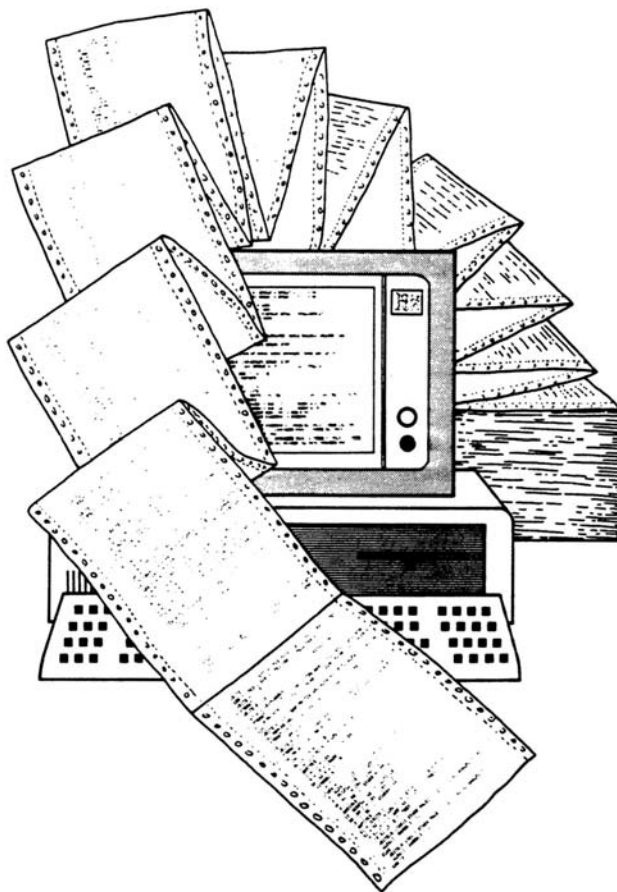


USER'S MANUAL FOR WATEQ4F, WITH
REVISED THERMODYNAMIC DATA BASE AND
TEST CASES FOR CALCULATING SPECIATION
OF MAJOR, TRACE, AND REDOX ELEMENTS
IN NATURAL WATERS



U.S. GEOLOGICAL SURVEY
Open-File Report 91-183

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TRACE, AND REDOX ELEMENTS IN NATURAL WATERS**

By James W. Ball and D. Kirk Nordstrom

U.S. GEOLOGICAL SURVEY

Open-File Report 91-183



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CONVERSION FACTORS AND ABBREVIATIONS

<u>Multiply</u>	<u>By</u>	<u>To obtain</u>
cal (calorie)	0.003968	Btu (British thermal unit)
cm ² (square centimeter)	0.1550	in ² (square inch)
kg (kilogram)	2.200	lb (pound)
L (liter)	0.2642	gal (gallon)
mg (milligram)	3.520 X 10 ⁻⁵	oz (ounce)

Explanation of abbreviations:

°C (degrees Celsius)
cu ft/sec (cubic feet per second)
kcal (kilocalories)
mg/L (milligrams per liter)
mol (molar, moles per liter)
: S (microSiemens, reciprocal megohms)

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ABSTRACT

A FORTRAN 77 version of the PL/1 computer program for the geochemical model WATEQ2, which computes major and trace element speciation and mineral saturation for natural waters, has been developed. The code WATEQ4F has been adapted to execute on an IBM PC¹ or compatible microcomputer with or without an 8087, 80287 or 80387 numeric coprocessor and, if recompilation is desired, a full-featured microcomputer FORTRAN compiler. The calculation procedure is identical to WATEQ2, which has been installed on many mainframes and minicomputers. Several data base revisions have been made that include the addition of Se (-II, 0, IV, VI) and U (III, IV, V, VI) species as well as the recently published values of Nordstrom and others (1990). A new set of redox options has been introduced so that all species that would exist in a disequilibrium system can be independently calculated, or selected species can be coupled, at the desire of the user. This report provides all the reactions and references for the complete data base, instructions for program operation, and an explanation of the input and output files. Attachments contain sample output from four water analyses used as test cases, and the complete source listings for WATEQ4F, its thermodynamic data base, input data preparation program WQ4FINPT, and a batch program to run WATEQ4F. The thermodynamic mass transfer program PHREEQE and the revised version of mass balance program BALANCE (BALN INPT) also have been adapted to execute on a personal microcomputer with the same specifications as those described above.

¹The use of trade, brand, or product names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

INTRODUCTION

Background

WATEQ4F is a chemical speciation code for natural waters. It uses field measurements of temperature, pH, Eh, dissolved oxygen and alkalinity, and the chemical analysis of a water sample as input and calculates the distribution of aqueous species, ion activities, and mineral saturation indices that indicate the tendency of a water to dissolve or precipitate a set of minerals (see Drever, 1988; Nordstrom and Munoz, 1986). The model assumes homogeneous aqueous phase equilibria, except for redox species. Equilibrium with respect to mineral solubilities is not assumed. The program results are used primarily to examine the tendency of a water to reach mineral solubility equilibria as a constraint on interpreting the chemistry of natural waters. Results also may be used for reaction modeling with the programs BALANCE and PHREEQE.

The original computer program, WATEQ (Truesdell and Jones, 1973, 1974), written in PL/1, has been translated into FORTRAN IV (WATEQF, Plummer and others, 1976). Trace elements have been added (WATEQ2, Ball and others, 1979, 1980); uranium species added (WATEQ3, Ball and others, 1981); and WATEQ2 was translated from PL/1 into FORTRAN 77 (Ball and others, 1987). Additional recommendations for the data base have been made, primarily on the aqueous aluminum species and forms of gibbsite (Nordstrom and others, 1984; Nordstrom and May, 1989). The code described in this report includes the major update and revision of Nordstrom and others (1990). This report describes a revised version of the FORTRAN 77 code for WATEQ4F that has been adapted for operation on a personal microcomputer with or without a math coprocessor, and is named WATEQ4F, Version 2.0. This report replaces the reports of Ball and others (1980, 1981, 1987) as the primary reference and user's manual for program WATEQ4F. The entire library of reactions and thermodynamic data used in WATEQ4F is included in this report. The original translation of WATEQ2 into FORTRAN 77 was made by Zachmann and Baethge (written commun., January, 1985).

The geochemical simulation program PHREEQE (Parkhurst and others, 1980) and a revised version of the mass balance program BALANCE (Parkhurst and others, 1982), which is known as BALN INPT, have been adapted for operation on a personal microcomputer. The reader is referred to the reports of Parkhurst and others (1980, 1982) for full instructions on the operation of PHREEQE and BALANCE. Otherwise, similarly to WATEQ4F, the requirements are a suitably configured IBM PC or compatible with or without a math coprocessor, the PHREEQE or BALN INPT program, and, if recompilation is desired, with a full-featured microcomputer FORTRAN compiler.

Purpose and Scope

This report supersedes earlier Open-File Report 87-50 (Ball and others, 1987), and marks significant changes to the WATEQ4F source code and data base and correction of some errors in the text of Open-File Report 87-50. The present version is designated Version 2.0, and is compatible with Microsoft FORTRAN, Version 4.00 or later, or its equivalent. An executable code that does not use an 8087, 80287 or 80387 numeric coprocessor can be created by recompiling the source code using appropriate compiler options.

The text of this report represents revision of Open-File Report 87-50 to reflect changes made in the code to adapt it to a more extensive variety of computer hardware and software. The primary changes made in the model are: 1) The addition of Se, U, five Fe, Mn, and Ba carbonate reactions, and the FeCl^+ and SrSO_4^0 complexes to the model calculations; 2) Revision of the user options for the control of redox calculations; 3) Significant revision of the thermodynamic data base, after Nordstrom and others (1990); 4) Inclusion of the entire WATEQ4F data base in the report. Model results for the test cases in Attachment A have been revised to show use of the new code, and are similar to results using the previous version of WATEQ4F. Most of the changes made to WATEQ4F since publication of Open-File Report 87-50 are described in a comment section at the beginning of the FORTRAN source code, found in Attachment C.

