(OH)6
6003002 'Jurbanite'          0.0000      3.8                                230.1289
  4    -1.000 330     1.000 030     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                    Al(SO4)(OH):5H2O
6003000 'AlOHSO4'            0.0000    3.2300                               140.0525
  4    -1.000 330     1.000 030     1.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1998                       AlOHSO4
6003001 'Basaluminite'       0.0000   -22.5000                              374.0632
  4   -10.000 330     4.000 030     1.000 732    10.000 002
  999.  999.  999.  999.  999.
  Nordstrom 1982                           Al4(SO4)(OH)10:5H2O
6003002 'Al2(SO4)3'          0.0000    -17.34                               342.1478
  2     2.000 030     3.000 732
  4.03342e+3  -2.40311e+5  6.64438e-1  -1.45453e+3  1.38921e+7
  EQ3/6 database: version mdas.3245        Al2(SO4)3
6003003 'Al2(SO4)3:6H2O'     0.0000      0.02                               450.2402
  3     2.000 030     3.000 732     6.000 002
  5.58796e+3  -3.21225e+5  8.64448e-1  -2.01352e+3  1.90246e+7
  EQ3/6 database: version mdas.3245        Al2(SO4)3:6H2O
6041000 'Alum-K'            -7.2200      5.74                               474.3904
  4     1.000 410     1.000 030     2.000 732    12.000 002
  4.13778e+3  -2.18043e+5  6.78201e-1  -1.51283e+3  1.24845e+7
  EQ3/6 database: version mdas.3245        KAl(SO4)2:12H2O
4250000 'Cryolite'           -9.09     33.84                               209.9413
  3     1.000 030     3.000 500     6.000 270
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       Na3AlF6
3006000 'Arsenolite'        -7.1850      1.46                               197.8414
  2     2.000 060    -3.000 002
  -1.52901e+2  9.27998e+3  -2.86049e-2  5.54944e+1  -4.93569e+5
  Reed and Spycher 1989: SOLVEQ database  As2O3(cubic)
3006001 'Claudetite'        -6.6650      1.32                               197.8414
  2     2.000 060    -3.000 002
  1.22322e+2  -7.06897e+3  7.36151e-3  -4.26809e+1  5.44557e+7
  Reed and Spycher 1989: SOLVEQ database  As2O3(mono)
3006100 'As2O5'              0.0000     -8.18                               229.8402
  2     2.000 061    -3.000 002
  5.92620e+3  -3.55529e+5  7.75626e-1  -2.11157e+3  2.23807e+7
  Reed and Spycher 1989: SOLVEQ database  As2O5
4306000 'AsI3'              -1.8920    -4.1575                              455.6350
  4     1.000 060     3.000 380     3.000 330    -3.000 002
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       AsI3
1006000 'Orpiment'         -82.8790    60.9689                              246.0412
  4     2.000 060     3.000 730     3.000 330    -6.000 002
  3.71682e+3  -2.03916e+5  5.38922e-1  -1.33479e+3  1.39110e+7
  Reed and Spycher 1989: SOLVEQ database  As2S3
1006001 'Realgar'            0.0000    20.8578                              106.9876
  5     1.000 060     1.000 730     2.000 330     1.000 001    -3.000 002
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       AsS
7203000 'AlAsO4:2H2O'        0.0000    -3.6649                              201.9313
  4     1.000 030     1.000 061     2.000 002    -3.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       AlAsO4:2H2O
7215000 'Ca3(AsO4)2:4H2O'    0.0000   -21.4669                              470.1335
  4     3.000 150     2.000 061     4.000 002    -6.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       Ca3(AsO4)2:4H2O
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7215001 'Ca3(AsO4)2'        32.2070  -22.7350                          398.0724
  3     3.000 150     2.000 061     -6.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      Ca3(AsO4)2
7223100 'Cu3(AsO4)2.6H2O'    0.0000   -4.6574                          576.5681
  4     3.000 231     2.000 061     6.000 002     -6.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      Cu3(AsO4)2:6H2O
7210000 'Ba3(AsO4)2'          0.0000    -23.18                         695.9062
  3     3.000 100     2.000 061     -6.000 330
  999.  999.  999.  999.  999.
  Robins 1985
2010000 'BaO'                 0.0000    -47.80                         153.3394
  3     1.000 100     1.000 002     -2.000 330
  3.88331e+2  -3.60608e+4  5.70315e-2  -1.40260e+2  1.32116e+6
  EQ3/6 database: version mdas.3245       BaO
4210000 'BaF2'               -1.0010    6.7369                         175.3238
  2     1.000 100     2.000 270
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      BaF
6010000 'Barite'              -6.35      9.97                          233.3906
  2     1.000 100     1.000 732
  -1.36035e+2  7.68041e+3  0.0000  4.8595e+1  0.0000
  Nordstrom et al. 1990                   BaSO4
5010000 'Witherite'          -0.703     8.562                          197.3362
  2     1.000 100     1.000 140
  -6.07642e+2  -1.21098e-1  2.001125e+4  2.364948e+2  0.0000
  Nordstrom et al. 1990                   BaCO3
1010000 'BaSO3'              -1.5120    8.8640                         217.3912
  2     1.000 100     1.000 733
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      BaSO3
1010001 'BaS2O3'              0.0000    4.7886                         249.4572
  2     1.000 100     1.000 735
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      BaS2O3
5295000 'Zn(BO2)2'            0.0000   -8.2886                         151.0096
  4    -2.000 002    -2.000 330     1.000 950     2.000 090
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      Zn(BO2)2
5260000 'Pb(BO2)2'            6.3580   -7.6692                         292.8196
  4    -2.000 002    -2.000 330     1.000 600     2.000 090
  999. 999. 999. 999. 999.
  Krupka et al. 1988                      Pb(BO2)2
6015002 'Ettringite'         88.2870  -58.7011                        1255.1072
  5   -12.000 330     6.000 150     2.000 030    38.000 002     3.000 732
  999. 999. 999. 999. 999.
  Krupka et al. 1988:                     Ca6Al2(SO4)3(OH)12:6H2O
5015000 'Aragonite'           2.589     8.336                          100.0872
  2     1.000 150     1.000 140
  1.719773e+2  -2.903293e+3  7.7993e-2  -7.1595e+1  0.0000
  Nordstrom et al. 1990                   CaCO3
5015001 'Calcite'             2.297     8.48                           100.0872
  2     1.000 150     1.000 140
  1.719065e+2  -2.839319e+3  7.7993e-2  -7.1595e+1  0.0000
  Nordstrom et al. 1990                   CaCO3
5015002 'Vaterite'            0.000     7.73                           100.0872
  2     1.000 150     1.000 140
  999.  999.  999.  999.  999.
  Robie et al. 1978                       CaCO3
4215000 'Fluorite'           -4.69      10.6                            78.0748
  2     1.000 150     2.000 270
  -6.6348e+1  4.2982e+3  0.0000  2.5271e+1  0.0000
  Nordstrom et al. 1990                   CaF2
6015000 'Anhydrite'           1.71      4.36                           136.1416
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  2     1.000 150     1.000 732
  -1.9752e+2  8.6698e+3  0.0000  6.9835e+1  0.0000
  Nordstrom et al. 1990                    CaSO4
6015001 'Gypsum'              0.109      4.58                              172.1722
  3     1.000 150     1.000 732     2.000 002
  -6.82401e+1  3.22151e+3  0.0000  2.50627e+1  0.0000
  Nordstrom et al. 1990                    CaSO4:2H2O
2015000 'Lime'              46.2640    -32.58                               56.0774
  3    -2.000 330     1.000 150     1.000 002
  4.57072e+2  -3.56860e+4  6.61520e-2  -1.64378e+2  1.51569e+6
  EQ3/6 database: version mdas.3245        CaO
2015001 'Portlandite'         31.0    -22.56                               74.0927
  3    -2.000 330     1.000 150     2.000 002
  4.24572e+2  -2.97871e+4  6.25954e-2  -1.53774e+2  1.29873e+6
  EQ3/6 database: version mdas.3245        Ca(OH)2
4115000 'Antarcticite'        0.0000   -4.1216                             219.0751
  3     1.000 150     2.000 180     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CaCl2:6H2O
4115001 'CaCl2:4H2O'          0.0000   -5.6997                             183.0445
  3     1.000 150     2.000 180     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CaCl2:4H2O
4115002 'Ca4Cl2(OH)6:19H2O' 0.0000  -68.7012                             567.4601
  4     4.000 150     2.000 180    19.000 002    -6.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Ca4Cl2(OH)6:19H2O
4115003 'Ca2Cl2(OH)2:3H2O'  0.0000  -26.5223                             203.0914
  4     2.000 150     2.000 180     3.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Ca2Cl2(OH)2:3H2O
5015005 'Gaylussite'          0.0000    9.4423                             296.1523
  4     1.000 150     2.000 500     2.000 140     5.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988: CaNa2(CO3)2:5H2O     CaNa2(CO3)2:5H2O
6050005 'Glauberite'          0.0000    5.2694                             278.1847
  3     2.000 500     1.000 150     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Na2Ca(SO4)2
6050006 'Labile-Salt'         0.0000    5.7165                             456.2584
  4     4.000 500     1.000 150     3.000 732     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Na4Ca(SO4)3:2H2O
5050004 'Pirssonite'          0.0000    9.2576                             242.1065
  4     2.000 500     1.000 150     2.000 140     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Na2Ca(CO3)2:2H2O
6041011 'Syngenite'           0.0000    7.2045                             328.4171
  4     2.000 410     1.000 150     2.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       K2Ca(SO4)2:H2O
7015003 'Hydroxyapatite'   38.9380     40.03                               502.3114
  4     5.000 150     3.000 580     1.000 002    -1.000 330
  8.34132e+3  -4.70345e+5  1.31607e+0  -3.00494e+3  2.83896e+7
  EQ3/6 database: version mdas.3245        Ca4(PO4)3(OH)
7015004 'Fluorapatite'     14.1270   59.0265                               504.3025
  3     5.000 150     3.000 580     1.000 270
  9.00668e+3  -5.01875e+5  1.42257e+0  -3.24533e+3  3.06459e+7
  EQ3/6 database: version mdas.3245        Ca4(PO4)3F
1015001 'CaSO3:0.5H2O'        3.2965     6.64                               129.1498
  3     1.000 150     1.000 733     0.500 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988 (H): Rai  1991a (K)  CaSO3:0.5H2O
0016000 'Cd(alpha)'           18.0000  -13.4935                             112.4110
  2     1.000 160     2.000 001
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd(alpha)
0016001 'Cd(gamma)'        18.1410  -13.5969                          112.4110
  2     1.000 160     2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd(gamma)
5016000 'Otavite'           0.5830    12.24                           172.4202
  2     1.000 160     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988 (H): Rai 1991b (K)   CdCO3
4116000 'CdCl2'             4.4740    0.6765                          183.3164
  2     1.000 160     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdCl2
4116001 'CdCl2:H2O'         1.8190    1.7130                          201.3317
  3     1.000 160     2.000 180     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdCl2:H2O
4116002 'CdCl2:2.5H2O'     -1.7075    1.9362                          228.3546
  3     1.000 160     2.000 180     2.500 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdCl2:2.5H2O
4216000 'CdF2'              9.7210    2.9803                          150.4078
  2     1.000 160     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdF2
2016001 'Cd(OH)2(c)'        0.0000    -13.86                          146.4257
  3    -2.000 330     1.000 160     2.000 002
  999.  999.  999.  999.  999.
  Rai et al. 1991c                      Cd(OH)2(c)
4116003 'CdOHCl'            7.4070   -3.5154                          164.8710
  4    -1.000 330     1.000 160     1.000 002     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdOHCl
6016000 'Cd3(OH)4SO4'       0.0000  -22.5261                          501.3260
  4    -4.000 330     3.000 160     4.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd3(OH)4(SO4)
6016001 'Cd3(OH)2(SO4)2'    0.0000   -6.7024                          563.3749
  4    -2.000 330     3.000 160     2.000 002     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd3(OH)2(SO4)2
6016002 'Cd4(OH)6(SO4)'     0.0000  -28.4010                          647.7516
  4    -6.000 330     4.000 160     6.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd4(OH)6(SO4)
2016002 'Monteponite'      24.7450  -15.1259                          128.4104
  3    -2.000 330     1.000 160     1.000 002
  3.55497e+2  -2.44962e+4  4.92981e-2  -1.27254e+2  1.04452e+6
  EQ3/6 database: version mdas.3245     CdO
7016000 'Cd3(PO4)2'         0.0000   32.5958                          527.1757
  2     3.000 160     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd3(PO4)2
8216000 'CdSiO3'           14.5770   -7.5556                          188.4947
  4    -1.000 002     1.000 160     1.000 770    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdSiO3
6016003 'CdSO4'            12.4030    0.1012                          208.4746
  2     1.000 160     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdSO4
6016004 'CdSO4:H2O'         7.5170    1.6573                          226.4899
  3     1.000 160     1.000 732     1.000 002
  999.  999.  999.  999.  999.
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  Krupka et al. 1988                    CdSO4:H2O
6016005 'CdSO4:2.7H2O'      4.5260    1.7282                          256.5754
  3     1.000 160     1.000 732     2.670 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdSO4:2.7H2O
1016000 'Greenockite'     -16.3520   15.9329                          144.4770
  3    -1.000 330     1.000 160     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdS
4016000 'CdBr2:4H2O'       -7.2270    2.4159                          344.2801
  3     1.000 160     2.000 130     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdBr2:4H2O
4316000 'CdI2'             -4.0670    3.6129                          366.2199
  2     1.000 160     2.000 380
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdI2
5216000 'Cd(BO2)2'          0.0000   -9.8367                          198.0306
  4    -2.000 002    -2.000 330     1.000 160     2.000 090
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cd(BO2)2
1216000 'CdSe'            -18.1590   18.0827                          191.3710
  3     1.000 760     1.000 160    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CdSe
2017100 'CeO2'              4.8279    8.1300                          172.1188
  3     1.000 171     2.000 002    -4.000 330
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  CeO2
2011700 'Ce2O3'           108.4489   60.9010                          328.2382
  3     2.000 170     3.000 002    -6.000 330
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Ce2O3
4117000 'CeCl3'            34.3933   15.4290                          246.4790
  2     1.000 170     3.000 180
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  CeCl3
1017000 'CeS'              52.3972   36.5180                          172.1840
  4     1.000 170     1.000 730     1.000 001    -1.000 330
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  CeS
6017000 'Ce2(SO4)3:8H2O'    0.0000   -8.6530                          572.4272
  3     2.000 170     3.000 732     8.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Ce2(SO4)3:8H2O
0020000 'Co(alpha)'        13.9100   -9.5288                           58.9332
  2     1.000 200     2.000 001
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Co
2020001 'CoO'              25.3550  -13.5602                           74.9326
  3    -2.000 330     1.000 200     1.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  CoO
2020002 'Co(OH)2(blue)'     0.0000  -13.7654                           92.9478
  3    -2.000 330     1.000 200     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Co(OH)2
2020003 'Co(OH)2(pink1)'   21.5400  -13.0325                           92.9478
  3    -2.000 330     1.000 200     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Co(OH)2
2020004 'Co(OH)2(pink2)'    0.0000  -12.3728                           92.9478
  3    -2.000 330     1.000 200     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                  Co(OH)2
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2020005 'Transvaalite'       0.0000  -12.0796                          92.9478
  3    -2.000 330      1.000 200     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(OH)2
2020100 'Co(OH)3'            8.3550    3.3424                          109.9551
  3    -3.000 330      1.000 201     3.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(OH)3
3020100 'Co-Spinel'        101.9900  -59.4011                          240.7972
  4    -8.000 330     -2.000 001     3.000 200     4.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co3O4
2020101 'Heterogenite'       0.0000   10.2251                          91.9399
  3    -3.000 330      1.000 201     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoOOH
4220000 'CoF2'               8.8120    5.1456                          96.9300
  2     1.000 200      2.000 270
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoF2
4120000 'CoCl2'             19.0760   -8.2519                          129.8392
  2     1.000 200      2.000 180
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoCl2
4120001 'CoCl2:H2O'         15.0910   -4.7263                          147.8544
  3     1.000 200      2.000 180     1.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoCl2:H2O
4120002 'CoCl2:2H2O'         9.8060   -4.6457                          165.8696
  3     1.000 200      2.000 180     2.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoCl2:2H2O
4120003 'CoCl2:6H2O'        -1.9340   -2.5640                          237.9304
  3     1.000 200      2.000 180     6.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoCl2:6H2O
7020000 'CoHPO4'             0.0000   19.0576                          154.9125
  3     1.000 200      1.000 580     1.000 330
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoHPO4
7020001 'Co3(PO4)2'          0.0000   34.6702                          366.7423
  2     3.000 200      2.000 580
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co3(PO4)2
5020000 'Spherocobaltite'    4.6000   10.1372                          118.9424
  2     1.000 200      1.000 140
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoCO3
1020000 'Jaipurite'         -4.8900    9.2942                          90.9932
  3    -1.000 330      1.000 200     1.000 730
  999.  999.  999.  999.  999.
  Peterson et al. 1987                    CoS
1020001 'Cattierite'       -14.2900   20.2011                          123.0532
  4    -2.000 330     -2.000 001     1.000 200     2.000 730
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoS2
1020002 'Linnaeite'        -27.2700   40.9885                          305.0396
  4    -4.000 330     -2.000 001     3.000 200     4.000 730
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co3S4
1020003 'Co-Pentlandite'   -44.6100   77.3592                          786.8788
  4    -8.000 330      9.000 200     8.000 730     2.000 001
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co9S8
6020000 'CoSO4'             18.9300   -2.9099                          154.9908
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  2     1.000 200      1.000 732
  999.  999.  999.  999.  999.
  Peterson et al. 19'6                    CoSO4
6020001 'Bieberite'        -2.7850    2.4628                          281.0972
  3     1.000 200      1.000 732      7.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoSO4:7H2O
6020002 'CoSO4:6H2O'       -0.2800    2.3089                          263.0820
  3     1.000 200      1.000 732      6.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoSO4:6H2O
6020003 'CoSO4:H2O'        12.5650    1.1801                          173.0060
  3     1.000 200      1.000 732      1.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoSO4:H2O
7220002 'Hodderite'        -55.8500   31.1225                         133.8548
  5    -4.000 002      1.000 200      1.000 061      5.000 330      7.000 001
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoAs
7220003 'Safflorite'       -121.1100   71.4074                         208.7764
  5    -8.000 002      1.000 200      2.000 061     10.000 330     12.000 001
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    CoAs2
7220000 'Co3(AsO4)2'         0.0000   -13.0471                         454.6380
  3    -6.000 330      3.000 200      2.000 061
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co3(AsO4)2
7220001 'Erythrite'          0.0000   -12.9885                         598.7596
  4    -6.000 330      3.000 200      2.000 061      8.000 002
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co3(AsO4)2:8H2O
4120100 'Co(NH3)5Cl3'       13.9590   -13.0926                         250.4442
  4    -5.000 330      1.000 201      5.000 490      3.000 180
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(NH3)5Cl3
4120101 'Co(NH3)5Cl3:H2O'   17.5740   -20.4151                         268.4594
  5    -5.000 330      1.000 201      5.000 490      1.000 002      3.000 180
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(NH3)5Cl3:H2O
4020100 'Co(NH3)6Br3'       16.5270   -26.9863                          400.8276
  4    -6.000 330      1.000 201      6.000 490      3.000 130
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(NH3)6Br3
5120101 'Co(NH3)6(NO3)3'    11.3900   -26.6411                         347.1303
  4    -6.000 330      1.000 201      6.000 490      3.000 492
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(NH3)6(NO3)3
4120102 'Co(NH3)6(ClO4)3'   14.5400   -25.8714                         459.4674
  4    -6.000 330      1.000 201      6.000 490      3.000 181
  999.  999.  999.  999.  999.
  Peterson et al. 1986                    Co(NH3)6(ClO4)3
6021200 'BaCrO4).05(SO4).95' 0.0000     9.8714                         234.3871
  3     1.000 100      0.050 212      0.950 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Ba(CrO4)0.05(SO4)0.95
6021201 'BaCrO4).10(SO4).90' 0.0000     9.9295                         235.3836
  3     1.000 100      0.100 212      0.900 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Ba(CrO4)0.10(SO4)0.90
6021202 'BaCrO4).15(SO4).85' 0.0000     9.9745                         236.3801
  3     1.000 100      0.150 212      0.850 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Ba(CrO4)0.15(SO4)0.85
6021203 'BaCrO4).20(SO4).80' 0.0000    10.0107                         237.3766
  3     1.000 100      0.200 212      0.800 732
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ba(CrO4)0.20(SO4)0.80
6021204 'BaCrO4).25(SO4).75' 0.0000   10.0410                    238.3731
  3     1.000 100     0.250 212     0.750 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ba(CrO4)0.25(SO4)0.75
4021100 'CrBr3'             0.0000  -24.6693                    291.7081
  4     1.000 211     3.000 130     1.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrBr3
4121100 'CrCl3'             0.0000  -18.2784                    158.3542
  4     1.000 211     3.000 180     1.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrCl3
4221100 'CrF3'              0.0000    9.9811                    108.9913
  4     1.000 211     3.000 270     1.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrF3
4321100 'CrI3'              0.0000  -25.0923                    432.7095
  4     1.000 211     3.000 380     1.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrI3
3021100 'Chromite'          0.0000  -12.7774                    223.8368
  4     2.000 211     1.000 280    -6.000 330     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeCr2O4
3021101 'Mg-Chromite'       0.0000  -21.6450                    192.2948
  4     2.000 211     1.000 460    -6.000 330     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgCr2O4
0021000 'Cr(metal)'        34.3000  -32.2440                     51.9961
  2     1.000 210     2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr(metal)
3021102 'Eskolaite'         0.0000    -7.64                     151.9904
  3     2.000 211    -4.000 330     1.000 002
 -3.37513e+3  1.65726e+5 -5.47981e-1  1.24476e+3 -9.33969e+6
  EQ3/6 database: version mdas.3245     Cr2O3
2021102 'Cr(OH)3(am)'       0.0000   -5.7539                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr(OH)3(am)
2021101 'Cr(OH)3(c)'        0.0000   -6.4723                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr(OH)3(c)
2021103 'Cr.99Fe.01(OH)3'   0.0000   -0.6963                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr0.99Fe0.01(OH)3
2021104 'Cr.95Fe.05(OH)3'   0.0000   -1.5759                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr0.95Fe0.05(OH)3
2021105 'Cr.90Fe.10(OH)3'   0.0000   -2.0890                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr0.90Fe0.10(OH)3
2021106 'Cr.80Fe.20(OH)3'   0.0000   -2.7487                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr0.80Fe0.20(OH)3
2021107 'Cr.70Fe.30(OH)3'   0.0000   -3.1885                    103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
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  Krupka et al. 1988                    Cr0.70Fe0.30(OH)3
2021108 'Cr.60Fe.40(OH)3'   0.0000   -3.9215                          103.0181
  3     1.000 211     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cr0.60Fe0.40(OH)3
4121000 'CrCl2'            19.7010  -15.8559                          122.9015
  2     1.000 210     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrCl2
3021200 'Ag2CrO4'         -14.3700   12.1983                          331.7301
  2     1.000 212     2.000 020
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ag2CrO4
3021201 'BaCrO4'           -6.7210   10.3006                          253.3207
  2     1.000 212     1.000 100
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    BaCrO4
3021202 'Cs2CrO4'          -7.7200    1.0863                          381.8046
  2     1.000 212     2.000 220
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cs2CrO4
3021203 'Cs2Cr2O7'        -23.4450   18.9381                          481.7989
  4     2.000 212     2.000 220     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cs2Cr2O7
3021204 'CuCrO4'           0.0000    6.0632                          179.5397
  2     1.000 212     1.000 231
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CuCrO4
3021205 'K2CrO4'           -4.4800    0.3474                          194.1903
  2     1.000 212     2.000 410
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2CrO4
3021206 'K2Cr2O7'         -18.6850   16.6527                          294.1846
  4     2.000 212     2.000 410     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2Cr2O7
3021207 'Li2CrO4'          10.4920   -4.2191                          129.8757
  2     1.000 212     2.000 440
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Li2Cr2O7
3021208 'MgCrO4'           20.9300   -4.7424                          140.2987
  2     1.000 212     1.000 460
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgCrO4
3021209 '(NH4)2CrO4'       -2.8780    0.2844                          152.0707
  2     1.000 212     2.000 490
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    (NH4)2CrO4
3021210 'Na2CrO4'           4.2000   -2.6343                          161.9732
  2     1.000 212     2.000 500
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2CrO4
3021211 'Na2Cr2O7'         -6.0450   11.1494                          261.9675
  4     2.000 212     2.000 500     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2Cr2O7
3021212 'PbCrO4'          -10.5540   14.3159                          323.1937
  2     1.000 212     1.000 600
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbCrO4
3021213 'Rb2CrO4'          -6.1980    0.6040                          286.9293
  2     1.000 212     2.000 680
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Rb2CrO4
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3021214 'SrCrO4'            2.0890    5.3075                          203.6137
  2     1.000 212     1.000 800
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    SrCrO4
2021200 'CrO3'              0.9150    3.8372                          99.9943
  3     1.000 212     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CrO3
3015000 'CaCrO4'            6.1090    2.8960                          156.0717
  2     1.000 150     1.000 212
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CaCrO4
3036000 'Hg2CrO4'           0.0000    9.3250                          517.1737
  2     1.000 360     1.000 212
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2CrO4
0023000 'Cu-metal'         -17.1300    8.7562                          63.5460
  2     1.000 230     1.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cu(metal)
4123000 'Nantokite'         -9.9700    6.7647                          98.9987
  2     1.000 230     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CuCl
4223000 'CuF'               12.3700   -7.0777                          82.5444
  2     1.000 230     1.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CuF
2023000 'Cuprite'           -6.2410     1.90                           143.0914
  3    -2.000 330     2.000 230     1.000 002
  2.33564e+2  -1.08508e+4  2.98087e-2  -8.51844e+1  5.88874e+5
  EQ3/6 database: version mdas.3245     Cu2O
1023000 'Chalcocite'       -49.0530    34.73                           159.1580
  3    -1.000 330     2.000 230     1.000 730
  5.06840e+2  -1.51767e+4  8.80870e-2  -1.87313e+2  1.42462e+6
  EQ3/6 database: version mdas.3245     Cu2S
1023001 'Djurleite'        -47.8835   33.9190                          154.9640
  4    -1.000 330     0.066 231     1.868 230     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cu0.07Cu1.85S
1023002 'Anilite'          -43.5380   31.8768                          143.2715
  4    -1.000 330     0.250 231     1.500 230     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cu0.25Cu1.50S
1023103 'Blaubleidender-I' 0.0000    24.1614                          101.9666
  4    -1.000 330     0.900 231     0.200 230     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cu0.9Cu0.2S
1023004 'Blaubleidender-II' 0.0000   27.2780                          121.0304
  4    -1.000 330     0.600 231     0.800 230     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Cu0.6Cu0.8S
1023100 'Covellite'        -23.9630    22.06                           95.6120
  3    -1.000 330     1.000 231     1.000 730
  999.  999.  999.  999.  999.
  Krupka 1988 (H); Shea-Helz 1988 (K)   CuS
1023101 'Bornite'           0.0000    102.44                          405.6410
  5     4.000 230     1.000 231     1.000 280     4.000 730   -4.000 330
  3.99567e+3  -1.90769e+5  6.19180e-1  -1.44769e+3  1.28209e+7
  EQ3/6 database: version mdas.3245     Cu5FeS4
1023103 'Chalcopyrite'     -30.2240    32.56                           183.5250
  4    -2.000 330     1.000 231     1.000 280     2.000 730
  2.08823e+3  -1.08453e+5  3.24527e-1  -7.54226e+2  6.89860e+6
  EQ3/6 database: version mdas.3245     CuFeS2
6023000 'Cu2SO4'            4.5610    1.9534                          223.1556
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  2     2.000 230     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988:                    Cu2SO4
3023000 'Cuprousferrite'    3.7960    8.9241                          151.3918
  4    -4.000 330     1.000 230     1.000 281     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuFeO2
4123100 'Melanothallite'   11.8190   -3.7258                          134.4514
  2     1.000 231     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuCl2
5023100 'CuCO3'             0.0000    9.6329                          123.5552
  2     1.000 231     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuCO3
4223100 'CuF2'             13.3200    0.6216                          101.5428
  2     1.000 231     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuF2
4223101 'CuF2:2H2O'         3.6500    4.5504                          137.5734
  3     1.000 231     2.000 270     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuF2:2H2O
2023100 'Cu(OH)2'           0.0000   -8.6697                           97.5607
  3    -2.000 330     1.000 231     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu(OH)2
4123101 'Atacamite'        18.6870   -7.3379                          213.5667
  4    -3.000 330     2.000 231     3.000 002     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu2Cl(OH)3
5123100 'Cu2(OH)3NO3'      15.0810   -8.7965                          240.1190
  4    -3.000 330     2.000 231     3.000 002     1.000 492
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu2(OH)3(NO3)
6023100 'Antlerite'         0.0000   -8.7526                          354.7310
  4    -4.000 330     3.000 231     4.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu3(SO4)(OH)4
6023101 'Brochantite'       0.0000    -15.44                          452.2916
  4    -6.000 330     4.000 231     6.000 002     1.000 732
  2.53570e+3  -1.45421e+5  3.68002e-1  -9.13059e+2  7.66161e+6
  EQ3/6 database: version mdas.3245      Cu4(SO4)(OH)6
6023102 'Langite'          39.6770  -17.2515                          470.3069
  4    -6.000 330     4.000 231     7.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuSO4:3Cu(OH)2:H2O
2023101 'Tenorite'         15.2350    -7.66                           79.5454
  3    -2.000 330     1.000 231     1.000 002
  4.42977e+2  -2.75333e+4  6.36684e-2  -1.58755e+2  1.38269e+6
  EQ3/6 database: version mdas.3245      CuO
6023103 'CuOCuSO4'         20.0960   -0.0572                          239.1550
  4    -2.000 330     2.000 231     1.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     CuOCuSO4
7023100 'Cu3(PO4)2'         0.0000   36.8530                          380.5807
  2     3.000 231     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu3(PO4)2
7023101 'Cu3(PO4)2:3H2O'    0.0000   35.1180                          434.6266
  3     3.000 231     2.000 580     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Cu3(PO4)2:3H2O
6023104 'Chalcocyanite'    17.4820    -2.92                           159.6096
  2     1.000 231     1.000 732
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  1.50687e+3  -8.68467e+4  2.34363e-1  -5.43405e+2  4.99916e+6
  EQ3/6 database: version mdas.3245        CuSO4
6023105 'Chalcanthite'      -1.4330    2.6387                          249.6860
  3     1.000 231     1.000 732     5.000 002
  1.17102e+3  -6.31834e+4  1.67193e-1  -4.22727e+2  3.52760e+6
  EQ3/6 database: version mdas.3245        CuSO4:5H2O
2023102 'Dioptase'           8.6700   -6.1336                          157.6450
  3    -2.000 330     1.000 231     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuSiO2(OH2)
3023100 'Cupricferrite'     50.2690   -5.8961                          239.2376
  4    -8.000 330     1.000 231     2.000 281     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuFe2O4
4023000 'CuBr'              -13.0790    8.2028                          143.4500
  2     1.000 230     1.000 130
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuBr
4323000 'CuI'               -20.1440   11.8971                          190.4505
  2     1.000 230     1.000 380
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuI
7060005 'Tsumebite'           0.0000    9.7919                          677.9852
  5    -3.000 330     2.000 600     1.000 231     1.000 580     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Pb2CuPO4(OH)3:3H2O
5023101 'Malachite'          16.2100      4.39                          221.1159
  4     2.000 231     2.000 002     1.000 140    -2.000 330
  2.26726e+3  -1.28353e+5  3.47802e-1  -8.16541e+2  7.50271e+6
  EQ3/6 database: version mdas.3245        Cu2(OH)2CO3
5023102 'Azurite'            23.7650     11.50                          344.6711
  4     3.000 231     2.000 002     2.000 140    -2.000 330
  4.13121e+3  -2.33907e+5  6.37133e-1  -1.48771e+3  1.38746e+7
  EQ3/6 database: version mdas.3245        Cu3(CO3)(OH)2
1023004 'CuSCN'             -20.4000   12.7517                          121.6297
  2     1.000 230     1.000 734
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuSCN
1223100 'Klockmannite'      -28.7300   26.4769                          142.5060
  3     1.000 760     1.000 231    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuSe
1223000 'Cu2Se(alpha)'      -51.0700   36.0277                          206.0520
  3     1.000 760     2.000 230    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Cu2Se(alpha)
1223101 'CuSe2'             -33.3800   33.3449                          221.4660
  4     2.000 760     1.000 231    -2.000 330    -2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuSe2
1223001 'Umangite'          -80.9800   63.3914                          348.5580
  4     2.000 760     2.000 230     1.000 231    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Cu3Se2
6123100 'Chalcomenite'        9.0300   -0.4977                          226.5348
  4     1.000 761     1.000 231     2.000 002    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       CuSeO3:2H2O
1102001 'Ag4Fe(CN)6:H2O'      0.0000   89.6909                          661.4415
  4     6.000 143     4.000 020     1.000 280     1.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Ag4Fe(CN)4:H2O
1102002 'AgCN'              -26.3850   16.2180                          133.8859
  2     1.000 143     1.000  20
  999.  999.  999.  999.  999.
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  Sehmel (1989)                          AgCN
1116001 'Cd2Fe(CN)6:7H2O'   0.0000   62.9824                          562.8824
  4     6.000 143     2.000 160     1.000 280     7.000   2
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Cd2Fe(CN)6:7H2O
1121001 'CrCN'              0.0000  -23.8880                           78.0138
  3     1.000 143     1.000 210     1.000   1
  999.  999.  999.  999.  999.
  Sehmel (1989)                          CrCN
1121002 'Cr2CN'             0.0000  -56.6450                          130.0099
  3     1.000 143     2.000 210     3.000   1
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Cr2CN
1123001 'CuCN'            -30.2000   19.4974                           89.5637
  2     1.000 143     1.000 230
  999.  999.  999.  999.  999.
  Sehmel (1989)                          CuCN
1123102 'Cu2Fe(CN)6'        0.0000   61.4168                          339.0454
  3     6.000 143     2.000 231     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Cu2Fe(CN)6
1138001 'CNI'              17.3090  -11.3114                           152.9222
  3     1.000 143     1.000 380    -2.000   1
  999.  999.  999.  999.  999.
  Sehmel (1989)                          CNI
1141001 'K12Ni8Fe(CN)6:7H2O' 0.000  431.0902                          2422.3737
  4    42.000 143    12.000 410     8.000 540     7.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K12Ni8Fe(CN)6:7H2O
1141002 'KCN(cub)'          -2.7400   -1.4403                           65.1160
  2     1.000 143     1.000 410
  999.  999.  999.  999.  999.
  Sehmel (1989)                          KCN(cub)
1141003 'K2CdFe(CN)6'       0.0000   63.0279                          402.5610
  4     6.000 143     2.000 410     1.000 160     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K2CdFe(CN)6
1141004 'K4Ni4(Fe(CN)6)3'   0.0000  183.5467                          1027.0135
  4    18.000 143     4.000 410     4.000 540     3.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K4Ni4(Fe(CN)6)3
1141005 'K4Fe(CN)6'       -95.6200   48.8241                          368.3466
  3     6.000 143     4.000 410     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K4Fe(CN)6
1141006 'K2Mn3(Fe(CN)6)2'   0.0000  121.0011                          666.9176
  4    12.000 143     2.000 410     3.000 470     2.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K2Mn3(Fe(CN)6)2
1141007 'K2Ni3(Fe(CN)6)2'   0.0000  123.1267                          678.1735
  4    12.000 143     2.000 410     3.000 540     2.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K2Ni3(Fe(CN)6)2
1141008 'K4Fe(CN)6:3H2O'  -99.1750   49.5424                          422.3925
  4     6.000 143     4.000 410     1.000 280     3.000   2
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K4Fe(CN)6:3H2O
1141009 'K12Cd8(Fe(CN)6)7'  0.0000  441.9853                          2852.1417
  4    42.000 143    12.000 410     8.000 160     7.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K12Cd8(Fe(CN)6)7
1141010 'KZn1.5Fe(CN)6'     0.0000   66.8086                          349.1367
  4     6.000 143     1.000 410     1.500 950     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          KZn1.5Fe(CN)6
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1141011 'K3Fe(CN)6'        -83.2900   54.6440                    329.2483
  3     6.000 143     3.000 410     1.000 281
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K3Fe(CN)6
1141012 'KMn6(Fe(CN)6)5'    0.0000  293.6849                   1702.1819
  4    30.000 143     8.000 410     6.000 470     5.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          KMn6(Fe(CN)6)5
1141013 'K2Cu2Fe(CN)6'      0.0000   72.5142                    417.2420
  4     6.000 143     2.000 410     2.000 230     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          K2Cu2Fe(CN)6
1147014 'Mn2Fe(CN)6'        0.0000   59.0272                    321.8295
  3     6.000 143     2.000 470     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Mn2Fe(CN)6
1150001 'NaCN(cub)'         0.5200   -2.2869                     49.0075
  2     1.000 143     1.000 500
  999.  999.  999.  999.  999.