Acknowledgments

The authors wish to gratefully acknowledge the contributions of Neil Dubrovsky (U.S. Geological Survey) for providing the analytical results for test problem number 3 for use in this report, and of Charles Alpers (McGill University, U.S. Geological Survey) for many helpful discussions and suggestions during development of this version of the WATEQ4F model.

SOLUTE SPECIATION CALCULATIONS

Program WATEQ4F solves a set of nonlinear mass action and mass balance equations using the mathematical method known as the continued fraction method (Wigley, 1977). The Davies equation (Davies, 1962) is used in most cases to calculate individual ion activity coefficients for the solute species, because the a parameter required for the Debye Hückel equation frequently cannot be estimated. The WATEQ Debye-Hückel equation developed by Truesdell and Jones (1974) and expanded by Plummer and Busenberg (1982) and Busenberg and others (1984) is used for the major cations and anions:

<u>Ion</u>	<u>a</u>	<u>b</u>
Ca ²⁺	5.0	0.165
Mg ²⁺	5.5	0.20
Na ⁺	4.0	0.075
K ⁺	3.5	0.015
Cl ⁻	3.5	0.015
SO ₄ ²⁻	5.0	-0.04
HCO ₃ ⁻	5.4	0.0
CO ₃ ²⁻	5.4	0.0
H ₂ CO ₃ ⁰	0.0	0.0
Sr ²⁺	5.26	0.121

The extended Debye-Hückel equation is used for the following species because it forms an integral part of the thermodynamic data used for the species (Plummer and Busenberg, 1982; Busenberg and others, 1984; Cloke, 1963a):

<u>Ion</u>	<u>a</u>
H ⁺	9.0
SrHCO ₃ ⁺	5.4
SrOH ⁺	5.0
SrCO ₃ ⁰	0.0
Cu(S ₄) ₂ ³⁻	23.0
CuS ₄ S ₅ ³⁻	25.0
S ₂ ²⁻	6.5
S ₃ ²⁻	8.0
S ₄ ²⁻	10.0
S ₅ ²⁻	12.0
S ₆ ²⁻	14.0
Ag(S ₄) ₂ ³⁻	22.0
AgS ₄ S ₅ ³⁻	24.0
Ag(HS)S ₄ ²⁻	15.0

SATURATION INDICES

The main objective of program WATEQ4F is to calculate saturation indices. As expressed so elegantly by Truesdell and Jones (1974):

A water sample when collected is usually no longer in contact with mineral phases, and these phases may not be accessible to observation. It is of interest then to determine with what mineral phases the water is saturated or nearly so. The calculated activities of the dissolved ions in a water may be combined to produce the appropriate activity product which may be compared with the solubility equilibrium constant to show the degree of saturation of the water with each mineral considered.

The saturation index (SI), $[= \log_{10} (IAP/K_{sp(T)})]$ is approximately equal to zero when a water is at equilibrium. When the SI is above zero the water is supersaturated with that mineral, and the mineral would tend to precipitate. When the SI is less than zero the water is undersaturated with respect to the mineral, and the mineral would tend to be dissolved by the water. Because of thermodynamic and analytical errors there will be a range of uncertainty for the SI that must be taken into account. This uncertainty will vary according to both the complexity of the mineral stoichiometry and input data errors. Users must be aware of these problems when interpreting output.

LIMITS

The temperature range over which WATEQ4F can be used is 0 to 100 degrees Celsius. However, users are cautioned that uncertainties increase considerably when there are large departures from 25°C. The effect of pressure is not calculated in WATEQ4F because for the majority of natural waters it can be neglected (Truesdell and Jones, 1974; Nordstrom and Munoz, 1986).

Speciation calculations show reliable results up to the ionic strength of seawater (0.72), although saturation indices frequently agree well with calculations using the Pitzer (1979) model at ionic strengths slightly greater than seawater. The discrepancies between the ion association model as calculated by WATEQ4F and the Pitzer specific ion interaction model depend upon the charge on the ions and the degree of certainty with which the equilibrium constants are known.

Charge imbalance is calculated using the following formula:

$$\text{) \%} = \frac{(\text{Sum of Cation Species} - \text{Sum of Anion Species}) * 100}{(\text{Sum of Cation Species} + \text{Sum of Anion Species}) / 2} \quad (1)$$

Thus, the maximum value of the result of this calculation is ± 200 percent. This means that a value for) % of zero denotes exact electrical balance, whereas departures of more than 10 percent suggest errors in the analytical input values. This charge imbalance calculation is twice the charge imbalance normally computed. However, it is more appropriate to compare the cation/anion imbalance with the average of the cations and anions than with their sum.

THERMODYNAMIC DATA

The number assigned to the specific chemical reaction used in the computer code, the reaction, selected reaction enthalpy () H_r°) and equilibrium reaction constant (log K_r°) values, and the sources of the thermodynamic data are given in table 2. Because of its length, table 2 follows the References in the text of this report. The most precise and internally consistent sets of data available for the solubility product

constants and ion association constants in the $\text{CaCO}_3\text{-CO}_2\text{-H}_2\text{O}$ system and in the $\text{SrCO}_3\text{-CO}_2\text{-H}_2\text{O}$ system are those of Plummer and Busenberg (1982) and Busenberg and others (1984), respectively. These data are included in WATEQ4F. Two errors in Nordstrom and others (1990) are corrected in this report. They are the enthalpy and log K values for the AlSO_4^+ and $\text{Al}(\text{SO}_4)_2^-$ aqueous species, reactions 87 and 88 in table 2, respectively. Thermodynamic data revisions for gypsum, talc, sepiolite, muscovite, and chlorite were made but the use of solubility product constants (K_{sp}) for smectites, illites, chlorites, micas, feldspars, amphiboles, pyroxenes and pyrophyllites is not recommended at this time, because these phases have not demonstrated reversible, equilibrium solubility behavior (Nordstrom and others, 1990). Bisulfate ion association constants are given or estimated for Fe^{2+} , Fe^{3+} , Ca^{2+} , and Al^{3+} because of their importance in very acid waters such as some mine waters issuing from oxidizing ore deposits. Data for uranium reactions are from Grenthe and others (1992) were available. Data for aqueous uranium (IV) phosphate complexes are not given. These complexes are known to exist, but reliable data are not available at this time (Grenthe and others, 1992). The number of significant figures given in table 2 is not consistent because uncertainties in thermodynamic data are reaction-specific.

PROGRAM OPERATION

System Requirements

Program WATEQ4F is written in FORTRAN 77, and requires a minimum configuration of an IBM PC or full compatible with at least 512 kilobytes (KB, 1KB=1024 bytes, or characters) of random access memory (RAM). The packed executable code and supporting files occupy about 350KB of disk storage. The FORTRAN source code occupies about 200KB of disk storage. The program described in this report has been compiled, linked, and executed correctly on an IBM PC/AT with 640KB of RAM, an 80287 numeric coprocessor, and a 20MB hard disk, using Microsoft FORTRAN, Version 4.00. It also has been compiled, linked, and executed correctly on several similarly configured 8088, 80286 and 80386 based IBM PC compatibles with and without numeric coprocessor, and using other full-featured microcomputer FORTRAN compilers. For linking of the object code, the linker supplied with the compiler should be used. It was found by experiment that substitute linkers produced object codes that would not execute.

The test cases were solved on the PC/AT in an average time of less than 20 seconds each, including output of the results to a disk file. This should represent an upper limit of execution time for this class of computer with a numeric coprocessor, since the first test case in particular contains a fairly comprehensive array of constituents and output options. The size of the output file varies as a function of the complexity of the input and the print options selected, but will occupy approximately 25-50KB of disk storage per data set. The results obtained using the PC are virtually identical to those obtained using the U.S. Geological Survey Prime 850 minicomputer, exhibiting minor differences in the fifth or greater significant digit for less than one percent of the calculated results.

Executing WATEQ4F

To execute WATEQ4F, initiate execution of batch program WQ4F.BAT by typing WQ4F and pressing Enter. To initiate execution of WATEQ4F external to WQ4F.BAT, verify that the input data file you want to process is named WATEQ4F.DAT, then type WATEQ4F and press Enter. To initiate execution of the BASIC version of WQ4FINPT external to WQ4F.BAT, type the command you normally use to invoke your BASIC language program, followed by a space and WQ4FINPT, and press Enter. For IBM PC DOS, the BASIC program should be named BASICA. For MS DOS, the name should be GWBASIC. Program WQ4F.BAT uses the BASICA command. If your BASIC language program is a name other than BASICA, you may either use a line editor to edit WQ4F.BAT so that the invoking command matches the name of your BASIC language program or copy or rename your BASIC program file to BASICA.EXE. If you do not have a BASIC language interpreter, you will have to use the FORTRAN version of WQ4FINPT. To modify WQ4F.BAT to execute the FORTRAN version, use a line editor to remove the "BASICA" from the beginning

of the line that invokes WQ4FINPT. To initiate execution of the FORTRAN version external to WQ4F.BAT, type WQ4FINPT and press Enter.

Input

The data base for the calculation of mineral and solute reactions and their accompanying thermodynamic data is read initially, from two separate files named TABLE1 and TABLE2. The use of two separate files facilitates future expansion of the data base, in that species are just appended to their respective file, rather than the file having to be expanded in the middle for insertion of data. Files TABLE3, TABL3A, and TABLE4 contain index numbers of all mineral phases, index numbers of a subset of mineral phases selected by the authors, and index numbers of all solute species, respectively.

User-supplied input of water analyses to WATEQ4F is read from a disk file that must be named WATEQ4F.DAT. The input format has been modified extensively to conform to constraints in the FORTRAN language, as compared with PL/1. The number of records per input data set is not fixed. To facilitate preparation of input data sets, a separate computer program, called WQ4FINPT, is included in this report. The interpreted BASIC source code for this program is found in Attachment D, and the source code for a FORTRAN version of WQ4FINPT is found in Attachment E. Batch program WQ4F.BAT, the code for which is found in Attachment F, has been written to facilitate formatting input data sets, running the program and producing printed output.

Expanded sets of printing (PRNT) and redox (EHOPT) options have been added to WATEQ4F. Generation of a printable disk file of the thermodynamic data base may be specified in addition to suppression of printing of some of the output. The CORALK, PRNT and PUNCH options are as follows:

CORALK	0 =	alkalinity input has NOT been corrected for noncarbonate alkalinity
	1 =	alkalinity input HAS been corrected for noncarbonate alkalinity
	2 =	alkalinity input is in terms of total inorganic carbon
PRNT	0 =	print minimum output (aqueous species \$ 1% of master species input, selected subset of mineral saturation indices, no mole ratios)
	1 =	include complete aqueous speciation and mineral solubility listing
	2 =	include mole ratios page
	3 =	1 plus 2
	4 =	0 plus generate thermodynamic data table
	5 =	1 plus generate thermodynamic data table
	6 =	2 plus generate thermodynamic data table
PUNCH	7 =	3 plus generate thermodynamic data table
	0 =	generate a disk file of selected parameters for input to plotting program
	1 =	omit generation of the disk file

Redox Options

To allow greater flexibility in the use of the various redox values calculated by WATEQ4F, a user now may specify in the input data set which one of 14 input or calculated Eh values known to WATEQ4F is to be used in 9 separate areas of the program where redox calculations are done. The areas of calculation using the above redox parameters are:

EHOPT id	1 =	Fe species distribution
	2 =	Mn species with a valence other than +2
	3 =	Cu species having a valence of +1

- 4 = As species distribution
- 5 = Se species distribution
- 6 = Ion activity product calculations
- 7 = Calculation of the partial pressure of atmospheric O₂
- 8 = Calculation of the activity of H₂S from input SO₄, pH and Eh
- 9 = U species distribution

The 14 possible Eh values that can be specified as an EHOPT parameter are:

- | | |
|------------|---|
| Eh index # | 0 = Measured Eh
1 = Eh calculated from the Fe ²⁺ /Fe ³⁺ activity ratio
2 = Eh calculated from the O ₂ /H ₂ O ₂ activity ratio using the Sato relation
3 = Eh calculated from the O ₂ /H ₂ O activity ratio using the classical relation
4 = Eh calculated from the NH ₄ /NO ₃ activity ratio
5 = Eh calculated from the S ⁼ /SO ₄ activity ratio
6 = Eh calculated from the NO ₂ /NO ₃ activity ratio
7 = Eh calculated from the S ⁼ /S(s) activity ratio
8 = Eh calculated from the As ³⁺ /As ⁵⁺ activity ratio
9 = Eh calculated from the As(s)/As ³⁺ activity ratio
10 = Eh calculated from the Se ⁴⁺ /Se ⁶⁺ activity ratio
11 = Eh calculated from the Se(s)/Se ⁴⁺ activity ratio
12 = Eh calculated from the Se ²⁻ /Se(s) activity ratio
13 = Eh calculated from the U ⁴⁺ /UO ₂ ²⁺ activity ratio |
|------------|---|

Input concentrations of the members of the couples must be supplied for a selected option to have any effect. It must be emphasized that the above species are the only ones for which redox calculations are done. Note specifically that redox distributions of S and N species are not performed, with the exception of the calculation of the activity of H₂S from input SO₄, pH and Eh. As an example of the use of the Eh options, suppose you have a water analysis that includes analytical values for Fe(II) and Fe(III) and dissolved oxygen, but has no measured Eh value. Now, suppose further that you want to use the Eh calculated from the activities of Fe²⁺ and Fe³⁺ to perform redox distribution of Mn and As and to calculate ion activity products of minerals, and to use the pe calculated from dissolved oxygen using the classical relation to perform redox distribution of Cu and to calculate the partial pressure of atmospheric O₂, but to use the pe calculated from dissolved oxygen using the Sato relation to calculate the activity of H₂S. You would set the EHOPT values as follows:

- | | |
|------------|---|
| EHOPT(1) = | 0 (would have no effect since the presence of redox species analysis takes precedence over the EHOPT settings) |
| EHOPT(2) = | 1 = Eh calculated from the Fe ²⁺ /Fe ³⁺ activity ratio |
| EHOPT(3) = | 3 = Eh calculated from the O ₂ /H ₂ O activity ratio using the classical relation |
| EHOPT(4) = | 1 = Eh calculated from the Fe ²⁺ /Fe ³⁺ activity ratio |
| EHOPT(5) = | 0 (no Se to distribute) |
| EHOPT(6) = | 1 = Eh calculated from the Fe ²⁺ /Fe ³⁺ activity ratio |
| EHOPT(7) = | 3 = Eh calculated from the O ₂ /H ₂ O activity ratio using the classical relation |
| EHOPT(8) = | 2 = Eh calculated from the O ₂ /H ₂ O ₂ activity ratio using the Sato relation |
| EHOPT(9) = | 0 (no U to distribute) |

As a second example of Eh option usage, suppose you have a set of samples with complete water analyses, but no analytical redox species, no dissolved oxygen measurement and no measured Eh value. You will have available the Eh calculations from NH₄/NO₃, NO₂/NO₃, and H₂S/SO₄, but you know from your previous experiences with geochemical modeling that Eh calculated from H₂S/SO₄ is seldom reflective of

solution Eh, and that the two species hardly ever exist at thermodynamic equilibrium in solution in measurable quantities. Furthermore, you know that at least one of the nitrogen species is usually present at a concentration near the detection limit, hence that its determination frequently is subject to large uncertainties. Unfortunately, which species this applies to varies from sample to sample. You decide that you want to test both of these calculated Eh values as fully as possible in each sample, so you can decide which one to use in each sample for all the calculations, in a subsequent run of WATEQ4F. You decide to set the Eh options as follows:

EHOPT(1) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
 EHOPT(2) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
 EHOPT(3) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
 EHOPT(4) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
 EHOPT(5) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
 EHOPT(6) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
 EHOPT(7) = 4 = Eh calculated from the NH_4/NO_3 activity ratio
 EHOPT(8) = 6 = Eh calculated from the NO_2/NO_3 activity ratio
 EHOPT(9) = 4 = Eh calculated from the NH_4/NO_3 activity ratio

As a final precautionary summary for geochemical modeling of oxidation-reduction reactions, the user should always remember the following:

1. There is no such thing as an "Eh" or "pe" of a natural water (Thorstenson, 1984; Hostetler, 1984).
2. Redox couples do not tend to reach equilibrium with each other in natural waters. Redox disequilibrium is the general rule (see, for example, Lindberg and Runnells, 1984).
3. Only dissolved iron, dissolved sulfide and possibly dissolved uranium and vanadium are likely to give reversible potential measurements for a platinum electrode, and then only when the concentrations are high enough.
4. Arsenic and Se, and probably all oxyanions, do not give reversible potentials at a platinum electrode (Runnells and Lindberg, 1990; Runnells and Skoda, 1990).
5. Redox reactions usually are kinetically controlled and many are microbially mediated. Hence, individual redox species must be analytically determined. The WATEQ4F program was designed for this contingency.
6. A useful general classification and guide for describing redox environments is presented by Berner (1981).