  Sehmel (1989)                          NaCN(cub)
1160001 'Pb2Fe(CN)6:3H2O'   0.0000   63.6011                    680.3993
  4     6.000 143     2.000 600     1.000 280     3.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Pb2Fe(CN)6:3H2O
1187001 'Tl4Fe(CN)6:2H2O'   0.0000   56.9162                   1065.5172
  4     6.000 143     4.000 870     1.000 280     2.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Tl4Fe(CN)6:2H2O
1195001 'Zn2Fe(CN)6:2H2O'   0.0000   61.2321                    378.7640
  4     6.000 143     2.000 950     1.000 280     2.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Zn2Fe(CN)6:2H2O
7714401 'AgOCN'           -13.1750    6.6159                    149.8853
  2     1.000 144     1.000 020
  999.  999.  999.  999.  999.
  Sehmel (1989)                          AgOCN
1102002 'Ag4Fe(CN)6'      -260.9100  193.9140                    133.8859
  3     6.000 143     4.000 020     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Ag4Fe(CN)6
1116002 'Cd2Fe(CN)6'        0.0000   28.2243                    436.7754
  3     6.000 143     2.000 160     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Cd2Fe(CN)6
1136100 'Hg(CN)2'         -60.7300   45.3791                    252.6255
  4     1.000 361     2.000 143     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Hg(CN)2
1160002 'Pb2Fe(CN)6'        0.0000   27.5895                    626.3534
  3     6.000 143     2.000 600     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Pb2Fe(CN)6
1195002 'Zn2Fe(CN)6'        0.0000   29.9263                    342.7334
  3     6.000 143     2.000 950     1.000 280
  999.  999.  999.  999.  999.
  Sehmel (1989)                          Zn2Fe(CN)6
2028001 'Fe(OH)2(ppt)'     21.9350  -11.6750                     89.8617
  3    -2.000 330     1.000 280     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Fe(OH)2(ppt)
2028100 'Fe(OH)3(am)'      19.8350   -4.8853                    106.8690
  3    -3.000 330     1.000 281     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Fe(OH)3(am)
2028101 'Fe3(OH)8'          0.0000  -20.2216                    303.5997
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  4    -8.000 330     2.000 281     1.000 280     8.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe3(OH)8
2028102 'Goethite'          14.5400       1.0                              88.8537
  3    -3.000 330     1.000 281     2.000 002
  999.  999.  999.  999.  999.
  Krupka 1988 (H): Nordstrom 1990 (K)     FeOOH
2028103 'Lepidocrocite'      0.0000    -1.3634                             88.8537
  3    -3.000 330     1.000 281     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeOOH(gamma)
2028104 'Maghemite'          0.0000    -6.3733                            159.6922
  3    -6.000 330     2.000 281     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe2O3
2028105 'Hematite'          31.1350     -0.11                             159.6922
  3    -6.000 330     2.000 281     3.000 002
  1.12732e+3  -6.70651e+4  1.75188e-1  -4.01988e+2  3.55270e+6
  EQ3/6 database: version mdas.3245       Fe2O3
2028106 'Fe(OH)3(soil)'      0.0000    -2.6864                            106.8690
  3    -3.000 330     1.000 281     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe(OH)3(soil)
2028107 'Fe(OH)3(ppt)'       19.8350    -3.4267                            106.8690
  3    -3.000 330     1.000 281     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe(OH)3(ppt)
4128100 'Fe(OH)2:7Cl'        0.0000     3.0406                            112.4026
  4    -2.700 330     1.000 281     2.700 002     0.300 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe(OH)2:7Cl
1028000 'FeS(ppt)'           0.0000     3.9134                             87.9130
  3    -1.000 330     1.000 280     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeS(ppt)
1028001 'Greigite'           0.0000    44.9613                            295.8050
  4    -4.000 330     2.000 281     1.000 280     4.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe3S4
1028002 'Mackinawite'        0.0000     4.6464                             87.9130
  3    -1.000 330     1.000 280     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeS
1028003 'Pyrite'           -12.8810    19.6484                            119.9790
  4    -2.000 330    -2.000 001     1.000 280     2.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeS2
1028004 'Pyrrhotite'         1.6020     5.8822                             87.9130
  3    -1.000 330     1.000 280     1.000 730
  2.33550e+3  -1.34160e+5  3.38581e-1  -8.38774e+2  8.24836e+6
  Reed and Spycher 1989: SOLVEQ database  FeS
6028100 'Fe2(SO4)3'          58.1500    -3.21                              399.8848
  2     2.000 281     3.000 732
  5.74414e+3  -3.35687e+5  8.95012e-1  -2.06672e+3  2.00563e+7
  EQ3/6 database: version mdas.3245       Fe2(SO4)4
6050000 'Jarosite-Na'        36.1820    11.1993                            484.7020
  5    -6.000 330     1.000 500     3.000 281     2.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NaFe3(SO4)2(OH)6
6041002 'Jarosite-K'         31.2820    14.8012                            500.8105
  5    -6.000 330     1.000 410     3.000 281     2.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KFe3(SO4)2(OH)6
6028101 'Jarosite-H'         55.1470    12.1023                            480.7355
  4    -5.000 330     3.000 281     2.000 732     7.000 002
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    H3OFe3(SO4)2(OH)6
3028000 'Magnetite'        51.0750    -10.47                          231.5386
  4    -8.000 330     2.000 281     1.000 280     4.000 002
  1.51389e+3  -9.25740e+4  2.32310e-1  -5.40230e+2  4.76[illegible]2e+6
  EQ3/6 database: version mdas.3245       Fe3O4
6028000 'Melanterite'        -4.91     2.209                           278.0176
  3     1.000 280     1.000 732     7.000 002
  -1.447e+0  0.0000  4.153e-3  0.0000  2.14949e+5
  Nordstrom et al. 1990                 FeSO4:7H2O
6028001 'FeSO4(s)'           0.0000     -2.66                          151.9086
  2     1.000 280     1.000 732
  1.85770e+3  -1.07971e+5  2.87403e-1  -6.69286e+2  6.41644e+6
  EQ3/6 database: version mdas.3245       FeSO4(s)
5028000 'Siderite'             2.48     10.52                          115.8562
  2     1.000 280     1.000 140
  1.88474e+3  -1.06032e+5  2.93106e-1  -6.78393e+2  6.45825e+6
  Nordstrom 1990 (H); EQ3/6 mdas.3245     FeCO3
7028100 'Strengite'          6.3960   25.9000                          186.8489
  3     1.000 281     1.000 580     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FePO4:2H2O
7028001 'Vivianite'          0.0000   36.0013                          501.6060
  3     3.000 280     2.000 580     8.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe3(PO4)2:8H2O
3028001 'Hercynite'         78.3750  -27.2282                          173.8077
  4    -8.000 330     1.000 280     2.000 030     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    FeAl2O4
3046001 'Mg-Ferrite'        66.6190  -16.7619                          199.9966
  4    -8.000 330     1.000 460     2.000 281     4.0[illegible] 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgFe2O4
0036000 'Hg-metal(l)'      -20.6025   13.4473                          200.5900
  2     0.500 360     1.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg(metal)
4036000 'Hg2Br2'           -32.5630   22.2226                          560.9880
  2     1.000 360     2.000 130
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2Br2
5036000 'Hg2CO3'             0.0000   13.9722                          461.1892
  2     1.000 360     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2CO3
4136000 'Calomel'          -24.6900   17.8357                          472.0854
  2     1.000 360     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2Cl2
4236000 'Hg2F2'              1.7950    4.1025                          439.1768
  2     1.000 360     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2F2
4336000 'Hg2I2'              0.0000   28.3885                          654.9889
  2     1.000 360     2.000 380
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2I2
2036000 'Hg2(OH)2'           0.0000   -5.2540                          435.1947
  3     1.000 360     2.000 002    -2.000 330
  999.  999.  999.  [illegible].  999.
  Krupka et al. 1988                    Hg2(OH)2
7036000 'Hg2HPO4'            0.0000   25.9821                          497.1593
  3     1.000 360     1.000 330     1.000 580
  999.  999.  999.  999.  999.
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  Krupka et al. 1988                    Hg2HPO4
1036000 'Hg2S'          -17.9980   41.8307                          433.2460
  3     1.000 360     1.000 730    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2S
6036000 'Hg2SO4'          -1.5630    6.1594                          497.2436
  2     1.000 360     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2SO4
6136000 'Hg2SeO3'          0.0000    6.9128                          528.1382
  3     1.000 360     1.000 761    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg2SeO3
4036100 'HgBr2'          -34.4330   25.3957                          360.3980
  4     1.000 361     2.000 130     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgBr2
5036100 'HgCO3'          -22.1350   28.6897                          260.5992
  4     1.000 361     1.000 140     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgCO3
4136100 'HgCl2'          -25.4400   20.2516                          271.4954
  4     1.000 361     2.000 180     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgCl2
4336100 'Coccinite'      -50.5530   34.7772                          454.3989
  4     1.000 361     2.000 380     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgI2
2036100 'Montroydite'     -5.1290    3.6554                          216.5894
  2     1.000 361    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgO(red)
2036102 'HgO(yellow)'     -5.0400    3.6327                          216.5894
  2     1.000 361    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgO(yellow)
2036103 'HgO(hex)'        -5.0400    3.6327                          216.5894
  2     1.000 361    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgO(hex)
2036101 'Hg(OH)2'          0.0000    3.5117                          234.6047
  1     1.000 361
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Hg(OH)2
1036100 'Cinnabar'       -61.4380   45.9229                          232.6560
  4     1.000 361     1.000 730     1.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgS(alpha)
1036101 'Metacinnabar'   -60.3380   45.4143                          232.6560
  4     1.000 361     1.000 730     1.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgS(beta)
6036100 'HgSO4'           -3.5140    9.4291                          296.6536
  4     1.000 361     1.000 732     2.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgSO4
6136100 'HgSeO3'           0.0000   12.7004                          327.5482
  4     1.000 361     1.000 761     1.000 330    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgSeO3
4336102 'HgI2:2NH3'      -33.8080   16.2554                          488.4601
  4     1.000 361     2.000 380     2.000 490    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgI2:2(NH3)
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4336103 'HgI2:6NH3'        18.6640  -33.6462                          556.5823
  5     1.000 361     2.000 380     6.000 490    -2.000 002    -4.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    HgI2:6(NH3)
6041003 'Arcanite'           0.0000     1.80                          174.2602
  2     2.000 410     1.000 732
  1.69935e+3  -9.48882e+4  2.64488e-1  -6.16295e+2  5.93995e+6
  EQ3/6 database: version mdas.3245     K2SO4
5041000 'Kalicinite'         0.0000     9.9305                        100.1154
  3     1.000 410     1.000 140     1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KHCO3
6041006 'Mercallite'         0.0000     1.2820                        136.1698
  3     1.000 410     1.000 330     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KHSO4
6041007 'Misenite'           0.0000     9.8337                        991.2792
  3     8.000 410     6.000 330     7.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KH6(SO4)7
5041001 'K2CO3:1.5H2O'       0.0000    -3.2929                        165.2287
  3     2.000 410     1.000 140     1.500 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2CO3:1.5H2O
5041002 'KH4(CO3)6:3H2O'     0.0000    33.3222                        730.9192
  4     8.000 410     4.000 330     6.000 140     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KH4(CO3)6:3H2O
6041010 'K3H(SO4)2'          0.0000     3.1672                        310.4300
  3     3.000 410     1.000 330     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K3H(SO4)2
4141001 'Sylvite'            0.0000    -1.0291                         74.5510
  2     1.000 410     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KCl
1041000 'K2SO3'              5.6300    -5.0473                        158.2608
  2     2.000 410     1.000 733
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2SO3
1041001 'KSCN'              -5.7890    -2.1462                         97.1820
  2     1.000 410     1.000 734
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KSCN
5046000 'Artinite'          28.5320    -9.33                          196.6797
  4    -2.000 330     2.000 460     1.000 140     5.000 002
  2.33983e+3  -1.35771e+5  3.52920e-1  -8.43075e+2  7.74465e+6
  EQ3/6 database: version mdas.3245     Mg2(OH)2CO3:3H2O
2046000 'Brucite'           27.2400    -16.30                          58.3197
  3     1.000 460     2.000 002    -2.000 330
  3.74982e+2  -2.58332e+4  5.35236e-2  -1.34555e+2  1.09761e+6
  EQ3/6 database: version mdas.3245     Mg(OH)2
5015002 'Dolomite(o)'         9.436     18.14                          184.4014
  3     1.000 150     1.000 460     2.000 140
  3.69590e+3  -2.07327e+5  5.77405e-1  -1.33217e+3  1.26073e+7
  EQ3/6 database: version mdas.3245     CaMg(CO3)2(ordered)
5015003 'Dolomite(d)'        11.09     16.54                          184.4014
  3     1.000 150     1.000 460     2.000 140
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                 CaMg(CO3)2(disordered)
5015004 'Huntite'           29.2390    31.02                          353.0298
  3     3.000 460     1.000 150     4.000 140
  7.48865e+3  -4.23192e+5  1.16431e+0  -2.69688e+3  2.55869e+7
  EQ3/6 database: version mdas.3245     CaMg3(CO3)4
6046000 'Epsomite'          -2.8240    2.1388                         246.4756
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  3     1.000 460     1.000 732     7.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgSO4:7H2O
7015002 'FCO3-Apatite'    -39.3900  114.4000                          967.3660
  6   9.496 150   0.360 500   0.144 460   4.800 580   1.200 140   2.480 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ca9Na0.4(PO4)5(CO3)F3
5046001 'Hydromagnesite'   58.0610    10.47                           467.6376
  4     5.000 460     4.000 140    -2.000 330     6.000 002
  8.03211e+3  -4.59360e+5  1.23337e+0  -2.89115e+3  2.71347e+7
  EQ3/6 database: version mdas.3245     Mg5(CO3)4(OH)2:4H2O
5046002 'Magnesite'         7.3400     8.04                             84.3142
  2     1.000 460     1.000 140
  1.82754e+3  -1.03113e+5  2.85094e-1  -6.58162e+2  6.21475e+6
  EQ3/6 database: version mdas.3245     MgCO3
5046003 'Nesquehonite'      5.7890    5.2115                           138.3600
  3     1.000 460     1.000 140     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgCO3:3H2O
2046001 'Periclase'        36.0850   -21.34                             40.3044
  3    -2.000 330     1.000 460     1.000 002
  4.49024e+2  -3.25083e+4  6.37032e-2  -1.60206e+2  1.43040e+6
  EQ3/6 database: version mdas.3245     MgO
3046000 'Spinel'           89.1090  -36.3934                           142.2657
  4    -8.000 330     1.000 460     2.000 030     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgAl2O4
4146000 'Bischofite'        0.0000   -4.4265                           203.3021
  3     1.000 460     2.000 180     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgCl2:6H2O
6050004 'Bloedite'          0.0000    2.3881                           334.4729
  4     2.000 500     1.000 460     2.000 732     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2Mg(SO4)2:4H2O
4141000 'Carnallite'        0.0000   -4.4302                           277.8531
  4     1.000 410     1.000 460     3.000 180     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KMgCl3:6H2O
6046001 'Hexahydrite'       0.0000    1.6661                           228.4603
  3     1.000 460     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgSO4:6H2O
6041004 'Kainite'           0.0000    0.0880                           248.9654
  5     1.000 410     1.000 460     1.000 180     1.000 732     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KMgCl(SO4):3H2O
6046002 'Kieserite'         0.0000    0.1422                           138.3839
  3     1.000 460     1.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgSO4:H2O
6041005 'Leonite'           0.0000    3.7492                           366.6899
  4     2.000 410     1.000 460     2.000 732     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2Mg(SO4)2:4H2O
4146001 'Mg2Cl(OH)3:7H2O'   0.0000  -26.0488                           207.1458
  4     2.000 460     1.000 180     7.000 002    -3.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mg2Cl(OH)3:7H2O
6041008 'Picromerite'       0.0000    4.1025                           402.7205
  4     2.000 410     1.000 460     2.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2Mg(SO4)2:6H2O
6041009 'Polyhalite'        0.0000   13.5294                           602.9426
  5     2.000 410     1.000 460     2.000 150     4.000 732     2.000 002
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2MgCa2(SO4)4:2H2O
4146002 'Tachyhydrite'      0.0000  -17.3175                          517.5876
  4     2.000 460     1.000 150     6.000 180     12.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CaMg2Cl6:12H2O
1046000 'MgSO3'            22.4700   -2.7707                          104.3692
  2     1.000 460     1.000 733
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MgSO3
3047100 'Bixbyite'         29.7460    0.9932                          157.8743
  3    -6.000 330     2.000 471     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mn2O3
2047101 'Manganite'         0.0000     25.34                           87.9448
  4    -3.000 330    -1.000 001     1.000 470     2.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                 MnOOH(gamma)
2047102 'Birnessite'        0.0000  -18.0681                           86.9368
  4    -4.000 330    -1.000 001     1.000 471     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnO2
2047103 'Nsutite'           0.0000  -17.4817                           86.9368
  4    -4.000 330    -1.000 001     1.000 471     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnO2(gamma)
2047104 'Pyrolusite'         65.11    -41.38                           86.9368
  4    -4.000 330    -2.000 001     1.000 470     2.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                 MnO2
2047105 'MnO2(beta)'        39.3400  -15.9637                           86.9368
  4    -4.000 330    -1.000 001     1.000 471     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnO2(beta)
2047000 'Hausmannite'       100.64    -61.03                          228.8117
  4    -8.000 330    -2.000 001     3.000 470     4.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                 Mn3O4
2047001 'Manganosite'       0.0000    -17.92                           70.9374
  3     1.000 470     1.000 002    -2.000 330
  3.36734e+2  -2.41791e+4  5.04209e-2  -1.21135e+2  9.90550e+5
  EQ3/6 database: version mdas.3245     MnO
2047003 'Pyrochroite'       0.0000     -15.2                           88.9527
  3    -2.000 330     1.000 470     2.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                 Mn(OH)2
5047000 'Rhodochrosite'     2.0600     10.52                          114.9473
  2     1.000 470     1.000 140
  1.91033e+3  -1.07074e+5  2.96178e-1  -6.88128e+2  6.55449e+6
  EQ3/6 database: version mdas.3245     MnCO3
4147000 'MnCl2:4H2O'        2.6270   -2.7091                          197.9046
  3     1.000 470     2.000 180     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnCl2:4H2O
1047000 'MnS(green)'        5.7680    0.4178                           87.0040
  3    -1.000 330     1.000 470     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnS(green)
6047000 'MnSO4'            15.4810   -2.6754                          151.0017
  2     1.000 470     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnSO4
6047100 'Mn2(SO4)3'        39.0630    5.7605                          398.0669
  2     2.000 471     3.000 732
  999.  999.  999.  999.  999.
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  Krupka et al. 1988                    Mn2(SO4)3
7047000 'Mn3(PO4)2'        -2.1050   23.8213                          354.7569
  2     3.000 470     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mn3(PO4)2
7047001 'MnHPO4(c)'         0.0000   25.2799                          150.9173
  3     1.000 470     1.000 580     1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnHPO4(c)
7247000 'Mn3(AsO4)2:8H2O'   0.0000  -10.1965                          586.7748
  4     3.000 470     2.000 061     8.000 002    -6.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mn3(AsO4)2:8H2O
7347000 'Mn(VO3)2'         22.1110   -4.8135                          252.8175
  4    -4.000 330     1.000 470     2.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mn(VO3)2
1247000 'MnSe'             13.4610   -5.3486                          133.8981
  3     1.000 760     1.000 470    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnSe
6147001 'MnSeO3:2H2O'      -2.0290   -0.9587                          217.9268
  4     1.000 761     1.000 470     2.000 002    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnSeO3:2H2O
6147000 'MnSeO3'            0.0000   -0.0425                          181.8963
  3     1.000 761     1.000 470    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MnSeO3
0048000 'Mo(metal)'        -34.7600   19.6586                           95.9400
  4     1.000 480     8.000 330     6.000 001    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mo(metal)
2048001 'MoO2'             -38.6300   29.9593                          127.9388
  4     1.000 480     4.000 330     2.000 001    -2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MoO2
2048002 'Molybdite'         -7.8960   12.0532                          143.9382
  3     1.000 480     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MoO3
2048003 'H2MoO4'           -11.5000   13.3403                          161.9535
  2     1.000 480     2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    H2MoO4(white)
1048000 'Molybdenite'      -92.1440   70.5703                          160.0720
  5     1.000 480     2.000 001     6.000 330     2.000 730    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    MoS2
7402000 'Ag2MoO4'          -12.9600   11.5460                          375.6740
  2     1.000 480     2.000 020
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ag2MoO4
7428100 'Fe2(MoO4)3'        0.0000   38.8995                          591.5068
  2     3.000 480     2.000 281
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe2(MoO4)3
7410000 'BaMoO4'           -0.3510    6.2252                          297.2646
  2     1.000 480     1.000 100
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    BaMoO4
7415000 'Powellite'         -0.1640    7.8349                          200.0156
  2     1.000 480     1.000 150
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CaMoO4
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7423100 'CuMoO4'            5.3200    6.7962                          223.4836
  2     1.000 480     1.000 231
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      CuMoO4
7428000 'FeMoO4'            2.8650   10.4538                          215.7846
  2     1.000 480     1.000 280
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      FeMoO4
7441000 'K2MoO4'            0.9800   -3.7793                          238.1342
  2     1.000 480     2.000 410
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      K2MoO4
7446000 'MgMoO4'           15.2400    0.8429                          184.2426
  2     1.000 480     1.000 460
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MgMoO4
7447000 'MnMoO4'            6.5110    4.5540                          214.8757
  2     1.000 480     1.000 470
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MnMoO4
7450000 'Na2MoO4'           2.2300   -0.8898                          205.9171
  2     1.000 480     2.000 500
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Na2MoO4
7450001 'Na2Mo2O7'        -13.1150   17.3087                          349.8553
  4     2.000 480     2.000 500     2.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Na2MoO7
7460000 'Wulfenite'       -12.4950   15.8332                          367.1376
  2     1.000 480     1.000 600
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      PbMoO4
7480000 'SrMoO4'            -3.6510   10.2625                          247.5576
  2     1.000 480     1.000 800
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      SrMoO4
7495000 'ZnMoO4'            8.6810    4.8172                          225.3276
  2     1.000 480     1.000 950
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      ZnMoO4
4148000 'MoCl6'            79.9520  -49.7550                          308.6562
  4     1.000 480     8.000 330     6.000 180    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MoCl6
4148001 'MoCl5'            39.0000  -21.0836                          273.2035
  5     1.000 480     8.000 330     5.000 180     1.000 001    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MoCl5
4148002 'MoCl4'            11.0480   -1.8325                          237.7508
  5     1.000 480     8.000 330     4.000 180     2.000 001    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MoCl4
2048004 'Ilsemannite'       0.0000   63.8136                          415.8152
  4     3.000 480     8.000 330     2.000 001    -4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Mo3O8
7428001 'Ferrimolybdite'    0.0000   36.0873                          853.7136
  4     3.520 480     9.880 002     1.040 330     2.000 281
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Fe2Mo3.52013.6:10H2O
4150000 'Halite'           -0.9510   -1.5627                           58.4425
  2     1.000 500     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      NaCl
6050001 'Mirabilite'      -18.9870    1.2116                          322.1959
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  3     2.000 500     1.000 732    10.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2SO4:10H2O
3050000 'Natron'          -15.7450    1.3113                          286.1415
  3     2.000 500     1.000 140    10.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2CO3:10H2O
6050002 'Thenardite'        0.4110    0.2881                          142.0431
  2     2.000 500     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2SO4
5050001 'Thermonatrite'     2.8020   -0.1253                          124.0040
  3     2.000 500     1.000 140     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2CO3:H2O
6050003 'Aphthitalite'      0.0000    3.4260                          332.4119
  3     1.000 500     3.000 410     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NaK3(SO4)2
5050002 'Burkeite'          0.0000    0.8099                          390.0750
  3     6.000 500     1.000 140     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na6(CO3)(SO4)2
5041003 'KNaCO3:6H2O'       0.0000    0.0015                          230.1890
  4     1.000 410     1.000 500     1.000 140     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    KNaCO3:6H2O
5041004 'K-Trona'           0.0000    8.8523                          258.2433
  5     2.000 410     1.000 500     1.000 330     2.000 140     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    K2NaH(CO3)2:2H2O
6050007 'Na3H(SO4)2'        0.0000    0.8459                          262.1044
  3     3.000 500     1.000 330     2.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NaH(SO4)2
5050005 'Na2CO3:7H2O'       0.0000    0.4838                          232.0957
  3     2.000 500     1.000 140     7.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2CO3:7H2O
5050003 'Nahcolite'         0.0000   10.7507                           84.0069
  3     1.000 500     1.000 330     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NaHCO3
5050007 'Trona'             0.0000   11.4045                          226.0262
  4     3.000 500     1.000 330     2.000 140     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na3H(CO3)2:2H2O
1050000 'Na2SO3'            6.0700   -1.4469                          126.0437
  2     2.000 500     1.000 733
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na2SO3
5054000 'NiCO3'            10.0500    6.8461                          118.6992
  2     1.000 540     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiCO3
5054001 'NiCO3:6H2O'        0.0000   12.4607                          226.7909
  3     1.000 540     1.000 140     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiCO3:6H2O
2054000 'Ni(OH)2'          22.9400  -12.7319                           92.7047
  3    -2.000 330     1.000 540     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ni(OH)2
6054000 'Ni4(OH)6SO4'      93.4510  -31.9266                          432.8676
  4    -6.000 330     4.000 540     1.000 732     6.000 002
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ni4(OH)6(SO4)
2054001 'Bunsenite'        23.9350  -12.4424                          74.6894
  3    -2.000 330     1.000 540     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiO
7054000 'Ni3(PO4)2'           0.0000   31.3204                        366.0127
  2     3.000 540     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ni3(PO4)2
1054000 'Millerite'         -2.4830    8.0533                         90.7560
  3    -1.000 330     1.000 540     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiS
6054001 'Retgersite'        -1.0880    2.0509                        262.8453
  3     1.000 540     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiSO4:6H2O(tetra)
6054002 'Morenosite'        -2.9240    2.0663                        280.8606
  3     1.000 540     1.000 732     7.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiSO4:7H2O
8054000 'Ni2SiO4'           33.0700  -14.3812                        209.4631
  3    -4.000 330     2.000 540     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ni2SiO4
1254000 'NiSe'               0.0000   17.7529                        137.6500
  3     1.000 760     1.000 540    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiSe
6154000 'Ahlfeldite'         7.4200   -2.7787                        221.6788
  4     1.000 761     1.000 540     2.000 002    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NiSeO3:2H2O
0060000 'Pb(metal)'          0.4060   -4.2799                        207.2000
  2     1.000 600     2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb(metal)
4160000 'Cotunnite'         -5.5910    4.7681                        278.1054
  2     1.000 600     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbCl2
4160001 'Matlockite'        -7.9380    9.4174                        261.6511
  3     1.000 600     1.000 180     1.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbFCl
4160002 'Phosgenite'         0.0000   19.8089                        545.3146
  3     2.000 600     2.000 180     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2Cl2CO3
5060000 'Cerrusite'         -4.8440     13.54                        267.2092
  2     1.000 600     1.000 140
  1.76426e+3  -9.75150e+4  2.76310e-1  -6.36537e+2  6.13623e+6
  EQ3/6 database: version mdas.3245     PbCO3
4260000 'PbF2'               0.7060    6.1475                        245.1968
  2     1.000 600     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbF2
2060000 'Massicot'          16.7800  -12.9057                        223.1994
  3    -2.000 330     1.000 600     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbO(yellow)
2060001 'Litharge'          16.3810   -12.64                         223.1994
  3    -2.000 330     1.000 600     1.000 002
  2.78403e+2  -1.86946e+4  3.95704e-2  -1.00918e+2  8.51025e+5
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  EQ3/6 database:  version mdas.3245      PbO(red)
2060002 'PbO:1.33H2O'       0.0000  -12.8432                          229.1444
  3    -2.000 330     1.000 600     1.330 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbO:1.33H2O
5060001 'Pb2OCO3'          11.4640    0.5080                          490.4086
  4    -2.000 330     2.000 600     1.000 002     1.000 140
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2OCO3
6060000 'Larnakite'         6.4480    0.2771                          526.4630
  4    -2.000 330     2.000 600     1.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2O(SO4)
6060001 'Pb3O2SO4'         20.7760  -10.8753                          749.6624
  4    -4.000 330     3.000 600     1.000 732     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb3O2(SO4)
6060002 'Pb4O3SO4'         35.0990  -22.0973                          972.8618
  4    -6.000 330     4.000 600     1.000 732     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb4O3(SO4)
7060001 'Cl-Pyromorphite'   0.0000   84.4296                          1356.3668
  3     5.000 600     3.000 580     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb5(PO4)3Cl
7060002 'OH-Pyromorphite'   0.0000   62.7911                          1337.9214
  4    -1.000 330     5.000 600     3.000 580     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb5(PO4)3OH
5060002 'Pb3O2CO3'         26.4280  -11.0219                          713.6080
  4    -4.000 330     3.000 600     1.000 140     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbO2(CO3)
7060003 'Plumbogummite'     0.0000   32.7871                          581.1393
  5    -5.000 330     1.000 600     3.000 030     2.000 580     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbAl3(PO4)2(OH)5:H2O
7060004 'Hinsdalite'        0.0000    2.4987                          581.2236
  6    -6.000 330     1.000 600     3.000 030     1.000 580     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbAl3(PO4)(SO4)(OH)6
8260000 'PbSiO3'            7.2120   -5.8170                          283.2837
  4    -1.000 002    -2.000 330     1.000 600     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbSiO3
8060000 'Pb2SiO4'          23.9730  -18.2652                          506.4831
  3    -4.000 330     2.000 600     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2SiO4
6060003 'Anglesite'        -2.1440     7.85                           303.2636
  2     1.000 600     1.000 732
  1.83327e+3  -1.02950e+5  2.83349e-1  -6.61509e+2  6.42205e+6
  EQ3/6 database: version mdas.3245     PbSO4
1060001 'Galena'           -19.3870    14.85                          239.2660
  3    -1.000 330     1.000 600     1.000 730
  9.93145e+2  -5.14485e+4  1.54011e-1  -3.59708e+2  3.41533e+6
  EQ3/6 database: version mdas.3245     PbS
2060003 'Plattnerite'      70.7360  -49.2903                          239.1988
  4    -4.000 330    -2.000 001     1.000 600     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    PbO2
3060000 'Pb2O3'             0.0000  -61.0378                          462.3982
  4    -6.000 330    -2.000 001     2.000 600     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2O3
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3060001 'Minium'          102.7760  -73.6847                          685.5976
  4    -8.000 330    -2.000 001     3.000 600     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb3O4(red)
2060004 'Pb(OH)2(c)'        13.9860   -8.1427                          241.2147
  3    -2.000 330     1.000 600     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb(OH)2(c)
4160003 'Laurionite'         0.0000   -0.6216                          259.6600
  4    -1.000 330     1.000 600     1.000 180     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbOCl
4160004 'Pb2(OH)3Cl'         0.0000   -8.7936                          500.8747
  4    -3.000 330     2.000 600     3.000 002     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb2(OH)3Cl
5060003 'Hydrocerrusite'     0.0000   18.8619                          775.6331
  4    -2.000 330     3.000 600     2.000 140     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb3(CO3)2(OH)2
2060005 'Pb2O(OH)2'          0.0000  -26.1991                          464.4141
  3    -4.000 330     2.000 600     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb2O(OH)2
4060000 'PbBr2'             -8.1030    5.1800                          367.0080
  2     1.000 600     2.000 130
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbBr2
4060001 'PbBrF'              0.0000    8.4828                          306.1024
  3     1.000 600     1.000 130     1.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbBrF
4360000 'PbI2'              -15.1530    8.0702                          461.0089
  2     1.000 600     2.000 380
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbI2
6060004 'Pb4(OH)6SO4'        0.0000  -21.0975                          1026.9076
  4    -6.000 330     4.000 600     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb4(OH)6(SO4)
7060006 'PbHPO4'            -10.5680   23.8044                          303.1793
  3     1.000 600     1.000 580     1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbHPO4
7060007 'Pb3(PO4)2'          -5.3800   44.3551                          811.5427
  2     3.000 600     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb3(PO4)2
1060000 'Pb(SCN)2'           -8.6340    4.6757                          323.3675
  2     1.000 600     2.000 734
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     Pb(SCN)2
1060002 'PbS2O3'             -5.6840    2.4049                          319.3302
  2     1.000 600     1.000 735
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbS2O3
1260000 'Clausthalite'      -27.9940   21.2258                          286.1600
  3     1.000 760     1.000 600    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbSe
6160000 'PbSeO4'             -3.8040    6.8541                          350.1576
  2     1.000 762     1.000 600
  999.  999.  999.  999.  999.
  Krupka et al. 1988                     PbSeO4
2085000 'ThO2(c)'            0.0000   -6.2849                          264.0374
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  3     1.000 850     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Langmuir and Herman (1980)
2085001 'Thorianite'          0.0000   -1.7768                              264.0374
  3     1.000 850     2.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Langmuir and Herman (1980)
4285000 'ThF4(c)'             0.0000    9.4207                              308.0316
  2     1.000 850     4.000 270
  999.  999.  999.  999.  999.
  Langmuir and Herman (1980)
6085000 'Th(SO4)2(c)'         0.0000    20.350                              424.1612
  2     1.000 850     2.000 732
  999.  999.  999.  999.  999.