Description of Input Variables

A list of all the optional analytical input constituents and their assigned reference numbers is in table 1. The required input is as follows:

Record	Variable Name	Variable	FORTTRAN Format	Comments
1	CHECK	start-of-data-set record	A4	four asterisks
2	CARD1	sample description	A80	
3	CARD2	Physical and chemical parameters carried through to plot program:		
		conductivity	F5.0	: S/cm ² at 25°C
		total dissolved solids	F6.0,1X	parts per million
		date, year, month, day	F6.0	yymmdd
		discharge	F8.0	cu ft/sec
		dissolved organic carbon	F8.0	mg/L
		salinity	F8.0	parts per thousand
		Cr, Co, Mo, V	4F8.0	
4		dummy record	A80	ignored by program
5	TEMP	temperature	F8.2,1X	°C, 0 to 100 only
	PH	pH, measured in field	F8.2,1X	
	EHM	Eh, measured in field	F8.2,1X	volts
	DOC	dissolved organic carbon	F8.2,1X	mg/L
	DOX	dissolved oxygen	F8.2,1X	mg/L
	CORALK	alkalinity correction flag	I8	0, 1 or 2
6		dummy record	A80	ignored by program
7	FLG	units in which remaining concentrations are expressed	A4	options: MQ/L, MG/L, PPM, MMOL, MOL
	DENS	density	F11.5	
	PRNT	print option	I6	0 through 7
	PUNCH	punch option	I6,6X	0 or 1
	EHOPT(1)	Eh option for Fe redox species	I3	0 through 13
	EHOPT(2)	Eh option for Mn redox species	I3	0 through 13
	EHOPT(3)	Eh option for Cu redox species	I3	0 through 13
	EHOPT(4)	Eh option for As redox species	I3	0 through 13
	EHOPT(5)	Eh option for Se redox species	I3	0 through 13
	EHOPT(6)	Eh option for IAP calculations	I3	0 through 13
	EHOPT(7)	Eh option for pO ₂ calculations	I3	0 through 13
	EHOPT(8)	Eh option for H ₂ S calculation	I3	0 through 13
	EHOPT(9)	Eh option for U redox species	I3	0 through 13
8		dummy record	A80	ignored by program
9	ITDS	analytical TDS	8X,F8.2,1X	parts per million
	COND	specific conductance	F8.2,1X	: S/cm ² at 25°C
	SIGMDO	dissolved oxygen sigma	F12.4	
	SIGMEH	Eh sigma	F12.4	
	SIGMPH	pH sigma	F12.4	
10		dummy record	A80	ignored by program
11	CUNITS(I)	Ca, Mg, Na, K, Cl, SO ₄	6F12.4	in FLG units
12		dummy record	A80	ignored by program
13	CUNITS(I)	HCO ₃ , Fe ^{tot} , H ₂ S, CO ₃ , SiO ₂ ^{tot} , NH ₄	6F12.4	in FLG units
14		dummy record	A80	ignored by program
15	CUNITS(I)	B ^{tot} , PO ₄ , Al, F, NO ₃	5F12.4	in FLG units
16		dummy record	A80	ignored by program
17 to n-1, where n=# of records in the data set		additional concentration values, sigma values, or replacement log ₁₀ K _r ^o values:		
	WORD	record type identifier	A4,1X	'CUN','SIGM','LOKT'
	J	subscript	I3,1X	0 to 653
	CUNITS(J), SIGMA(J), LOGKTO(J)	concentration, sigma, or log K values	F12.5	numerical value for referenced quantity
n		blank-final record in a data set		REQUIRED

Table 1. Reference Numbers for Optional Analytical Input Constituents

Number	Ionic Constituent	Charge	Number	Ionic Constituent	Charge
7	Fe	2	204	Ni	2
8	Fe	3	212	Ag	1
48	Cs	1	249	As total	0
80	Li	1	261	As ³ tot	0
87	Sr	2	262	As ⁵ tot	0
89	Ba	2	284	Fulvate	-2
94	Rb	1	285	Humate	-2
96	I	-1	298	Se total	0
97	Br	-1	299	H ₂ Se	0
109	Mn	2	300	Se ⁴ tot	0
130	Cu	2	301	Se ⁶ tot	0
145	Zn	2	316	U total	0
160	Cd	2	317	U	4
182	Pb	2	359	U ⁶ tot	0
202	NO ₂	-1			

Output

For the water analysis data, output is placed in a disk file named WATEQ4F.OUT. First, a listing of the input data is written, which includes the species name, index number, and input concentration of each species, as well as the values of all other parameters entered. Results of the anion mass balance calculations follow in the form: CO₂, SO₄, F, PO₄, Cl, H₂S, fulvic, and humic. When mass balance convergence to within 0.1 percent is obtained (or 40 iterations have been done), a table of distribution of aqueous species is written. If convergence to 0.1 percent or better is not obtained after 40 iterations, a warning message is printed and execution continues as though convergence were obtained. Both the sums of analytical and calculated milliequivalents per kilogram cation and anion values, and analytical and calculated specific conductance are listed for comparison. The percentage differences in the input and calculated charge balances are computed and displayed. The total (based on the input data) and the effective (calculated after speciation) ionic strengths are displayed for comparison. Numerous input and calculated solution parameters also are listed, including temperature, pH, and Eh and pe calculated using various redox couples.

The concentration of each aqueous species with a value greater than one mole percent of the input concentration of its master species, or all species greater than 1×10^{-78} molal, as selected by user option, is listed in parts per million, molality, mole percent of master species, and activity, as well as the individual ion activity coefficient and the negative log activity of each species. This is followed by a table of analytical molality ratios and log activity ratios, if selected by user option. A table follows of the mineral equilibrium calculations for a selected subset of, or all (as selected by user option) solid phases for which an activity product has been calculated, printed in the following order: the reaction number, the name of the solid phase, the computed saturation index ($\log_{10}(\text{IAP}/K_{\text{sp(T)}})$), the $\log_{10}(\text{IAP})$, the analytical propagated standard deviation in the $\log_{10}$ of the ion activity product, $\log_{10}(K_{\text{sp(T)}})$, and the uncertainty in the $\log_{10}$ of the equilibrium constant. The lists of solute and mineral species have been arranged in alphabetical order for convenience in locating species of interest. All the above is written to the disk file WATEQ4F.OUT for subsequent

printing.

By specifying a value for PRNT of 4, 5, 6 or 7 in an input data set, WATEQ4F can be directed to produce a disk file containing the permanent data base in tabular form, followed by a table of the analytical expressions for the temperature dependence of selected equilibrium constants, and by a listing of the names and reference numbers of all possible analytical input constituents. This information is written into a separate file, named TABLES.OUT, on the default disk drive, for later printing at the user's convenience.