  Langmuir and Herman (1980)
0076000 'Se(hex-black)'      -3.8000    7.7110                               78.9600
  3     1.000 760    -1.000 330    -2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Se(hex-black)
0076001 'Se(am)'             -2.6000    7.1246                               78.9600
  3     1.000 760    -1.000 330    -2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Se(am)
1228001 'Ferroselite'         0.0000   18.6119                              213.7670
  4     2.000 760     1.000 280    -2.000 330    -2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      FeSe2
1228000 'FeSe'               -0.5050    7.1554                              134.8070
  3     1.000 760     1.000 280    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      FeSe
1295000 'ZnSe'               -6.3190   11.4140                              144.3500
  3     1.000 760     1.000 950    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      ZnSe
2076100 'SeO2'               -0.3350   -0.1217                              110.9588
  3     1.000 761     1.000 330    -1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      SeO2
6110000 'BaSeO3'              6.2790   -4.1546                              264.2852
  3     1.000 761     1.000 100    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      BaSeO3
6115000 'CaSeO3:2H2O'         4.6490   -2.7853                              203.0668
  4     1.000 761     1.000 150     2.000 002    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      CaSeO3:2H2O
6128100 'Fe2(SeO3)3:2H2O'     0.0000   20.6606                              528.5992
  4     3.000 761     2.000 281     2.000 002    -3.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Fe2(SeO3)3:2H2O
6128101 'Fe2(OH)4SeO3'        0.0000   -1.5253                              306.6816
  4     1.000 761     2.000 281     4.000 002    -5.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Fe2(OH)4(SeO3)
6146000 'MgSeO3:6H2O'        -1.2500   -3.9515                              259.3549
  4     1.000 761     1.000 460     6.000 002    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      MgSeO3:6H2O
6180000 'SrSeO3'              0.0000   -0.2639                              214.5782
  3     1.000 761     1.000 800    -1.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      SrSeO3
2076200 'SeO3'               34.9750  -21.0330                              126.9582
  3     1.000 762     2.000 330    -1.000 002
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    SeO3
6110001 'BaSeO4'          -2.0110    5.2064                          280.2846
  2     1.000 762     1.000 100
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    BaSeO4
6115001 'CaSeO4:2H2O'      1.6480    3.0961                          219.0662
  3     1.000 762     1.000 150     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    CaSeO4:2H2O
6180001 'SrSeO4'          -2.7010    6.7222                          230.5776
  2     1.000 762     1.000 800
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    SrSeO4
2077000 'Chalcedony'      -4.6200    3.73                             60.0843
  2    -2.000 002     1.000 770
  6.72519e+2  -4.42002e+4  7.56149e-2  -2.34550e+2  3.31575e+6
  EQ3/6 database: version mdas.3245     SiO2
2077001 'Cristobalite'    -4.7800    3.45                             60.0843
  2    -2.000 002     1.000 770
  6.56659e+2  -4.31487e+4  7.41828e-2  -2.29102e+2  3.22675e+6
  EQ3/6 database: version mdas.3245     SiO2
2077002 'Quartz'          -5.4000    4.00                             60.0843
  2    -2.000 002     1.000 770
  6.35196e+2   -4.18406e+4  7.08653e-2  -2.21131e+2  3.16747e+6
  EQ3/6 database: version mdas.3245     SiO2
2077003 'SiO2(am)'        -3.9100    2.71                             60.0843
  2    -2.000 002     1.000 770
  6.32244e+2  -4.06305e+4  7.40829e-2  -2.21557e+2  2.92383e+6
  EQ3/6 database:  version mdas.3245    SiO2
2077004 'SiO2(ppt)'       -3.9100    2.87                             60.0843
 2     -2.000 002     1.000 770
 999.  999.  999.  999.  999.
 Felmy et al. (1984)                    SiO2
8015001 'Ca-Olivine'      54.7430  -37.7318                          172.2391
  3    -4.000 330     1.000 770     2.000 150
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ca2SiO4
8015002 'Larnite'         57.2860   -38.47                           172.2391
  3    -4.000 330     1.000 770     2.000 150
  1.33604e+3  -9.30130e+4  1.77916e-1  -4.74917e+2  5.29495e+6
  EQ3/6 database: version mdas.3245     Ca2SiO4
8015003 'Monticellite'    49.4700   -29.59                           156.4661
  4    -4.000 330     1.000 770     1.000 150     1.000 460
  1.42273e+3  -9.66417e+4  1.85934e-1  -5.03923e+2  5.62807e+6
  EQ3/6 database: version mdas.3245     CaMgSiO4
8015004 'Merwinite'       107.2080   -68.51                           328.7052
  4    -8.000 330     2.000 770     1.000 460     3.000 150
  2.65576e+3  -1.83711e+5  3.50326e-1  -9.41954e+2  1.05126e+7
  EQ3/6 database: version mdas.3245     Ca3MgSi2O8
8015005 'Akermanite'      74.1320   -45.32                           272.6278
  5    -1.000 002    -6.000 330     2.000 770     2.000 150     1.000 460
  2.34579e+3  -1.60069e+5  3.01874e-1  -8.29458e+2  9.61937e+6
  EQ3/6 database: version mdas.3245     Ca2MgSi2O7
8015006 'Gehlenite'       109.3610   -54.59                           274.2004
  5   -10.000 330     2.000 030     1.000 770     2.000 150     3.000 002
  2.23810e+3  -1.51758e+5  3.23473e-1  -7.95872e+2  7.92038e+6
  EQ3/6 database: version mdas.3245     Ca2Al2SiO7
8015007 'Ca3SiO5'         106.3860  -73.9068                          228.3165
  4    -6.000 330     1.000 770     3.000 150     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ca3SiO5
8046000 'Forsterite'      53.3790   -27.86                           140.6931
  3    -4.000 330     2.000 460     1.000 770
  1.40532e+3  -9.54000e+4  1.83305e-1  -4.96825e+2  5.46755e+6
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  EQ3/6 database: version mdas.3245       Mg2SiO4
8215000 'Diopside'          35.1990    -20.97                              216.5504
  5    -2.000 002     1.000 150     1.000 460     2.000 770    -4.000 330
  2.66145e+3  -1.63194e+5  3.58876e-1  -9.49947e+2  9.64580e+6
  EQ3/6 database: version mdas.3245       CaMgSi2O6
8215001 'Tremolite'         109.5230    -61.24                              812.3665
  5    -8.000 002     2.000 150     5.000 460     8.000 770   -14.000 330
  7.95405e+3  -5.25396e+5  9.83256e-1  -2.80093e+3  3.41802e+7
  EQ3/6 database: version mdas.3245       Ca2Mg5Si8O22(OH)2
8215002 'Wollastonite'      19.5470    -13.76                              116.1617
  4    -1.000 002    -2.000 330     1.000 770     1.000 150
  9.85741e+2  -6.64976e+4  1.23802e-1  -3.48017e+2  4.24653e+6
  EQ3/6 database: version mdas.3245       CaSiO3
8215003 'Ps-Wollastonite'  21.1170   -13.9274                              116.1617
  4    -1.000 002    -2.000 330     1.000 770     1.000 150
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      CaSiO3
8246000 'Enstatite'         22.2940    -11.47                              100.3887
  4    -1.000 002     1.000 460     1.000 770    -2.000 330
  1.44901e+3  -8.91876e+4  1.95500e-1  -5.16695e+2  5.23471e+6
  EQ3/6 database: version mdas.3245       MgSiO3
8415000 'Leonhardite'       85.4170   -16.5633                              922.8587
  5    -1.000 002   -16.000 330     2.000 150     8.000 770     4.000 030
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Ca2Al4Si8O24:7H2O
8415001 'Anorthite'         70.6800    -24.87                              278.2073
  4     1.000 150     2.000 030     2.000 770    -8.000 330
  2.69626e+3  -1.77098e+5  3.63645e-1  -9.52002e+2  1.06773e+7
  EQ3/6 database: version mdas.3245       CaAl2Si2O8
8415002 'Laumontite'         0.0000    -11.96                              470.4370
  4     1.000 150     2.000 030     4.000 770    -8.000 330
  4.06074e+3  -2.63514e+5  5.12205e-1  -1.42889e+3  1.72564e+7
  EQ3/6 database: version mdas.3245       CaAl2Si4O12:4H2O
8415003 'Wairakite'         63.1760    -16.37                              434.4064
  5     1.000 150     2.000 030     4.000 770    -8.000 330    -2.000 002
  4.00970e+3  -2.63106e+5  5.07929e-1  -1.40937e+3  1.71013e+7
  EQ3/6 database: version mdas.3245       CaAl2Si4O12:2H2O
8441000 'Kalsilite'         29.0290    -10.04                              158.1629
  4    -4.000 330     1.000 770     1.000 030     1.000 410
  1.19654e+3  -7.79562e+4  1.59789e-1  -4.23124e+2  4.82165e+6
  EQ3/6 database: version mdas.3245       KAlSiO4
8441001 'Leucite'           22.2450   -6.7501                              218.2472
  5    -2.000 002    -4.000 330     2.000 770     1.000 030     1.000 410
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      KAlSi2O6
8441002 'K-Feldspar'        12.5200     1.13                              278.3315
  5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
  2.53904e+3  -1.64744e+5  3.11524e-1  -8.91701e+2  1.13997e+7
  EQ3/6 database: version mdas.3245       KAlSi3O8
8441003 'High-Sanidine'     14.4620    -0.07                              278.3315
  5    -4.000 002    -4.000 330     3.000 770     1.000 030     1.000 410
  2.57218e+3  -1.67522e+5  3.14802e-1  -9.02903e+2  1.15523e+7
  EQ3/6 database: version mdas.3245       KAlSi3O8
8447000 'Rhodonite'          0.0000    -9.73                              131.0222
  4     1.000 470     1.000 770    -2.000 330    -1.000 002
  1.02106e+3  -6.75054e+4  1.28539e-1  -3.60189e+2  4.31740e+6
  EQ3/6 database: version mdas.3245       MnSiO3
8450000 'Magadiite'          0.0000   14.3064                              532.6483
  4    -1.000 330    -9.000 002     1.000 500     7.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      NaSi7O13(OH)3:3H2O
8450001 'Analcime'          21.9440    -5.32                              220.1540
  5     1.000 500     1.000 030     2.000 770    -1.000 002    -4.000 330
  2.06838e+3  -1.33447e+5  2.59593e-1  -7.28364e+2  8.78191e+6
  EQ3/6 database: version mdas.3245       NaAlSi2O6:H2O
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8450002 'Low-Albite'        17.3740     -1.91                                  262.2230
  5     1.000 500     1.000 030     3.000 770    -4.000 330    -4.000 002
  2.65845e+3  -1.73401e+5  3.24270e-1  -9.33008e+2  1.18437e+7
  EQ3/6 database: version mdas.3245        NaAlSi3O8
8450003 'High-Albite'       19.9740     -3.29                                  262.2230
  5     1.000 500     1.000 030     3.000 770    -4.000 330    -4.000 002
  3.09719e+3  -2.01130e+5  3.78396e-1  -1.08788e+3  1.36211e+7
  EQ3/6 database: version mdas.3245        NaAlSi3O8
8450004 'Nepheline'         33.2240    -12.95                                  142.0544
  4    -4.000 330     1.000 770     1.000 030     1.000 500
  1.34951e+3  -8.82443e+4  1.78187e-1  -4.76819e+2  5.35646e+6
  EQ3/6 database: version mdas.3245        NaAlSiO4
8450005 'Phillipsite'        0.0000   -3.4524                                  576.5851
  6   1.000 500    1.000 410    2.000 030    6.000 770   -8.000 330   -6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       NaKAl2Si6O16:2H2O
8603000 'Halloysite'        39.7580   -8.9739                                  258.1604
  4     2.000 030     2.000 770     1.000 002    -6.000 330
  999. 999. 999. 999. 999.
  Krupka et al. 1988                       Al2Si2O5(OH)4
8603001 'Kaolinite'            35.3    -7.435                                  258.1604
  4     2.000 030     2.000 770     1.000 002    -6.000 330
  5.56367e+3  -3.29275e+5  7.56645e-1  -1.98589e+3  1.97043e+7
  Reed and Spycher 1989: SOLVEQ database   Al2Si2O5(OH)4
8603002 'Pyrophyllite'      28.4150      1.27                                   360.3138
  4     2.000 030     4.000 770    -4.000 002    -6.000 330
  3.65068e+3  -2.36667e+5  4.56616e-1  -1.28179e+3  1.59977e+7
  EQ3/6 database: version mdas.3245        Al2Si4O10(OH)2
8615000 'Margarite'          0.0000   -37.65                                   398.1867
  5     1.000 150     4.000 030     2.000 770     4.000 002   -14.000 330
  3.69943e+3  -2.39083e+5  5.23335e-1  -1.31098e+3  1.35763e+7
  EQ3/6 database: version mdas.3245        CaAl2(Al2Si2)O10(OH)2
8615001 'Ca-Nontronite'      0.0000     11.86                                   424.2930
  6  -7.320 330    -2.680 002     0.330 030     2.000 281     0.167 150     3.670 770
  3.88576e+3  -2.45242e+5  4.98229e-1  -1.36822e+3  1.65074e+7
  EQ3/6 database: version mdas.3245        Ca.167Fe2Al.33Si3.67O10(OH)2
8615002 'Prehnite'           78.0590   -33.28                                   412.3843
  4     2.000 150     2.000 030     3.000 770   -10.000 330
  6.63611e+3  -3.93553e+5  9.21366e-1  -2.37573e+3  2.26174e+7
  EQ3/6 database: version mdas.3245        Ca2Al2Si3O10(OH)2
8615002 'Ca-Montmorillonite' 0.0000    -1.07                                   366.0480
  6   0.165 150     0.330 460     1.670 030     4.000 770    -6.000 330    -4.000 002
  3.80666e+3  -2.45776e+5  4.77352e-1  -1.33832e+3  1.65248e+7
  EQ3/6 database: version mdas.3245        Ca.165Mg.33Al1.7Si4O10(OH)2
8628000 'Greenalite'         0.0000   -22.67                                   371.7384
  4    -6.000 330     3.000 280     2.000 770     1.000 002
  2.57530e+3  -1.65949e+5  3.34204e-1  -9.12023e+2  1.02883e+7
  EQ3/6 database: version mdas.3245        Fe3Si2O5(OH)4
8628001 'Chlorite-Fe-1'      0.0000  -23.7250                                  659.1330
  6   2.470 770    3.130 030    3.290 280    1.050 460    8.120 002  -18.070 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Mg1.05Fe3.29Al3.13Si2.47O10(OH)8
8628002 'Chlorite-Fe-2'      0.0000  -22.4970                                  634.9880
  7  2.840 770 2.910 030  2.610 280  1.160 460  0.120 281  6.640 002  -16.630 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       Mg1.16Fe2.61Al2.91Si2.84O10(OH)8
8633000 'H-Nontronite'       0.0000     12.82                                   418.0149
  5     0.330 030     2.000 281     3.670 770    -6.990 330    -2.680 002
  3.82157e+3  -2.41420e+5  4.88120e-1  -1.34497e+3  1.63128e+7
  EQ3/6 database: version mdas.3245        H0.33Fe2Al0.33Si3.67O10(OH)2
8641000 'Muscovite'          59.4250   -11.02                                   398.3081
  4     1.000 410     3.000 030     3.000 770   -10.000 330
  3.65024e+3  -2.33771e+5  4.83735e-1  -1.28827e+3  1.47877e+7
  EQ3/6 database: version mdas.3245        KAl3Si3O10(OH)2
8641001 'Annite'             65.7700  -23.4196                                  511.8860
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  5     1.000 410     3.000 280     1.000 030     3.000 770   -10.000 330
  3.66297e+3  -2.37818e+5  4.76959e-1  -1.29460e+3  1.48705e+7
  EQ3/6 database: version mdas.3245       KFe3AlSi3O10(OH)2
8641002 'K-Nontronite'      0.0000     12.15                              430.5830
  6  -7.320 330  -2.680 002   0.330 030   2.000 281    0.330 410    3.670 770
  3.90054e+3  -2.45701e+5  4.99716e-1  -1.37394e+3  1.65745e+7
  EQ3/6 database: version mdas.3245       K0.3Fe2Al0.33Si3.67O10(OH)2
8641003 'Illite'            49.8550     -7.06                              383.9010
  6   0.600 410    0.250 460    2.300 030    3.500 770   -8.000 330   -2.000 002
  3.72181e+3  -2.39110e+5  4.81177e-1  -1.31170e+3  1.55908e+7
  EQ3/6 database: version mdas.3245       K0.6Mg0.25Al2.3Si3.5O10(OH)2
8641004 'K-Montmorillonite' 0.0000     -0.72                              372.3385
  6   0.330 410    0.330 460    1.670 030    4.000 770   -6.000 330   -4.000 002
  3.90054e+3  -2.45701e+5  4.99716e-1  -1.37394e+3  1.65745e+7
  EQ3/6 database: version mdas.3245       K0.33Mg0.33Al1.67Si4O10(OH)2
8646000 'Chrysotile'          46.8     -32.20                             277.1124
  4    -6.000 330     3.000 460     2.000 770     1.000 002
  -1.3248e+1  -1.02171e+4  0.0000  6.1894e+0  0.0000
  Nordstrom et al. 1990                   Mg3Si2O5(OH)4
8646001 'Phlogopite'        42.3000     -36.59                             417.2600
  5   -10.000 330     1.000 410     3.000 460     1.000 030     3.000 770
  3.77709e+3  -2.46922e+5  4.87728e-1  -1.33444e+3  1.52093e+7
  EQ3/6 database: version: mdas.3245      KMg3AlSi3O10(OH)2
8646002 'Talc'              43.3460     -21.14                             379.2657
  4    -4.000 002     3.000 460     4.000 770    -6.000 330
  3.83698e+3  -2.52438e+5  4.67988e-1  -1.34914e+3  1.66606e+7
  EQ3/6 database: version mdas.3245       Mg3Si4O10(OH)2
8646003 'Sepiolite(c)'      0.0000     -30.44                             323.9152
  4    -1.000 002     4.000 460     6.000 770    -8.000 330
  5.54850e+3  -3.63459e+5  6.64905e-1  -1.95181e+3  2.41360e+7
  EQ3/6 database: version mdas.3245       Mg2Si3O7.5(OH):3H2O
8646004 'Sepiolite(am)'     0.0000   -18.7736                             323.9152
  4    -0.500 002     2.000 460     3.000 770    -4.000 330
  999.  999.  999.  999.  999.
  EQ3/6 database: version mdas.3245       Mg2Si3O7.5(OH):3H2O
8646005 'Mg-Nontronite'     0.0000     11.90                              421.6910
  6  -7.320 330   -2.680 002    0.330 030    2.000 281    0.167 460    3.670 770
  3.89253e+3  -2.45887e+5  4.98406e-1  -1.37025e+3  1.65435e+7
  EQ3/6 database: version mdas.3245       Mg0.167Fe2Al0.33Si3.67O10(OH)2
8646006 'Mg-Montmorillonite' 0.0000    -0.96                              363.4463
  5     0.495 460     1.670 030     4.000 770    -6.000 330    -4.000 002
  3.83122e+3  -2.47304e+5  4.80371e-1  -1.34688e+3  1.66089e+7
  EQ3/6 database: version mdas.3245       Mg0.495Al1.67Si4O10(OH)2
8646007 'Chlorite-Mg-Fe-2'  0.0000   -51.8140                             573.8980
  7   2.99 770   2.40 030   3.52 460   0.21 281   0.57 280   6.04 002 -16.01 330
  999.  999.  999.  999.  999.
  Krupka et al 1988                       Mg3.52Fe.57Fe.21Al2.4Si2.99O10(OH)8
8646008 'Chlorite-Mg'      158.6200   -73.7040                             555.7970
  5   5.000 460   2.000 030   3.000 770   6.000 002 -16.000 330
  999.  999.  999.  999.  999.