TEST CASES AND PROGRAM LISTINGS

Attachment A contains a listing of the output from WATEQ4F of calculations for four test problems. The first two test cases appear in Ball and others (1980, 1987), and are from Nordstrom and others (1979). The third test case is the analysis of a well water containing measurable concentrations of Se (IV), Se (VI) and total As. The fourth test case is the U test case of Ball and others (1981), taken from Potter and others (1979). Test case 1 is a seawater analysis, which contains concentrations for virtually every species available for consideration by WATEQ4F, and is of relatively high (0.7) ionic strength. Test case 2 is a surface water analysis and is much more dilute, but also contains a fairly complete array of analytical values. These two test cases are described in more detail by Nordstrom and others (1979). Test case 2 demonstrates the capability of the model for computing independent Eh (pe) values based on analytical determinations of Fe (II/III), dissolved oxygen, NO₃, NO₂, NH₃, and S (VI/II). Test case 3 is a real analysis that demonstrates the model's capability for computing Eh (pe) values based on total As plus measured Eh, and on Se (IV/VI) determinations. These analyses were provided to us by Neil Dubrovsky of the California District Office, Water Resources Division, U.S. Geological Survey. Test case 4 is a real analysis of a U-containing water which demonstrates the capabilities of WATEQ4F for U speciation and mineral equilibrium calculations.

Users are cautioned that the Davies and Debye-Hückel equations are used in WATEQ4F to calculate the activity coefficients of all charged species except Ca, Mg, Na, K, Cl, SO₄, HCO₃, CO₃, H₂CO₃ and Sr. The ion-association models on which these two equations are based become less valid as ionic strengths increase above the seawater value of 0.7. Hence, results obtained for solutions of ionic strengths significantly higher than 0.7 always should be interpreted with caution.

Attachment B gives a listing of the five permanent data base files used by WATEQ4F. Attachment C gives a listing of the Version 2.0 FORTRAN source code. Attachment D gives the interpreted BASIC source code for WQ4FINPT, and the source code for a FORTRAN version of this program is given in Attachment E. The listing for batch program WQ4F.BAT is found in Attachment F.

PROGRAM PHREEQE

PHREEQE (Parkhurst and others, 1980) is a FORTRAN 77 computer program designed to model geochemical reactions, and is, like WATEQ4F, based on an ion pairing aqueous model. This program can calculate pH, redox potential, and mass transfer (amounts of solid or gaseous phases entering or leaving the aqueous phase) as a function of reaction progress, and can calculate the composition of solutions in equilibrium with multiple phases. PHREEQE is an attractive alternative tool for the interpretation and investigation of geochemical processes, and is well-suited to adaptation for execution on a microcomputer. Thus, PHREEQE was modified to be run on an IBM PC or compatible with or without an 8087, 80287 or 80387 numeric coprocessor, using the report of Parkhurst and others (1980) as a source of program documentation and running instructions.

PROGRAM BALANCE

PC BALN INPT (Prestemon, E. C., written commun., 1989) is a FORTRAN 77 computer program adapted from the mainframe version of BALN INPT, which is a revision of program BALANCE (Parkhurst and others, 1982). BALN INPT calculates the mass transfer necessary to account for the observed change in composition between two solutions. The program also can help to define and quantify chemical reactions that take place between ground water and minerals. BALN INPT also is particularly well-suited for execution on a microcomputer. Program documentation and running instructions can be found in Parkhurst and others (1982).

SUMMARY

The WATEQ2 geochemical model by Ball and others has been translated into FORTRAN 77, and Se and U have been added to the model. This WATEQ version is called WATEQ4F, Version 2.0. WATEQ4F, the PHREEQE geochemical reaction simulation program by Parkhurst and others, and the BALN INPT mass transfer calculation program by Parkhurst and others have been adapted for operation on an IBM or compatible personal microcomputer with or without an 8087, 80287 or 80387 math coprocessor or FORTRAN compiler. The codes are known to execute correctly on an IBM PC/AT with 20MB hard disk and 640KB RAM, and on many similarly configured 8088, 80286 and 80386 microcomputers. For WATEQ4F, the data base and computer code have been extensively revised from WATEQ2, and many changes have been made in the calculation options and in the appearance of the output. This program has been used for a wide variety of natural waters, including many types of ground waters, acid mine drainage waters, river waters and lake waters that occur in a wide variety of host rocks. WATEQ4F can be very useful as one of several tools used for the interpretation of the chemistry of natural waters.

The source code and documentation for WATEQ4F, PC PHREEQE and PC BALN INPT may be obtained by contacting:

U.S. Geological Survey
Water Resources Division
437 National Center
12201 Sunrise Valley Drive
Reston, Virginia 22092

Attn: Robin Sevin

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Table 2. Thermodynamic Data

) H_r° is enthalpy of reaction; $\log K_r^\circ$ is equilibrium constant for the reaction; kcal/mol is kilocalories per mole; 1F is the uncertainty in the listed value.

I ¹	Species	Reaction	) $H_r^\circ \pm 1F$ (kcal/mol)	Source	$\log K_r^\circ \pm 1F$	Source
0	kFe +3	$Fe^{2+} \rightleftharpoons Fe^{3+} + e^-$	9.68±0.5	47	-13.02±0.01	47
1	kFeOH +2	$Fe^{3+} + H_2O \rightleftharpoons FeOH^{2+} + H^+$	10.4±0.2	47	-2.19±0.02	47
2	kFeOH +	$Fe^{2+} + H_2O \rightleftharpoons FeOH^+ + H^+$	13.2±1.6	3	-9.5±0.1	3
3	kFe(OH)3 -	$Fe^{2+} + 3H_2O \rightleftharpoons Fe(OH)_3 + 3H^+$	30.3±3.6	3	-31.0±1.5	3
4	kFeSO4 +	$Fe^{3+} + SO_4^{2-} \rightleftharpoons FeSO_4^+$	3.91	47	4.04	47
5	kFeCl +2	$Fe^{3+} + Cl^- \rightleftharpoons FeCl^{2+}$	5.6	69	1.48	69
6	kFeCl2 +	$Fe^{3+} + 2Cl^- \rightleftharpoons FeCl_2^+$	--- ²	--- ²	2.13	69
7	kFeCl3 aq	$Fe^{3+} + 3Cl^- \rightleftharpoons FeCl_3^0$	--- ²	--- ²	1.13	79
8	kFeSO4 aq	$Fe^{2+} + SO_4^{2-} \rightleftharpoons FeSO_4^0$	3.23	4,45	2.25	4,45,69
9	Siderite (d) ³	$FeCO_3 \rightleftharpoons Fe^{2+} + CO_3^{2-}$	--- ²	--- ²	-10.45	47
10	Magnesite	$MgCO_3 \rightleftharpoons Mg^{2+} + CO_3^{2-}$	-6.169	64	-8.029	32
11	Dolomite (d)	$CaMg(CO_3)_2 \rightleftharpoons Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	-11.09	47	-16.54	47
12	Calcite	$CaCO_3 \rightleftharpoons Ca^{2+} + CO_3^{2-}$	-2.297±0.3 ⁴	53	-8.48±0.02	53
$\log K_r = -171.9065 - 0.077993T + 2839.319/T + 71.595 \log_{10} T$						
13	kH3SiO4 -	$H_4SiO_4^0 \rightleftharpoons H^+ + H_3SiO_4^-$	6.12 ⁴	47	-9.83	47
$\log K_r = -302.3724 - 0.050698T + 15669.69/T - 1.119669 \cdot 10^6/T^2 + 108.18466 \log_{10} T$						
14	kH2SiO4 -2	$H_4SiO_4^0 \rightleftharpoons 2H^+ + H_2SiO_4^{2-}$	17.6 ⁴	47	-23.0	47
$\log K_r = -294.0184 - 0.07265T + 11204.49/T - 1.119669 \cdot 10^6/T^2 + 108.18466 \log_{10} T$						
15	kHPO4 -2	$H + PO_4^{3-} \rightleftharpoons HPO_4^{2-}$	-3.49±0.9	21	12.5±0.03	21
16	kH2PO4 -	$2H^+ + PO_4^{3-} \rightleftharpoons H_2PO_4^-$	-4.35±1.1	21	19.56±0.03	21
17	Anhydrite	$CaSO_4 \rightleftharpoons Ca^{2+} + SO_4^{2-}$	-1.71 ⁴	47	-4.36	47
$\log K_r = 197.52 - 8669.8/T - 69.835 \log_{10} T$						
18	Gypsum	$CaSO_4 \cdot 2H_2O \rightleftharpoons Ca^{2+} + SO_4^{2-} + 2H_2O$	-0.109 ⁴	47	-4.58±0.02	47
$\log K_r = 68.2401 - 3221.51/T - 25.0627 \log_{10} T$						
19	Brucite	$Mg(OH)_2 + 2H^+ \rightleftharpoons Mg^{2+} + 2H_2O$	-27.1	47	16.84	47
20	Chrysotile	$Mg_3Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 3Mg^{2+} + 2H_4SiO_4^0 + H_2O$	-46.8 ⁴	47	32.20	47
$\log K_r = 13.248 + 10217.1/T - 6.1894 \log_{10} T$						
21	Aragonite	$CaCO_3 \rightleftharpoons Ca^{2+} + CO_3^{2-}$	-2.589±0.3 ⁴	53	-8.336±0.020	53
$\log K_r = -171.9773 - 0.077993T + 2903.293/T + 71.595 \log_{10} T$						