  Krupka et al 1988                       Mg5Al2Si3O10(OH)8
8646009 'Chlorite-Mg-Fe-1'  0.0000   -53.2050                             584.0570
  7   2.97 770   2.47 030   3.24 460   0.99 280   0.07 281   6.12 002 -16.08 330
  999.  999.  999.  999.  999.
  Krupka et al 1988                       Mg3.24Fe.99Fe.07Al2.47Si2.97O10(OH)8
8646010 'Kerolite'          0.0000     -25.79                             397.3041
  4     3.000 460     4.000 770    -6.000 330    -3.000 002
  999.  999.  999.  999.  999.
  Nordstrom et al. 1990                   Mg3Si4O10(OH)2:H2O
8650000 'Paragonite'        0.0000     -14.96                             382.2010
  4   1.00 500   3.00 030   3.00 770 -10.00 330
  3.69690e+3  -2.37884e+5  4.88045e-1  -1.30418e+3  1.49009e+7
  EQ3/6 database: version mdas.3245       NaAl3Si3O10(OH)2
8650001 'Na-Nontronite'     0.0000     11.81                              425.2670
  6  -7.32 330  -2.68 002   0.33 030    2.00 281   0.33 500   3.67 770
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  3.87984e+3  -2.44635e+5  4.96340e-1  -1.36632e+3  1.64795e+7
  EQ3/6 database: version mdas.3245        Na.33Fe2Al0.33Si3.67O10(OH)2
8650002 'Na-Montmorillonite' 0.000      -1.06                              367.0215
  6   0.33 500   0.33 460   1.67 030   4.00 770  -6.00 330  -4.00 002
  3.83920e+3  -2.47432e+5  4.80551e-1  -1.35013e+3  1.66400e+7
  EQ3/6 database: version mdas.3245        Na.33Mg.33Al1.67Si4O10(OH)2
1074000 'Stibnite'          -69.2897  60.1343                              339.6800
  4     2.000 740     3.000 730     3.000 330     -6.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb2S3
2074000 'Sb2O3'             -4.4949    8.4806                              291.4982
  2     2.000 740    -3.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb2O3
2074001 'Sb2O4'             16.2723   -3.4033                              307.4976
  4     2.000 740    -2.000 002    -2.000 330    -2.000 001
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb2O4
2074100 'Sb2O5'              0.0000   19.6540                              323.4970
  3     2.000 741     2.000 330    -7.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb2O5
2074002 'Sb4O6(cub)'        -14.6016   19.6610                              582.9964
  2     4.000 740    -6.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb4O6(cub)
2074003 'Sb4O6(ortho)'      -8.9850   17.0156                              582.9964
  2     4.000 740    -6.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb4O6(ortho)
2074004 'Sb(OH)3'            0.0000     7.095                              172.7719
  1     1.000 740
  999.  999.  999.  999.  999.
  Sehmel (1989)                            Sb(OH)3
4174000 'SbCl3'              8.4132   -0.5923                              228.1090
  4     1.000 740     3.000 180     3.000 330     -3.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            SbCl3
4074000 'SbBr3'              5.0739   -1.0532                              361.4620
  4     1.000 740     3.000 130     3.000 330     -3.000 002
  999.  999.  999.  999.  999.
  Sehmel (1989)                            SbBr3
6080000 'Celestite'           1.037      6.63                              183.6836
  2     1.000 800     1.000 732
  1.48059622e+4  -7.56968533e+5  2.466092e+0  -5.4363588e+3  4.055360e+7
  Nordstrom et al. 1990                    SrSO4
4280000 'SrF2'              -1.2540    8.3641                              125.6168
  2     1.000 800     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                       SrF2
5080000 'Strontianite'        0.40     9.271                              147.6292
  2     1.000 800     1.000 140
  -1.550305e+2  7.239594e+3  0.0000  5.658638e+1  0.0000
  Nordstrom et al. 1990                    SrCO3
2080000 'SrO'                0.0000    -41.89                              103.6194
  3     1.000 800     1.000 002    -2.000 330
  4.93520e+2  -4.08680e+4  6.96659e-2  -1.77107e+2  1.69968e+6
  EQ3/6 database: version mdas.3245        SrO
2080001 'Sr(OH)2'            0.0000    -27.52                              121.6348
  3     1.000 800     2.000 002    -2.000 330
  3.97958e+2  -2.95065e+4  5.30278e-2  -1.43504e+2  1.13433e+6
  EQ3/6 database: version mdas.3245        Sr(OH)2
2089100 'Uraninite'          18.630     4.700                              270.0278
  3    -4.000 330     1.000 891     2.000 002
  999.  999.  999.  999.  999.
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  NEA (1989)                                  UO2
2089101 'UO2(am)'            26.230    -0.934                          270.0278
  3    -4.000 330     1.000 891     2.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  UO2(am)
3089100 'U409(c)'            101.235    3.384                          1096.1106
  4   -18.000 330    -2.000 001     4.000 891     9.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U409(c)
3089101 'U308(c)'            116.020   -21.107                          842.0822
  4   -16.000 330    -4.000 001     3.000 891     8.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U308(c)
8089100 'Usio4(c)'           14.548     7.620                          330.1121
  3    -4.000 330     1.000 891     1.000 770
  999.  999.  999.  999.  999.
  NEA (1989)                                  Usio4(c)
4289100 'UF4(c)'             18.900    18.606                          314.0226
     2     1.000 891     4.000 270
  999.  999.  999.  999.  999.
  NEA (1989)                                  UF4(c)
4289101 'UF4:2.5H20'          0.588    27.570                          359.0606
  3     1.000 891     4.000 270     2.500 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  UF4:2.5H20
7089100 'U(HP04)2:4H20'      -3.840    51.584                          502.0486
  4     1.000 891     2.000 580     2.000 330     4.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U(HP04)2:4H20
7015000 'Ningyoite'           2.270    53.906                          504.0822
  4     1.000 891     1.000 150     2.000 580     2.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  CaU(P04)2:2H20
2089300 'U03(c)'             19.315    -7.719                          286.0272
  3    -2.000 330     1.000 893     1.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U03(c)
2089301 'Gummite'            23.015   -10.403                          286.0272
  3    -2.000 330     1.000 893     1.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U03
2089302 'B-U02(OH)2'         13.730    -5.544                          304.0424
  3    -2.000 330     1.000 893     2.000   2
  999.  999.  999.  999.  999.
  NEA (1989)                                  B-U02(OH)2
2089303 'Schoepite'           0.000    -4.820                          322.0576
  3    -2.000 330     1.000 893     3.000 002
  999.  999.  999.  999.  999.
  NEA (1989)                                  U03:2H20
5089300 'Rutherfordine'       0.000    14.450                          330.0370
  2     1.000 893     1.000 140
  999.  999.  999.  999.  999.
  NEA (1989)                                  U02(C03)
7089300 '(U02)3(P04)2'      -94.900    49.037                          1000.0262
  2     3.000 893     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                                  (U02)3(P04)2
7089301 'H-Autunite'          3.600    47.931                          732.0144
  3     2.000 330     2.000 893     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                                  H2(U02)2(P04)2
7050000 'Na-Autunite'         0.460    47.409                          775.9780
  3     2.000 500     2.000 893     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                                  Na2(U02)2(P04)2
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7041000 'K-Autunite'          -5.860    48.244                              808.2024
  3     2.000 410     2.000 893     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              K2(UO2)2(PO4)2
7049000 'Uramphite'           -9.700    51.749                              766.0756
  3     2.000 893     2.000 490     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              (NH4)2(UO2)(PO4)2
7046000 'Saleeite'            20.180    43.646                              754.3104
  3     2.000 893     1.000 460     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Mg(UO2)2(PO4)2
7015001 'Autunite'            14.340    43.927                              770.0784
  3     2.000 893     1.000 150     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Ca(UO2)2(PO4)2
7080000 'Sr-Autunite'         13.050    44.457                              817.6184
  3     2.000 893     1.000 800     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Sr(UO2)2(PO4)2
7010000 'Uranocircite'        10.100    44.631                              867.3384
  3     2.000 893     1.000 100     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Ba(UO2)2(PO4)2
7028000 'Bassetite'           19.900    44.485                              785.8454
  3     2.000 893     1.000 280     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Fe(UO2)2(PO4)2
7023102 'Torbernite'          15.900    45.279                              793.5444
  3     2.000 893     1.000 231     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Cu(UO2)2(PO4)2
7060000 'Przhevalskite'       11.000    44.365                              937.1883
  3     2.000 893     1.000 600     2.000 580
  999.  999.  999.  999.  999.
  NEA (1989)                              Pb(UO2)2(PO4)2
8015000 'Uranophane'           0.000   -17.490                              766.5176
  4    -6.000 330     2.000 893     1.000 150     2.000 770
  999.  999.  999.  999.  999.
  NEA (1989)                              Ca(UO2)2Si2O7:H2O
5189300 'UO2(NO3)2'           20.140   -12.369                              394.0380
  2     1.000 893     2.000 492
  999.  999.  999.  999.  999.
  NEA (1989)                              UO2(NO3)2
5189301 'UO2(NO3)2:2H2O'       6.060    -4.851                              430.0690
  3     1.000 893     2.000 492     2.000   2
  999.  999.  999.  999.  999.
  NEA (1989)                              UO2(NO3)2:2H2O
5189302 'UO2(NO3)2:3H2O'       2.405    -3.642                              448.0840
  3     1.000 893     2.000 492     3.000   2
  999.  999.  999.  999.  999.
  NEA (1989)                              UO2(NO3)2:3H2O
5189303 'UO2(NO3)2:6H2O'      -4.770    -2.300                              502.1300
  3     1.000 893     2.000 492     6.000   2
  999.  999.  999.  999.  999.
  NEA (1989)                              UO2(NO3)2:6H2O
7550000 'Na3UO4'              85.635   -59.183                              370.9960
  5     3.000 500     0.500 891     0.500 893     3.000 002    -6.000 330
  999.  999.  999.  999.  999.
  NEA (1989)                              Na3UO4
7550001 'Na2UO4'              42.490   -30.317                              348.0060
  4     2.000 500     1.000 893     2.000 002    -4.000 330
  999.  999.  999.  999.  999.
  NEA (1989)                              Na2UO4
7550002 'Na2U2O7'             42.905   -23.966                              634.0030
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  4     2.000 500     2.000 893     3.000 002    -6.000 330
  999.  999.  999.  999.  999.
  NEA (1989)                              Na2U2O7
0090000 'V(metal)'          0.0000  -42.3665                          50.9415
  2     1.000 901     3.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      V(metal)
2090000 'VO'                0.0000  -13.0940                          66.9409
  4    -2.000 330     1.000 901     1.000 002     1.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VO
4190000 'VCl2'              0.0000  -16.5127                          121.8469
  3     1.000 901     2.000 180     1.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VCl2
3090100 'Karelianite'       0.0000    -9.94                           149.8812
  3    -6.000 330     2.000 901     3.000 002
 -3.00650e+3  1.34522e+5 -5.14146e-1  1.12020e+3 -6.51017e+6
  EQ3/6 database:  version mdas.3245      V2O3
2090100 'V(OH)3'            0.0000   -7.6414                          101.9635
  3    -3.000 330     1.000 901     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      V(OH)3
4190100 'VCl3'              0.0000  -21.7784                          157.2996
  2     1.000 901     3.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VCl3
4190101 'VOCl'              0.0000   -9.4841                          102.3936
  4     1.000 901     1.000 180     1.000 002    -2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VOCl
3090200 'V2O4'             28.1200   -8.5393                          165.8806
  3    -4.000 330     2.000 902     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      V2O4
2090200 'VO(OH)2'           0.0000   -5.8199                          100.9556
  3    -2.000 330     1.000 902     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988: uttonite?           VO(OH)2
4290200 'VF4'              44.9850  -12.8587                          126.9351
  4    -1.000 002     1.000 902     4.000 270     2.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VF4
6090200 'VOSO4(c)'         20.7150   -3.7001                          163.0045
  2     1.000 902     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VOSO4(c)
7090200 '(VO)3(PO4)2'       0.0000   25.1560                          390.7654
  2     3.000 902     2.000 580
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      (VO)3(PO4)2
4190200 'VOCl2'            28.2040  -12.7671                          137.8463
  2     1.000 902     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      VOCl2
3090300 'V2O5'              8.3350    1.4623                          181.8800
  3    -2.000 330     2.000 903     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      V2O5
7315001 'Ca(VO3)2'         20.2790   -5.7019                          237.9574
  4    -4.000 330     1.000 150     2.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                      Ca(VO3)2
7315002 'Ca3(VO4)2'        70.1470  -39.0146                          350.1122
  4    -8.000 330     3.000 150     2.000 903     4.000 002
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  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ca3(VO4)2
7315003 'Ca2V2O7'          38.1430  -17.4033                        294.0348
  4    -6.000 330     2.000 150     2.000 903     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ca2V2O7
7328000 'Fe(VO3)2'         14.7450    3.8790                        253.7264
  4    -4.000 330     1.000 280     2.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Fe(VO3)2
7346000 'Mg(VO3)2'         32.6800  -11.2880                        222.1844
  4    -4.000 330     1.000 460     2.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mg(VO3)2
7346001 'Mg2V2O7'          61.0250  -26.3325                        262.4888
  4    -6.000 330     2.000 460     2.000 903     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Mg2V2O7
7349000 'NH4VO3'            3.5991   -2.6901                        116.9782
  4    -2.000 330     1.000 490     1.000 903     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    (NH4)VO3
7350000 'NaVO3'             7.1150   -3.7910                        121.9295
  4    -2.000 330     1.000 500     1.000 903     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    NaVO3
7350001 'Na3VO4'           44.3100  -36.8259                        183.9084
  4    -4.000 330     3.000 500     1.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na3VO4
7350002 'Na4V2O7'          47.9250  -37.3184                        305.8379
  4    -6.000 330     4.000 500     2.000 903     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Na4V2O7
7360000 'Pb3(VO4)2'        17.3980   -6.0962                        851.4782
  4    -8.000 330     3.000 600     2.000 903     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb3(VO4)2
7360001 'Pb2V2O7'           6.4770    1.9769                        628.2788
  4    -6.000 330     2.000 600     2.000 903     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Pb2V2O7
7302000 'AgVO3'             0.0000   -0.7762                        206.8079
  4    -2.000 330     1.000 020     1.000 903     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    AgVO3
7302001 'Ag2HVO4'           0.0000   -1.4865                        331.6834
  4    -3.000 330     2.000 020     1.000 903     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    AgHVO4
7302002 'Ag3H2VO5'          0.0000   -5.1888                        456.5590
  4    -4.000 330     3.000 020     1.000 903     3.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Ag3H2VO5
4190300 'VO2Cl'             9.6520   -2.8469                        118.3930
  2     1.000 903     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    VO2Cl
3090101 'V3O5'             23.5300   -1.8251                        232.8215
  4    -4.000 330     3.000 902     2.000 002     2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    V3O5
3090201 'V4O7'             39.1650   -7.1723                        315.7618
  4    -6.000 330     4.000 902     3.000 002     2.000 001
  999.  999.  999.  999.  999.
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  Krupka et al. 1988                    V407
3090202 'V6013'          -64.8250   61.2225                          513.6412
  4    -2.000 330     6.000 903     1.000 002     4.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    V6013
5095002 'Hydrozincite'     0.0000  -12.6806                          549.0124
  4     5.000 950     2.000 140     6.000 002    -6.000 330
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn5(OH)6(CO3)2
0095000 'Zn(metal)'       36.7810  -25.7629                           65.3900
  2     1.000 950     2.000 001
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(metal)
4195000 'ZnCl2'           17.4860   -7.0279                          136.2954
  2     1.000 950     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnCl2
5093000 'Smithsonite'      4.3610    9.87                            125.3992
  2     1.000 950     1.000 140
  1.82545e+3  -1.02118e+5  2.86246e-1  -6.57963e+2  6.19169e+6
  EQ3/6 database: version mdes.3245     ZnCO3
5095001 'ZnCO3:H2O'        0.0000   10.2662                          143.4145
  3     1.000 950     1.000 140     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnCO3:H2O
4295000 'ZnF2'           378.4770    1.5180                          103.3868
  2     1.000 950     2.000 270
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnF2
2095000 'Zn(OH)2(am)'      0.0000  -12.4519                           99.4047
  3    -2.000 330     1.000 950     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(OH)2(am)
2095001 'Zn(OH)2(c)'       0.0000  -12.1991                           99.4047
  3    -2.000 330     1.000 950     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(OH)2(c)
2095002 'Zn(OH)2(beta)'   19.9910  -11.8802                           99.4047
  3    -2.000 330     1.000 950     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(OH)2(beta)
2095003 'Zn(OH)2(gamma)'   0.0000  -11.8289                           99.4047
  3    -2.000 330     1.000 950     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(OH)2(gamma)
2095004 'Zn(OH)2(eps)'    19.6710  -11.6090                           99.4047
  3    -2.000 330     1.000 950     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(OH)2(eps)
4195001 'Zn2(OH)3Cl'       0.0000  -15.1764                          217.2547
  4    -3.000 330     2.000 950     3.000 002     1.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn2(OH)3Cl
4195002 'Zn5(OH)8Cl2'      0.0000  -38.4985                          533.9141
  4    -8.000 330     5.000 950     8.000 002     2.000 180
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn5(OH)8Cl2
6095000 'Zn2(OH)2SO4'      0.0000   -7.5006                          260.8583
  4    -2.000 330     2.000 950     2.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn2(OH)2SO4
6095001 'Zn4(OH)6SO4'      0.0000  -28.3988                          459.6676
  4    -6.000 330     4.000 950     6.000 002     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn4(OH)6(SO4)
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5195000 'Zn(NO3)2:6H2O'    -6.6370   -2.5581                          297.4916
  3     1.000 950     2.000 492     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn(NO3)2:6H2O
2095006 'Zincite'           21.8560    -11.21                           81.3894
  3    -2.000 330     1.000 950     1.000 002
  3.92034e+2  -2.58668e+4  5.75170e-2  -1.40373e+2  1.21831e+6
  EQ3/6 database: version mdas.3245       ZnO
6095002 'Zn3O(SO4)2'        62.0090  -19.0195                          404.2966
  4    -2.000 330     3.000 950     2.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn3O(SO4)2
7095000 'Zn3(PO4)2:4H2O'     0.0000   32.1824                          458.1738
  3     3.000 950     2.000 580     4.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn3(PO4)2:4H2O
1095000 'ZnS(am)'           -3.6700    9.0516                           97.4560
  3    -1.000 330     1.000 950     1.000 730
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnS(am)
1095001 'Sphalerite'        -8.2420     11.44                           97.4560
  3    -1.000 330     1.000 950     1.000 730
  1.07379e+3  -5.78346e+4  1.65144e-1  -3.87264e+2  3.61312e+6
  EQ3/6 database: version mdas.3245       ZnS
1095002 'Wurtzite'          -5.0520     9.16                           97.4560
  3    -1.000 330     1.000 950     1.000 730
  2.03701e+3  -1.13443e+5  2.99995e-1  -7.33247e+2  6.89374e+6
  EQ3/6 database: version mdas.3245       ZnS
8295000 'ZnSiO3'            16.2210   -2.9268                          141.4737
  4    -2.000 330    -1.000 002     1.000 950     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnSiO3
8095000 'Willemite'         31.3220  -13.8329                          222.8631
  3    -4.000 330     2.000 950     1.000 770
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    Zn2SiO4
6095003 'Zincosite'         19.2070   -3.5198                          161.4536
  2     1.000 950     1.000 732
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnSO4
6095004 'ZnSO4:H2O'         10.6360    0.5732                          179.4689
  3     1.000 950     1.000 732     1.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnSO4:H2O
6095005 'Bianchite'          0.1630    1.7658                          269.5453
  3     1.000 950     1.000 732     6.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnSO4:6H2O
6095006 'Goslarite'         -3.2930    1.9593                          287.5606
  3     1.000 950     1.000 732     7.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnSO4:7H2O
4095000 'ZnBr2:2H2O'         7.5170   -5.2093                          261.2286
  3     1.000 950     2.000 130     2.000 002
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnBr2:2H2O
4395000 'ZnI2'             112.8830   -7.2272                          319.1989
  2     1.000 950     2.000 380
  999.  999.  999.  999.  999.