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
22	kMgF +	$Mg^{2+} + F^- \rightleftharpoons MgF^+$	3.2	47	1.82	47
23	kCaSO4 aq	$Ca^{2+} + SO_4^{2-} \rightleftharpoons CaSO_4^0$	1.65	47	2.30	47
24	kMgOH +	$Mg^{2+} + H_2O \rightleftharpoons MgOH^+ + H^+$	15.952 ⁵	39	-11.44±0.05	47
25	kH3BO3 aq	$H_3BO_3^0 \rightleftharpoons H^+ + H_2BO_3^-$	3.224	40	-9.240	40
26	kNH3 aq	$NH_4^+ \rightleftharpoons NH_3^0 + H^+$	12.48	44	-9.252	44
27	Forsterite	$Mg_2SiO_4 + 4H^+ \rightleftharpoons 2Mg^{2+} + H_4SiO_4^0$	-48.578 ⁵	64	28.306 ⁵	64
28	Diopside	$CaMgSi_2O_6 + 4H^+ + 2H_2O \rightleftharpoons Ca^{2+} + Mg^{2+} + 2H_4SiO_4^0$	-32.348 ⁵	64	19.894 ⁵	64
29	Clinoenstatite	$MgSiO_3 + 2H^+ + H_2O \rightleftharpoons Mg^{2+} + H_4SiO_4^0$	-20.049 ⁵	64	11.342 ⁵	64
30	kNaHPO4 -	$Na^+ + HPO_4^{2-} \rightleftharpoons NaHPO_4^-$	--- ²	---	0.29	54
31	Tremolite	$Ca_2Mg_5Si_8O_{22}(OH)_2 + 14H^+ + 8H_2O \rightleftharpoons 2Ca^{2+} + 5Mg^{2+} + 8H_4SiO_4^0$	-96.853 ⁵	64	56.574 ⁵	64
32	kKHPO4 -	$K^+ + HPO_4^{2-} \rightleftharpoons KHPO_4^-$	--- ²	---	0.29	54
33	kMgHPO4 aq	$Mg^{+2} + HPO_4^{2-} \rightleftharpoons MgHPO_4^0$	3.3	15	2.870	67
34	kCaHPO4 aq	$Ca^{+2} + HPO_4^{2-} \rightleftharpoons CaHPO_4^0$	3.3	15	2.739	15
35	kH2CO3 aq	$HCO_3^- + H^+ \rightleftharpoons H_2CO_3^0$	-2.247 ⁴	53	6.351±0.01	53
$\log K_f = 356.3094 + 0.0609196T - 21834.37/T - 126.8339 \log_{10} T + 1684915/T^2$						
36	Sepiolite(c)	$Mg_2Si_3O_7 \cdot 5OH \cdot 3H_2O + 0.5H_2O + 4H^+ \rightleftharpoons 2Mg^{2+} + 3H_4SiO_4^0$	-10.7	47	15.76	47
37	Talc	$Mg_3Si_4O_{10}(OH)_2 + 4H_2O + 6H^+ \rightleftharpoons 3Mg^{2+} + 4H_4SiO_4^0$	-46.352	63	21.399±2.0	63
38	Hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O + 2H^+ \rightleftharpoons 5Mg^{2+} + 4CO_3^{2-} + 6H_2O$	-52.244 ⁵	62	-8.762 ⁵	62
39	Adularia	$KAlSi_3O_8 + 8H_2O \rightleftharpoons K^+ + Al(OH)_4^- + 3H_4SiO_4^0$	30.82	64	-20.573	64
40	Albite	$NaAlSi_3O_8 + 8H_2O \rightleftharpoons Na^+ + Al(OH)_4^- + 3H_4SiO_4^0$	25.896	64	-18.002	64
41	Anorthite	$CaAl_2Si_2O_8 + 8H_2O \rightleftharpoons Ca^{2+} + 2Al(OH)_4^- + 2H_4SiO_4^0$	11.58	44	-19.714	44
42	Analcime	$NaAlSi_2O_6 \cdot H_2O + 5H_2O \rightleftharpoons Na^+ + Al(OH)_4^- + 2H_4SiO_4^0$	18.206	64	-12.701	64
43	Kmica	$KAl_3Si_3O_{10}(OH)_2 + 10H^+ \rightleftharpoons K^+ + 3Al^{3+} + 3H_4SiO_4^0$	-59.376	63	12.703±1.3	63
44	Phlogopite	$KMg_3AlSi_3O_{10}(OH)_2 + 10H^+ \rightleftharpoons K^+ + 3Mg^{2+} + Al^{3+} + 3H_4SiO_4^0$	-42.3±4.0	42,63 ⁶	43.3±3.0	7,42 ⁶
45	Illite	$K_{0.6}Mg_{0.25}Al_{2.3}Si_{3.5}O_{10}(OH)_2 + 11.2H_2O \rightleftharpoons 0.6K^+ + 0.25Mg^{+2} + 2.3Al(OH)_4^- + 3.5H_4SiO_4^0 + 1.2H^+$	54.684	22	-40.267	22
46	Kaolinite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{3+} + 2H_4SiO_4^0 + H_2O$	-35.3	47	7.435	47
47	Halloysite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{3+} + 2H_4SiO_4^0 + H_2O$	-39.82 ⁵	64	12.498 ⁵	64
48	Beidellite	$(Na,K,1/2Mg)_{0.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2 + 12H_2O \rightleftharpoons 0.33(Na,K,1/2Mg)^+ + 2.33Al(OH)_4^- + 3.67H_4SiO_4^0 + 2H^+$	60.355	22	-45.272	22

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	) H _r ^o ±1F (kcal/mol)	Source	Log K _r ^o ±1F	Source
49	Chlorite 14A	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈ +16H ⁺ W 5Mg ²⁺ +2Al ³⁺ +3H ₄ SiO ₄ ^o +6H ₂ O	-151.494	23	68.380±6.0	23
50	Alunite	KAl ₃ (SO ₄) ₂ (OH) ₆ W K ⁺ +3Al ³⁺ +2SO ₄ ²⁻ +6OH ⁻	-50.25	47	-1.4	47
51	Gibbsite (c)	Al(OH) ₃ + 3H ⁺ W Al ³⁺ + 3H ₂ O	-22.8	47	8.11±0.2	47
52	Boehmite	AlOOH + 3H ⁺ W Al ³⁺ + 2H ₂ O	-28.181 ⁵	64	8.584 ⁵	64
53	Pyrophyllite	Al ₂ Si ₄ O ₁₀ (OH) ₂ + 12H ₂ O W 2Al(OH) ₃ ⁺ + 4H ₄ SiO ₄ ^o + 2H ⁺	--- ²	--- ²	-48.314	59
54	Phillipsite	Na _{0.5} K _{0.5} AlSi ₃ O ₈ "H ₂ O+7H ₂ O W 0.5Na ⁺ +0.5K ⁺ +Al(OH) ₄ ⁻ + 3H ₄ SiO ₄ ^o	--- ²	--- ²	-19.874	26
55	Erionite	NaAlSi _{3.5} O ₉ "3H ₂ O + 6H ₂ O W Na ⁺ + Al(OH) ₄ ⁻ + 3.5H ₄ SiO ₄ ^o	--- ²	--- ²	--- ²	--- ²
56	Clinoptilolite	(K,Na)AlSi ₅ O ₁₂ "3.5H ₂ O+8.5H ₂ O W (K,Na) ⁺ +Al(OH) ₄ ⁻ +5H ₄ SiO ₄ ^o	--- ²	--- ²	--- ²	--- ²
57	Mordenite	(Na,K)AlSi _{4.5} O ₁₁ "3H ₂ O+8H ₂ O W (Na,K) ⁺ +Al(OH) ₄ ⁻ +4.5H ₄ SiO ₄ ^o	--- ²	--- ²	--- ²	--- ²
58	Nahcolite	NaHCO ₃ W Na ⁺ + HCO ₃ ⁻	3.72	34	-0.548	34
59	Trona	NaHCO ₃ "Na ₂ CO ₃ "2H ₂ O W 2H ₂ O + 3Na ⁺ + CO ₃ ²⁻ + HCO ₃ ⁻	-18.0	34,35,74	-0.795	34,35,74
60	Natron	Na ₂ CO ₃ "10H ₂ O W 2Na ⁺ + CO ₃ ²⁻ + 10H ₂ O	15.745	74,77	-1.311	74,77
61	Thermonatrite	Na ₂ CO ₃ "H ₂ O W 2Na ⁺ + CO ₃ ²⁻ + H ₂ O	-2.802	34,77	0.125	34,77
62	Fluorite	CaF ₂ W Ca ²⁺ + 2F ⁻	4.69 ⁴	47	-10.6±0.02	47
log K _r = 66.348-4298.2/T-25.271Log ₁₀ T						
63	Montmorillonite (Ca)	Ca _{0.17} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂ + 12H ₂ O W 0.17Ca ⁺² + 2.33Al(OH) ₄ ⁻ + 3.67H ₄ SiO ₄ ^o + 2H ⁺	58.373	22	-45.027	22
64	Halite	NaCl W Na ⁺ + Cl ⁻	0.918	64	1.582	64
65	Thenardite	Na ₂ SO ₄ W 2Na ⁺ + SO ₄ ²⁻	-0.572	64	-0.179	64
66	Mirabilite	Na ₂ SO ₄ "10H ₂ O W 2Na ⁺ + SO ₄ ²⁻ + 10H ₂ O	18.987	64	-1.114	64
67	Mackinawite	FeS + H ⁺ W Fe ²⁺ + HS ⁻	--- ²	--- ²	-4.648	5
68	kHCO ₃ -	H ⁺ + CO ₃ ²⁻ W HCO ₃ ⁻	-3.167 ⁴	53	10.33±0.01	53
log K _r = 107.8871+0.03252849T-5151.79/T-38.92561Log ₁₀ T+563713.9/T ²						
69	kNaCO ₃ -	Na ⁺ + CO ₃ ²⁻ W NaCO ₃	8.91	47	1.27	47
70	NaHCO ₃ aq	Na ⁺ + HCO ₃ ⁻ W NaHCO ₃ ^o	--- ²	--- ²	-0.250	20
71	kNaSO ₄ -	Na ⁺ + SO ₄ ²⁻ W NaSO ₄	1.12	45	0.70±0.05	45
72	kKSO ₄ -	K ⁺ + SO ₄ ²⁻ W KSO ₄	2.25±1.0	45	0.85±0.05	45
73	kMgCO ₃ aq	Mg ²⁺ + CO ₃ ²⁻ W MgCO ₃ ^o	2.713 ⁴	47	2.98±0.03	47
log K _r = 0.9910 + 0.00667T						

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	ΔH_f° (kcal/mol)	Source	Log K _r ±1F	Source
74	kMgHCO ₃ +	Mg ²⁺ + HCO ₃ ⁻ W MgHCO ₃ ⁺ log K _r = -59.215+2537.455/T+20.92298Log ₁₀ T	0.79 ⁴	47	1.07±0.03	47
75	kMgSO ₄ aq	Mg ²⁺ + SO ₄ ²⁻ W MgSO ₄ ⁰	4.55	47	2.37±0.02	47
76	kCaOH +	Ca ²⁺ + H ₂ O W CaOH ⁺ + H ⁺	--- ²	---	-12.78	47
77	kCaHCO ₃ +	Ca ²⁺ + HCO ₃ ⁻ W CaHCO ₃ ⁺ log K _r = 1209.12+0.31294T-34765.05/T-478.782Log ₁₀ T	5.410 ⁴	53	1.11±0.07	53
78	kCaCO ₃ aq	Ca ²⁺ + CO ₃ ²⁻ W CaCO ₃ ⁰ log K _r = -1228.732-0.299444T+35512.75/T+485.818Log ₁₀ T	4.030 ⁴	53	3.22±0.14	53
79	kSrHCO ₃ +	Sr ²⁺ + HCO ₃ ⁻ W SrHCO ₃ ⁺ log K _r = -3.248 + 0.014867T	6.047 ⁴	11	1.18	11
80	kAlOH +2	Al ³⁺ + H ₂ O W AlOH ²⁺ + H ⁺ log K _r = -38.253-656.27/T+14.327Log ₁₀ T	11.49 ⁴	47	-5.00±0.02	47
81	kAl(OH) ₂ +	Al ³⁺ + 2H ₂ O W Al(OH) ₂ ⁺ + 2H ⁺ log K _r = 88.5-9391.6/T-27.121Log ₁₀ T	26.90 ⁴	47	-10.1±0.2	47
82	kAl(OH) ₄ -	Al ³⁺ + 4H ₂ O W Al(OH) ₄ ⁻ + 4H ⁺ log K _r = 51.578-11168.9/T-14.865Log ₁₀ T	42.30 ⁴	47	-22.7±0.3	47
83	kAlF +2	Al ³⁺ + F ⁻ W AlF ²⁺	1.06	47	7.0	47
84	kAlF ₂ +	Al ³⁺ + 2F ⁻ W AlF ₂ ⁺	1.98	47	12.7	47
85	kAlF ₃ aq	Al ³⁺ + 3F ⁻ W AlF ₃ ⁰	2.16	47	16.8	47
86	kAlF ₄ -	Al ³⁺ + 4F ⁻ W AlF ₄ ⁻	2.20	47	19.4	47
87	kAlSO ₄ +	Al ³⁺ + SO ₄ ²⁻ W AlSO ₄ ⁺	2.29	47	3.5	47
88	kAl(SO ₄) ₂ -	Al ³⁺ + 2SO ₄ ²⁻ W Al(SO ₄) ₂ ⁻	3.11	47	5.0	47
89	kHSO ₄ -	H ⁺ + SO ₄ ²⁻ W HSO ₄ ⁻ log K _r = -56.889+0.006473T+2307.9/T+19.8858Log ₁₀ T	3.85 ⁴	47	1.988	47
90	kH ₂ S/SO ₄	SO ₄ ²⁻ + 10H ⁺ + 8e ⁻ W H ₂ S ⁰ + 4H ₂ O	-65.440	44	40.644	44
91	kH ₂ S aq	H ₂ S W H ⁺ + HS ⁻	5.300	44	-6.994	44
92	kHS -	HS ⁻ W H ⁺ + S ²⁻	12.100	44	-12.918	44
93	koxy	0.5H ₂ O W 0.25O ₂ (g) + H ⁺ + e ⁻	34.158	17	-20.769	17
94	Siderite (c)	FeCO ₃ W Fe ²⁺ + CO ₃ ²⁻	-2.48	47	-10.89	47