  Krupka et al. 1988                    ZnI2
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APPENDIX F

COMPLETE LISTING OF THE GAS_RDX.DAT(4.00) DATA FILE

APPENDIX F

COMPLETE LISTING OF THE GAS_RDX.DAT(4.00) DATA FILE

```
GAS_RDX.DAT  Thermochemical Data for Monitored Species
File History:
Date      Version  Person  Action
08/03/90           LJC     New Database PHREEQE (1990)
09/23/91  4.00     TE      Changed input to 4-line, free format.

-----------------------------------------------------------------
1: ID    Name                    delta H    log K         GFW
2: n     S1 ID   S2  ID  .... etc
3: a1  a2  a3  a4  a5
4: Reference
-----------------------------------------------------------------
STOP.
Version 4.00
2802810 'Fe+2=>Fe+3'                9.68    -13.01         0.0000
 3     1.000 280    -1.000 281    -1.000 001
 9.06142e+3  -5.11520e+5  1.28888e+0  -3.26601e+3  3.00780e+7
 EQ3/6 database: version mdas.3245
2302310 'Cu+=>Cu+2'               -1.6500     -2.72         0.0000
 3     1.000 230    -1.000 231    -1.000 001
 -2.75908e+2  1.63422e+4  -4.29484e-2  9.76193e+1  -9.22882e+5
 EQ3/6 database: version mdas.3245
4704710 'Mn+2=>Mn+3'                25.8    -25.59         0.0000
 3     1.000 470    -1.000 471    -1.000 001
 2.58652e+3  -1.44821e+5  3.96914e-1  -9.43973e+2  8.09604e+6
 EQ3/6 database: version mdas.3245
7307320 'HS-=>SO4-2'              -60.1460    -33.68         0.0000
 5   1.000 730   4.000 002  -1.000 732   -9.000 330  -8.000 001
 -8.60888e+2  4.49047e+4  -1.40723e-1  3.05790e+2  -3.38712e+6
 EQ3/6 database: version mdas.3245
2002010 'Co+2=>Co+3'              -35.9000    -32.99         0.0000
 3     1.000 200    -1.000 201    -1.00 001
 -2.07235e+2  4.10862e+3  -3.49395e-2  7.22422e+1  -7.00140e+5
 EQ3/6 database: version mdas.3245
2112120 'Cr(OH)+2=>CrO4-2'         0.0000   -72.7744         0.0000
 5   1.000 211   3.000 002  -1.000 212  7.000 330  -3.000 001
 999.  999.  999.  999.  999.
 Krupke et al. 1988.
4914920 'NO2-=>NO3-'                43.76    -27.76         0.0000
 5   1.000 491   1.000 002  -1.000 492  -2.000 330  -2.000 001
 -2.04746e+1  -6.12591e+3  -4.09355e-3  6.49242e+0  -1.40884e+5
 EQ3/6 database: version mdas.3245
4904920 'NH4+=>NO3-'              187.6200   -119.14         0.0000
 5   1.000 490   3.000 002  -1.000 492 -10.000 330  -8.000 001
 -5.53007e+2  -8.90406e+2  -9.48586e-2  1.97936e+2  -2.19086e+6
 EQ3/6 database: version mdas.3245
4904910 'NH4+/NO2-'                 0.0000    -91.38         0.0000
 5   1.000 490   2.000 002  -1.000 491  -8.000 330  -6.000 001
 -5.32532e+2  5.23549e+3  -9.07651e-2  1.91443e+2  -2.04998e+6
 EQ3/6 database: version mdas.3245
0600610 'H3AsO3=>H3AsO4'           30.015    -19.39         0.0000
 5   1.000 060   1.000 002  -1.000 061  -2.000 330   -2.000 001
 -1.09542e+3  4.94122e+4  -2.05605e-1  4.05960e+2  -2.92594e+6
 EQ3/6 database: version mdas.3245
0020030 'H2O=>O2(g)'              68.3150    -41.55         0.0000
 3     1.000 002    -2.000 330    -2.000 001
 3.92367e+0  -1.27448e+4  -2.46917e-3  -5.13625e-1  -6.40957e+4
 EQ3/6 database: version mdas.3245
0020031 'H2O=>O2(aq)'              66.917    -43.00         0.0000
 4     1.000 002    -0.500 003    -2.000 330   -2.000 001
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 -1.08243e+2  -5.99929e+3  -1.19015e-2  3.77861e+1  -4.07137e+5
 EQ3/6 database: version mdas.3245
4704720 'Mn+2=>MnO4-'          196.6210   -127.80        0.0000
 5     1.000 470  4.000 002  -1.000 472  -8.000 330  -5.000 001
 -1.27131e+2  -2.97109e+4  -3.23536e-2  4.72056e+1  -7.26945e+5
 EQ3/6 database: version mdas.3245
4704730 'Mn+2=>MnO4-2'         169.9510   -118.41        0.0000
 5     1.000 470  4.000 002  -1.000 473  -8.000 330  -4.000 001
 -1.14776e+3  3.34410e+4  -1.87231e-1  4.13262e+2  -4.40629e+6
 EQ3/6 database: version mdas.3245
7607610 'HSe-=>HSeO3-'          78.1650    -44.87        0.0000
 5     1.000 760  3.000 002  -1.000 761 -7.000 330  -6.000 001
 7.71832e+1  -1.54742e+4  2.74837e-3  -2.93362e+1  1.43484e+5
 EQ3/6 database: version mdas.3245
7617620 'HSeO3-=>SeO4-2'         0.0000    -36.31        0.0000
 5    1.000 761  1.000 002  -1.000 762  -3.000 330  -2.000 001
 -7.62991e+2  3.50262e+4  -1.24522e-1  2.74127e+2  -2.84204e+6
 EQ3/6 database: version mdas.3245
8918930 'U+4=>UO2+2'             0.0000     -9.05        0.0000
 5    1.000 891  2.000 002  -1.000 893  -4.000 330  -2.000 001
 2.31292e+3  -1.39347e+5  3.15528e-1  -8.24585e+2  8.15020e+6
 EQ3/6 database: version mdas.3245
8918920 'U+4=>UO2+'              0.0000     -7.58        0.0000
 5    1.000 891  2.000 002  -1.000 892  -4.000 330  -1.000 001
 4.12489e+3  -2.51222e+5  5.57852e-1  -1.46692e+3  1.54298e+7
 EQ3/6 database: version mdas.3245
8928930 'UO2+=>UO2+2'            0.0000     -1.47        0.0000
 3    1.000 892   -1.000 893   -1.000 001
 2.82442e+4  -1.43703e+6  4.65652e+0  -1.03731e+4  7.58528e+7
 EQ3/6 database: version mdas.3245
9009010 'V+2=>V+3'               0.0000      4.25        0.0000
 3     1.000 900    -1.000 901   -1.000 001
 999.  999.  999.  999.  999.
 Krupka et al. 1988.
9019020 'V+3=>VO+2'              0.0000     -5.79        0.0000
 5     1.000 901  1.000 002  -1.000 902  -2.000 330  -1.000 001
 -1.66576e+3  7.78520e+4  -2.83951e-1  6.16755e+2  -3.78868e+6
 EQ3/6 database: version mdas.3245
9029030 'VO+2=>VO2+'             0.0000    -16.93        0.0000
 5     1.000 902  1.000 002  -1.000 903  -2.000 330  -1.000 001
 2.07615e+2  -1.78783e+4  3.16060e-2  -7.41954e+1  8.52351e+5
 EQ3/6 database: version mdas.3245
4804810 'Mo+3=>MoO4-2'           0.0000    -29.77        0.0000
 5     1.000 480  4.000 002  -1.000 481  -8.000 330  -3.000 001
 999.  999.  999.  999.  999.
 Krupka et al. 1988
7407410 'Sb(OH)3=>Sb(OH)6-'      0.0000   -29.3707        0.0000
 5    1.000 740   3.000 002  -1.000 741  -3.000 330  -2.000 001
 999.  999.  999.  999.  999.
 Krupka et al. 1988
1701710 'Ce+3=>Ce+4'            38.0019   29.4651        0.0000
 3     1.000 170    -1.000 171     -1.000 001
 999.  999.  999.  999.  999.
 Peterson et al. 1986
3301403 'CO2(g)'                -0.962    18.149         41.0100
 3     1.000 140     2.000 330    -1.000 002
 3.54181e+2  -1.99751e+4  7.33674e-2  -1.24722e+2  1.57398e+6
 Nordstrom et al. 1990
7330020 'SO2(g)'                 0.000     8.94          64.0628
 3     1.000 733     2.000 330    -1.000 002
 -3.52737e+1  2.01450e+3  2.64371e-2  1.23639e+1  -9.07027e+4
 Goldberg and Parker 1985
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0000000
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References

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Nordstrom, D. K., L. N. Plummer, D. Langmuir, E. Busenberg, H. M. May, B. F. Jones, and D. L. Parkhurst. 1990. "Revised Chemical Equilibrium Data for Major Water-Mineral Reactions and Their Limitations." In Chemical Modeling of Aqueous Systems, II, eds. D. C. Melchior and R. L. Bassett, pp. 398-413, ACS Symposium Series 416, Am. Chem. Soc., Washington, DC.

Peterson, S. R., B. E. Opitz, M. J. Graham, and L. E. Eary. 1986. An Overview of the Geochemical Code MINTEQ: Applications to Performance Assessment for Low-Level Wastes. PNL-6112/UC-70 prepared for the U.S. Dept. of Energy under Contract DE-AC06-76RLO 1830, Pacific Northwest Laboratory, Richland, Washington.

APPENDIX G

COMPLETE LISTING OF THE PRCOEF.DAT(4.00) DATA FILE

APPENDIX G

COMPLETE LISTING OF THE PRCOEF.DAT(4.00) DATA FILE

```
PRCOEF.DAT datafile containing coefficients for correcting
  equilibrium constants for pressure. Created by B. Sass
  and W. Howden (1985).

Data description:  Line 1: ID number, species name, and values
                           of constants a1, b1, and c1 for
                           describing molar volumes as a
                           polynomial function of temperature.
                   Line 2: Values of constants a2, b2, and c2 for
                           describing compressibilities as
                           polynomial functions of temperature.
STOP.
Version 4.00
3300020 OH-          -0.2575E+02   0.2416E+00  -0.3767E-02
                     -0.6927E-02   0.9990E-04  -0.2700E-07
4607320 MgSO4(aq)     0.1439E+02  -0.3708E+00   0.5408E-02
                      0.1826E-01  -0.1956E-03   0.2212E-05
1507320 CaSO4(aq)     0.3155E+02  -0.3810E+00   0.4899E-02
                      0.8860E-02  -0.1956E-03   0.2212E-05
5007320 NaSO4-        0.2259E+02  -0.3814E+00   0.4394E-02
                      0.1556E-01  -0.2757E-03   0.3212E-05
4707320 MnSO4(aq)     0.1392E+02  -0.3810E+00   0.4808E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
2317320 CuSO4(aq)     0.1602E+02  -0.2840E+00   0.3808E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
9507320 ZnSO4(aq)     0.1592E+02  -0.3575E+00   0.4828E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
5407320 NiSO4(aq)     0.7320E+01  -0.3540E+00   0.4688E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
3301400 HCO3-         0.2981E+02  -0.1150E+00   0.1816E-02
                      0.5740E-02  -0.9300E-04   0.1896E-05
3307320 HSO4-         0.2294E+02  -0.1149E+00   0.2597E-02
                      0.1043E-01  -0.2240E-03   0.3056E-05
3307301 S-2          -0.3100E+02   0.2014E+00  -0.2294E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
2817340 FeSCN+2       0.2050E+02  -0.1691E+00   0.1211E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
2113300 Cr+3          0.2732E+02  -0.1840E-01   0.4620E-03
                      0.0000E+00   0.0000E+00   0.0000E+00
2123302 Cr2O7-2       0.6397E+02  -0.6138E+00   0.4897E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
6041001 Alunite       0.1385E+03  -0.5899E+00   0.6746E-02
                      0.0000E+00   0.0000E+00   0.0000E+00
6015000 Anhydrite     0.5629E+02  -0.3810E+00   0.4899E-02
                      0.1786E-01  -0.1956E-03   0.2212E-05
5015000 Aragonite     0.6250E+02  -0.3970E+00   0.5155E-02
                      0.1847E-01  -0.1956E-03   0.2212E-05
5046000 Artinite      0.5896E+02  -0.4276E+00   0.6109E-02
                      0.2411E-01  -0.3227E-03   0.7033E-05
4210000 BaF2          0.5746E+02  -0.3958E+00   0.5169E-02
                      0.2001E-01  -0.2336E-03   0.1476E-05
6010000 Barite        0.5834E+02  -0.4254E+00   0.4849E-02
                      0.1930E-01  -0.1956E-03   0.2212E-05
2003001 Boehmite      0.2540E+02   0.1840E-01  -0.4620E-03
                      0.0000E+00   0.0000E+00   0.0000E+00
2046000 Brucite       0.1061E+02  -0.6840E-01   0.1138E-02
                      0.6796E-02  -0.3380E-04   0.1422E-05
5015001 Calcite       0.6528E+02  -0.3970E+00   0.5155E-02
                      0.1847E-01  -0.1956E-03   0.2212E-05
```

6080000	Celestite	0.5543E+02	-0.2922E+00	0.3208E-02
		0.1947E-01	-0.1946E-03	0.2212E-05
8646000	Chrysotile	0.4783E+02	-0.2512E+00	0.4569E-02
		0.2583E-01	0.5410E-04	-0.1399E-05
8246000	Clinoenstite	0.1723E+02	-0.9600E-01	0.1831E-02
		0.9777E-02	0.5950E-04	-0.1977E-05
2077001	Cristobalite	0.7349E+01	-0.1840E-01	0.4620E-03
		0.2464E-02	0.6220E-04	-0.2266E-05
2003002	Diaspore	0.2362E+02	0.1840E-01	-0.4620E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8215000	Diopside	0.3490E+02	-0.2022E+00	0.3153E-02
		0.1915E-01	0.1190E-03	-0.3954E-05
5015002	Dolomite	0.1238E+03	-0.7838E+00	0.1082E-01
		0.3734E-01	-0.3912E-03	0.4424E-05
6046000	Epsomite	0.3267E+02	-0.3064E+00	0.3791E-02
		0.1464E-01	-0.4133E-03	0.1014E-04
8646003	Sepiolit(c)	0.4454E+02	-0.1782E+00	0.3315E-02
		0.2021E-01	0.7235E-04	-0.2255E-05
6028100	Fe2(SO4)3	0.1904E+03	-0.8520E+00	0.1142E-01
		0.0000E+00	0.0000E+00	0.0000E+00
4215000	Fluorite	0.5025E+02	-0.3514E+00	0.5219E-02
		0.1857E-01	-0.2336E-03	0.1476E-05
8046000	Forsterite	0.3370E+02	-0.1736E+00	0.3200E-02
		0.1709E-01	0.5680E-04	-0.1688E-05
2003003	Gibbsite(c)	0.1965E+02	0.2760E-01	-0.6930E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2028102	Goethite	0.2818E+02	0.1840E-01	-0.4620E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8628000	Greenalite	0.6657E+02	-0.2137E+00	0.2449E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6015001	Gypsum	0.4870E+02	-0.3626E+00	0.4437E-02
		0.1683E-01	-0.2578E-03	0.4478E-05
4150000	Halite	0.1394E+02	-0.1870E+00	0.1850E-02
		0.7640E-02	-0.1637E-03	0.1800E-05
2028105	Hematite	0.6316E+02	0.2760E-01	-0.6930E-03
		0.0000E+00	0.0000E+00	0.0000E+00
5015003	Hunitite	0.2441E+03	-0.1557E+01	0.2215E-01
		0.7508E-01	-0.7824E-03	0.8848E-05
5046001	Hydromagnesit	0.1601E+03	-0.1579E+01	0.2287E-01
		0.8021E-01	-0.9406E-03	0.1480E-04
6050000	Jarosite-Na	0.1584E+03	-0.6102E+00	0.6816E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6041002	Jarosite-K	0.1527E+03	-0.5899E+00	0.6746E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6028101	Jarosite-H	0.1300E+03	-0.5036E+00	0.5999E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1028002	Mackinawite	0.2900E+02	-0.1656E+00	0.1827E-02
		0.0000E+00	0.0000E+00	0.0000E+00
5046002	Magnesite	0.5908E+02	-0.3868E+00	0.5664E-02
		0.1887E-01	-0.1956E-03	0.2212E-05
3028000	Magnetite	0.8524E+02	-0.3750E-01	-0.3070E-04
		0.0000E+00	0.0000E+00	0.0000E+00
6028000	Melanterite	0.3605E+02	-0.2939E+00	0.3084E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6050001	Mirabilite	0.3544E+02	-0.3868E+00	0.2670E-02
		0.1552E-01	-0.6384E-03	0.1470E-04
5046003	Nesquehonite	0.5202E+02	-0.3592E+00	0.4971E-02
		0.1732E-01	-0.2889E-03	0.5611E-05
8646001	Phlogopite	0.8752E+02	-0.3375E+00	0.5316E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2077002	Quartz	0.4298E+01	-0.1840E-01	0.4620E-03
		0.2464E-02	0.6220E-04	-0.2266E-05
8646004	Sepiolite(am)	0.4454E+02	-0.1782E+00	0.3315E-02
		0.2021E-01	0.7235E-04	-0.2255E-05
5028000	Siderite	0.6412E+02	-0.3743E+00	0.4957E-02

		0.0000E+00	0.0000E+00	0.0000E+00
2077003	SiO2(a,gl)	0.8880E+01	-0.1840E-01	0.4620E-03
		0.2464E-02	0.6220E-04	-0.2266E-05
4280000	SrF2	0.5417E+02	-0.2626E+00	0.3528E-02
		0.2018E-01	-0.2326E-03	0.1476E-05
5080000	Strontianite	0.6619E+02	-0.3082E+00	0.3464E-02
		0.2008E-01	-0.1946E-03	0.2212E-05
8646002	Talc	0.5697E+02	-0.2972E+00	0.5724E-02
		0.3128E-01	0.2096E-03	-0.7064E-05
6050002	Thenardite	0.5067E+02	-0.4788E+00	0.4980E-02
		0.2069E-01	-0.3274E-03	0.3368E-05
8215001	Tremolite	0.1313E+03	-0.7016E+00	0.7203E-01
		0.6959E-01	0.4476E-03	-0.1497E-04
5010000	Witherite	0.7005E+02	-0.4414E+00	0.5105E-02
		0.1991E-01	-0.1956E-03	0.2212E-05
5047000	Rhodochrosit	0.5931E+02	-0.3970E+00	0.5064E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4147000	MnCl2:4H2O	0.1254E+02	-0.2394E+00	0.2604E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6047000	MnSO4	0.5386E+02	-0.3810E+00	0.4808E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1023101	Covellite	0.3068E+02	-0.9130E-01	0.9333E-03
		0.0000E+00	0.0000E+00	0.0000E+00
4223100	CuF2	0.5786E+02	-0.2544E+00	0.4128E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4223101	CuF2:2H2O	0.4447E+02	-0.2360E+00	0.3666E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2023100	Cu(OH)2	0.2039E+02	0.1840E-01	-0.4620E-03
		0.0000E+00	0.0000E+00	0.0000E+00
4123101	Atacamite	0.4144E+02	-0.6200E-01	0.5710E-03
		0.0000E+00	0.0000E+00	0.0000E+00
5123100	Cu2(OH)3NO3	0.4650E+02	-0.1612E+00	0.1291E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6023100	Antlerite	0.9229E+02	-0.2472E+00	0.2884E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6023101	Brochantite	0.1064E+03	-0.2288E+00	0.2422E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2023101	Tenorite	0.2181E+02	0.9200E-02	-0.2310E-03
		0.0000E+00	0.0000E+00	0.0000E+00
6023104	CuSO4	0.5938E+02	-0.2840E+00	0.3808E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6023105	Chalcanthite	0.3662E+02	-0.2380E+00	0.2653E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2023102	Dioptase	0.2080E+02	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00
1023102	Chalcopyrite	0.6246E+02	-0.2569E+00	0.2760E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4195000	ZnCl2	0.3689E+02	-0.2527E+00	0.3548E-02
		0.0000E+00	0.0000E+00	0.0000E+00
5095000	Smithsonite	0.5982E+02	-0.3735E+00	0.5084E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4295000	ZnF2	0.4978E+02	-0.3279E+00	0.5148E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2095000	Zn(OH)2(am)	0.1901E+02	-0.5510E-01	0.5580E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2095001	Zn(OH)2(c)	0.1901E+02	-0.5510E-01	0.5580E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2095002	Zn(OH)2(b)	0.1901E+02	-0.5510E-01	0.5580E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2095003	Zn(OH)2(g)	0.1901E+02	-0.5510E-01	0.5580E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2095004	Zn(OH)2(e)	0.1901E+02	-0.5510E-01	0.5580E-03
		0.0000E+00	0.0000E+00	0.0000E+00
5195000	ZnNO3)2:6H2O	0.6810E+01	-0.3959E+00	0.3602E-02
		0.0000E+00	0.0000E+00	0.0000E+00

2095005	ZnO(active)	0.1897E+02	-0.6430E-01	0.7890E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2095006	Zincite	0.1897E+02	-0.6430E-01	0.7890E-03
		0.0000E+00	0.0000E+00	0.0000E+00
1095001	Sphalerite	0.2913E+02	-0.1648E+00	0.1953E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1095002	Wurtzite	0.2915E+02	-0.1648E+00	0.1953E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8295000	ZnSiO3	0.2760E+02	-0.8270E-01	0.1251E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8095000	Willemite	0.4329E+02	-0.1470E+00	0.2040E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6095003	Zincosite	0.5511E+02	-0.3575E+00	0.4828E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6095005	Bianchite	0.3472E+02	-0.3023E+00	0.3442E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6095006	Goslarite	0.3215E+02	-0.2931E+00	0.3211E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4395000	ZnI2	0.2321E+02	-0.3669E+00	0.3920E-02
		0.0000E+00	0.0000E+00	0.0000E+00
5016000	Otavite	0.6434E+02	-0.3742E+00	0.4951E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4116000	CdCl2	0.3386E+02	-0.2534E+00	0.3415E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4116002	CdCl2:2.5H2O	0.1178E+02	-0.2304E+00	0.2837E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4216000	CdF2	0.5005E+02	-0.3286E+00	0.5015E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2016000	Cd(OH)2(am)	0.1496E+02	-0.5580E-01	0.4247E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2016001	Cd(OH)2(c)	0.1496E+02	-0.5580E-01	0.4247E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2016002	Montoponite	0.1871E+02	-0.6500E-01	0.6557E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8216000	CdSiO3	0.2297E+02	-0.8340E-01	0.1118E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6016003	CdSO4	0.5648E+02	-0.3582E+00	0.4695E-02
		0.0000E+00	0.0000E+00	0.0000E+00
6016004	CdSO4:1H2O	0.5363E+02	-0.3490E+00	0.4464E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1016000	Greenockite	0.3373E+02	-0.1655E+00	0.1820E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4316000	CdI2	0.1891E+02	-0.3676E+00	0.3787E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4160000	Cotunnite	0.3135E+02	-0.2535E+00	0.3101E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4160002	Phosgenite	0.9870E+02	-0.6278E+00	0.7739E-02
		0.0000E+00	0.0000E+00	0.0000E+00
5060000	Cerrusite	0.6633E+02	-0.3743E+00	0.4637E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4260000	PbF2	0.5286E+02	-0.3287E+00	0.4701E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2060000	Massicot	0.2198E+02	-0.6510E-01	0.3423E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2060001	Litharge	0.2274E+02	-0.6510E-01	0.3423E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8260000	PbSiO3	0.2409E+02	-0.8350E-01	0.8043E-03
		0.0000E+00	0.0000E+00	0.0000E+00
6060003	Anglesite	0.5569E+02	-0.3583E+00	0.4381E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1060001	Galena	0.3099E+02	-0.1656E+00	0.1507E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4060000	PbBr2	0.2615E+02	-0.2873E+00	0.3065E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4360000	PbI2	0.2486E+02	-0.3677E+00	0.3473E-02

	0.0000E+00	0.0000E+00	0.0000E+00
2054000 Ni(OH)2	0.1120E+02	-0.5160E-01	0.4180E-03
	0.0000E+00	0.0000E+00	0.0000E+00
2054001 Bunsenite	0.1800E+02	-0.6080E-01	0.6490E-03
	0.0000E+00	0.0000E+00	0.0000E+00
1054000 Millerite	0.2459E+02	-0.1613E+00	0.1813E-02
	0.0000E+00	0.0000E+00	0.0000E+00
6054001 Retgersite	0.3352E+02	-0.2988E+00	0.3302E-02
	0.0000E+00	0.0000E+00	0.0000E+00
6054002 Morenosite	0.3255E+02	-0.2896E+00	0.3071E-02
	0.0000E+00	0.0000E+00	0.0000E+00
4002000 Bromyrite	0.8151E+01	-0.1735E+00	0.1613E-02
	0.0000E+00	0.0000E+00	0.0000E+00
4102000 Cerargyrite	0.1147E+02	-0.1566E+00	0.1631E-02
	0.0000E+00	0.0000E+00	0.0000E+00
5002000 Ag2CO3	0.5840E+02	-0.4340E+00	0.4798E-02
	0.0000E+00	0.0000E+00	0.0000E+00
4302000 Iodyrite	0.9950E+01	-0.2137E+00	0.1817E-02
	0.0000E+00	0.0000E+00	0.0000E+00
2002000 Ag2O	0.1855E+02	-0.1248E+00	0.5030E-03
	0.0000E+00	0.0000E+00	0.0000E+00
6002000 Ag2SO4	0.5223E+02	-0.4180E+00	0.4542E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8450001 Analcime	0.5170E+02	-0.1066E+00	0.8170E-03
	0.0000E+00	0.0000E+00	0.0000E+00
8603000 Halloysite	0.5629E+02	0.9200E-02	-0.2310E-03
	0.0000E+00	0.0000E+00	0.0000E+00
8603001 Kaolinite	0.5629E+02	0.9200E-02	-0.2310E-03
	0.0000E+00	0.0000E+00	0.0000E+00
8415000 Leonhardite	0.1928E+03	-0.2032E+00	0.2413E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8450002 Low-Albite	0.5406E+02	-0.1342E+00	0.1510E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8450003 Analbite	0.5442E+02	-0.1342E+00	0.1510E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8641000 Muscovite	0.9576E+02	-0.7710E-01	0.5160E-03
	0.0000E+00	0.0000E+00	0.0000E+00
8641001 Annite	0.1030E+03	-0.3000E+00	0.3196E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8415001 Anorthite	0.9534E+02	-0.9700E-01	0.1091E-02
	0.0000E+00	0.0000E+00	0.0000E+00
8603002 Pyrophyllite	0.6598E+02	-0.3680E-01	0.9240E-03
	0.0000E+00	0.0000E+00	0.0000E+00
8415002 Laumontite	0.9142E+02	-0.9700E-01	0.1091E-02
	0.0000E+00	0.0000E+00	0.0000E+00
5023101 Malachite	0.8322E+02	-0.2816E+00	0.3602E-02
	0.0000E+00	0.0000E+00	0.0000E+00
5023102 Azurite	0.1558E+03	-0.5816E+00	0.7666E-02
	0.0000E+00	0.0000E+00	0.0000E+00
2015001 Portlandite	0.1633E+02	-0.7860E-01	0.6290E-03
	0.6396E-02	-0.3380E-04	0.1422E-05
2028000 Wustite	0.1849E+02	-0.6116E-01	0.6150E-03
	0.0000E+00	0.0000E+00	0.0000E+00
2046001 Periclase	0.1540E+02	-0.7760E-01	0.1369E-02
	0.7313E-02	-0.2700E-05	0.2890E-06
3028001 Hercynite	0.7847E+02	-0.3750E-01	-0.3070E-04
	0.0000E+00	0.0000E+00	0.0000E+00
3046000 Spinel	0.7375E+02	-0.5000E-01	0.6760E-03
	0.0000E+00	0.0000E+00	0.0000E+00
4250000 Cryolite	0.1412E+03	-0.1055E+01	0.1414E-01
	0.0000E+00	0.0000E+00	0.0000E+00
8215002 Wollastonite	0.2298E+02	-0.1062E+00	0.1322E-02
	0.9377E-02	0.5950E-04	-0.1977E-05
8015001 Ca-Olivine	0.4360E+02	-0.1940E+00	0.2182E-02
	0.1629E-01	0.5680E-04	-0.1688E-05

8015002	Larnite	0.3609E+02	-0.1940E+00	0.2182E-02
		0.1629E-01	0.5680E-04	-0.1688E-05
8015003	Monticellite	0.3856E+02	-0.1838E+00	0.2691E-02
		0.1669E-01	0.5680E-04	-0.1688E-05
8015005	Akerminite	0.6306E+02	-0.2900E+00	0.4013E-02
		0.2607E-01	0.1163E-03	-0.3665E-05
8015004	Merwinite	0.7609E+02	-0.3778E+00	0.4873E-02
		0.3298E-01	0.1136E-03	-0.3376E-05
8441000	Kalsilite	0.4000E+02	-0.7710E-01	0.5160E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8441001	Leucite	0.5011E+02	-0.9550E-01	0.9780E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8441002	Microcline	0.5205E+02	-0.1139E+00	0.1440E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8441003	H-Sanidine	0.5238E+02	-0.1139E+00	0.1440E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8450004	Nepheline	0.4627E+02	-0.9740E-01	0.5860E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8015006	Gehlenite	0.1046E+03	-0.1664E+00	0.1489E-02
		0.0000E+00	0.0000E+00	0.0000E+00
2028103	Lepidocrocit	0.2906E+02	0.1840E-01	-0.4620E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8650000	Na-Nontronit	0.1031E+03	-0.5680E-01	0.8125E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8641002	K-Nontronite	0.1014E+03	-0.5010E-01	0.7894E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8615000	Ca-Nontronit	0.1049E+03	-0.4086E-01	0.8013E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8646005	Mg-Nontronit	0.1044E+03	-0.3915E-01	0.8863E-03
		0.0000E+00	0.0000E+00	0.0000E+00
2048002	Molybdite	0.2543E+02	-0.2875E+00	0.2404E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7410000	BaMoO4	0.5613E+02	-0.4197E+00	0.3214E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7415000	Powellite	0.4331E+02	-0.3753E+00	0.3264E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7441000	K2MoO4	0.4382E+02	-0.4325E+00	0.3205E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7446000	MgMoO4	0.8247E+02	-0.3651E+00	0.3773E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7450000	Na2MoO4	0.4608E+02	-0.4731E+00	0.3345E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7460000	PbMoO4	0.4756E+02	-0.3526E+00	0.2746E-02
		0.0000E+00	0.0000E+00	0.0000E+00
7480000	SrMoO4	0.4967E+02	-0.2865E+00	0.1573E-02
		0.0000E+00	0.0000E+00	0.0000E+00
5050007	Trona	0.9716E+02	-0.8738E+00	0.9424E-02
		0.3644E-01	-0.6653E-03	0.8846E-05
8615001	Prehnite	0.1014E+03	-0.1940E+00	0.2182E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8450005	Phillipsite	0.6049E+02	-0.1149E+00	0.1244E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8641003	Illite	0.4801E+02	-0.8636E-01	0.1172E-02
		0.0000E+00	0.0000E+00	0.0000E+00
8615002	Montmoril-Ca	0.9931E+02	-0.4105E-01	0.8022E-03
		0.0000E+00	0.0000E+00	0.0000E+00
8646009	Chlorite-Mg	0.1028E+03	-0.3788E+00	0.6614E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1050000	Na2SO3	0.4967E+02	-0.4088E+00	0.3172E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1041001	KSCN	0.1197E+02	-0.2462E+00	0.1727E-02
		0.0000E+00	0.0000E+00	0.0000E+00
1060002	PbS2O3	0.4864E+02	-0.2736E+00	0.2146E-02
		0.0000E+00	0.0000E+00	0.0000E+00
4021100	CrBr3	0.6652E+02	-0.3379E+00	0.4200E-02

	0.0000E+00	0.0000E+00	0.0000E+00
4121100 CrCl3	0.7508E+02	-0.2872E+00	0.4254E-02
	0.0000E+00	0.0000E+00	0.0000E+00
4221100 CrF3	0.1047E+03	-0.4000E+00	0.6654E-02
	0.0000E+00	0.0000E+00	0.0000E+00
4321100 CrI3	0.5439E+02	-0.4585E+00	0.4812E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021100 FeCr2O4	0.1310E+03	-0.7430E-01	0.8933E-03
	0.0000E+00	0.0000E+00	0.0000E+00
3021101 MgCr2O4	0.1268E+03	-0.8680E-01	0.1600E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021102 Cr2O3	0.1082E+03	-0.9200E-02	0.2310E-03
	0.0000E+00	0.0000E+00	0.0000E+00
3021201 BaCrO4	0.5822E+02	-0.4437E+00	0.3374E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021202 Ca2CrO4	0.3699E+02	-0.4459E+00	0.2989E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021205 K2CrO4	0.4276E+02	-0.4565E+00	0.3365E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021206 K2Cr2O7	0.8619E+02	-0.7680E+00	0.5929E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021209 (NH4)2CrO4	0.3092E+02	-0.2751E+00	0.2210E-03
	0.0000E+00	0.0000E+00	0.0000E+00
3021210 Na2CrO4	0.5300E+02	-0.4971E+00	0.3505E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021212 PbCrO4	0.5621E+02	-0.3766E+00	0.2906E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021213 Rb2CrO4	0.4318E+02	-0.4675E+00	0.3533E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3021214 SrCrO4	0.5711E+02	-0.3105E+00	0.1733E-02
	0.0000E+00	0.0000E+00	0.0000E+00
3301403 CO2(g)	0.2482E+05	-0.3092E+00	0.4295E-02
	0.1156E-01	-0.1929E-03	0.1923E-05

APPENDIX H

COMPLETE LISTING OF THE ALK.DAT(4.00) DATA FILE

APPENDIX H

COMPLETE LISTING OF THE ALK.DAT(4.00) DATA FILE

```
Data description: Line 1: ID number and alkalinity factor.
STOP.
Version 4.00
0303302  1.00
3307701  2.00
3307700  1.00
3305800  1.00
3307301  2.00
3300020  1.00
    580  3.00
    730  1.00
0
```

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