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f^\circ \pm 1F$	Source
95	Hydroxyapatite	$\text{Ca}_5(\text{PO}_4)_3\text{OH} + 4\text{H}^+ \text{ W } 5\text{Ca}^{2+} + 3\text{HPO}_4^{2-} + \text{H}_2\text{O}$	-36.223 ⁵	64	-3.421 ⁵	10
96	Fluorapatite	$\text{Ca}_5(\text{PO}_4)_3\text{F} + 3\text{H}^+ \text{ W } 5\text{Ca}^{2+} + 3\text{HPO}_4^{2-} + \text{F}^-$	-20.07	13,38	-17.6	13,38
97	Chalcedony	$\text{SiO}_2 + 2\text{H}_2\text{O} \text{ W } \text{H}_4\text{SiO}_4^\circ$	4.72 ⁴	47	-3.55	47
$\log K_f = -0.09 - 1032/T$						
98	Magadiite	$\text{NaSi}_2\text{O}_7(\text{OH})_3 \cdot 3\text{H}_2\text{O} + \text{H}^+ + 9\text{H}_2\text{O} \text{ W } \text{Na}^+ + 7\text{H}_4\text{SiO}_4^\circ$	--- ²	--- ²	-14.300	9
99	Cristobalite	$\text{SiO}_2 + 2\text{H}_2\text{O} \text{ W } \text{H}_4\text{SiO}_4^\circ$	5.500	64	-3.587	64
100	Silica gel	$\text{SiO}_2 + 2\text{H}_2\text{O} \text{ W } \text{H}_4\text{SiO}_4^\circ$	4.440	64	-3.018	64
101	Quartz	$\text{SiO}_2 + 2\text{H}_2\text{O} \text{ W } \text{H}_4\text{SiO}_4^\circ$	5.99 ⁴	47	-3.98	47
$\log K_f = 0.41 - 1309/T$						
102	kFe(OH) ₂ +	$\text{Fe}^{3+} + 2\text{H}_2\text{O} \text{ W } \text{Fe}(\text{OH})_2^+ + 2\text{H}^+$	17.1	47	-5.67±0.1	47
103	kFe(OH) ₃ aq	$\text{Fe}^{3+} + 3\text{H}_2\text{O} \text{ W } \text{Fe}(\text{OH})_3^0 + 3\text{H}^+$	24.8	47	-12.56	47
104	kFe(OH) ₄ -	$\text{Fe}^{3+} + 4\text{H}_2\text{O} \text{ W } \text{Fe}(\text{OH})_4^- + 4\text{H}^+$	31.9	47	-21.6±0.2	47
105	Fe(OH) ₂ aq	$\text{Fe}^{2+} + 2\text{H}_2\text{O} \text{ W } \text{Fe}(\text{OH})_2^0 + 2\text{H}^+$	28.6±2.9	3	-20.5±1.0	3
106	Vivianite	$\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O} \text{ W } 3\text{Fe}^{2+} + 2\text{PO}_4^{3-} + 8\text{H}_2\text{O}$	--- ²	--- ²	-36.000	50
107	Magnetite	$\text{Fe}_3\text{O}_4 + 8\text{H}^+ \text{ W } 2\text{Fe}^{3+} + \text{Fe}^{2+} + 4\text{H}_2\text{O}$	-50.460	64	3.737	64
108	Hematite	$\text{Fe}_2\text{O}_3 + 6\text{H}^+ \text{ W } 2\text{Fe}^{3+} + 3\text{H}_2\text{O}$	-30.845	64	-4.008	64
109	Maghemite	$\text{Fe}_2\text{O}_3 + 6\text{H}^+ \text{ W } 2\text{Fe}^{3+} + 3\text{H}_2\text{O}$	--- ²	--- ²	6.386	32
110	Goethite	$\text{FeOOH} + 3\text{H}^+ \text{ W } \text{Fe}^{3+} + 2\text{H}_2\text{O}$	-14.48 ⁵	64	-1.0±0.8	47
111	Greenalite	$\text{Fe}_3\text{Si}_2\text{O}_5(\text{OH})_4 + 6\text{H}^+ \text{ W } 3\text{Fe}^{2+} + 2\text{H}_4\text{SiO}_4^\circ + \text{H}_2\text{O}$	--- ²	--- ²	20.81 ⁵	54
112	Ferrihydrite	$\text{Fe}(\text{OH})_3 + 3\text{H}^+ \text{ W } \text{Fe}^{3+} + 3\text{H}_2\text{O}$	--- ²	--- ²	4.891	32
113	Annite	$\text{KFe}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2 + 10\text{H}_2\text{O} \text{ W } \text{K}^+ + 3\text{Fe}^{2+} + \text{Al}(\text{OH})_4^- + 3\text{H}_4\text{SiO}_4^\circ$	62.480	22	-85.645	22
114	Pyrite	$\text{FeS}_2 + 2\text{H}^+ + 2\text{e}^- \text{ W } \text{Fe}^{2+} + 2\text{HS}^-$	11.300	64	-18.479	64
115	Montmorillonite	$(\text{H}, \text{Na}, \text{K})_{0.28}\text{Mg}_{0.29}\text{Fe}_{0.23}^{3+}\text{Al}_{1.58}\text{Si}_{3.93}\text{O}_{10}(\text{OH})_2 + 10.04\text{H}_2\text{O} \text{ W}$	--- ²	--- ²	-34.913	30
	Belle Fourche	$0.28(\text{H}, \text{Na}, \text{K})^+ + 0.29\text{Mg}^{2+} + 0.23\text{Fe}^{3+} + 1.58\text{Al}(\text{OH})_4^- + 3.93\text{H}_4\text{SiO}_4^\circ$				
116	Montmorillonite	$(\text{H}, \text{Na}, \text{K})_{0.42}\text{Mg}_{0.45}\text{Fe}_{0.34}^{3+}\text{Al}_{1.47}\text{Si}_{3.82}\text{O}_{10}(\text{OH})_2 + 9.16\text{H}_2\text{O} +$	--- ²	--- ²	-29.688	31
	Aberdeen	$0.84\text{H}^+ \text{ W } 0.42(\text{H}, \text{Na}, \text{K})^+ + 0.45\text{Mg}^{2+} + 0.34\text{Fe}^{3+} + 1.47\text{Al}(\text{OH})_4^- + 3.82\text{H}_4\text{SiO}_4^\circ$				
117	Huntite	$\text{CaMg}_3(\text{CO}_3)_4 \text{ W } 3\text{Mg}^{2+} + \text{Ca}^{2+} + 4\text{CO}_3^{2-}$	-25.760	25	-29.968	25
118	Greigite	$\text{Fe}_3\text{S}_4 + 4\text{H}^+ \text{ W } 2\text{Fe}^{3+} + \text{Fe}^{2+} + 4\text{HS}^-$	--- ²	--- ²	-45.035 ⁷	54
119	FeS ppt	$\text{FeS} + \text{H}^+ \text{ W } \text{Fe}^{2+} + \text{HS}^-$	--- ²	--- ²	-3.915	5
120	kFeH ₂ PO ₄ +	$\text{Fe}^{2+} + \text{H}_2\text{PO}_4^- \text{ W } \text{FeH}_2\text{PO}_4^+$	--- ²	--- ²	2.700	50

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f \pm 1F$	Source
121	kCaPO4 -	$\text{Ca}^{2+} + \text{PO}_4^{3-} \rightleftharpoons \text{CaPO}_4^-$	3.100	15	6.459	15
122	kCaH2PO4 +	$\text{Ca}^{2+} + \text{H}_2\text{PO}_4^- \rightleftharpoons \text{CaH}_2\text{PO}_4^+$	3.400	15	1.408	15
123	kMgPO4 -	$\text{Mg}^{2+} + \text{PO}_4^{3-} \rightleftharpoons \text{MgPO}_4^-$	3.100	74	6.589	74
124	kMgH2PO4 +	$\text{Mg}^{2+} + \text{H}_2\text{PO}_4^- \rightleftharpoons \text{MgH}_2\text{PO}_4^+$	3.400	74	1.513	74
125	Chlorite 7A	$\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8 + 16\text{H}^+ \rightleftharpoons 5\text{Mg}^{2+} + 2\text{Al}^{3+} + 3\text{H}_4\text{SiO}_4^0 + 6\text{H}_2\text{O}$	-155.261	23	71.752±6.0	23
126	kLiSO4 -	$\text{Li}^+ + \text{SO}_4^{2-} \rightleftharpoons \text{LiSO}_4^-$	--- ²	--- ²	0.640	67
127	kNH4/NO3	$\text{NH}_4^+ + 3\text{H}_2\text{O} \rightleftharpoons \text{NO}_3^- + 10\text{H}^+ + 8\text{e}^-$	187.055 ⁸	44	-119.077 ⁸	44
128	Laumontite	$\text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot 4\text{H}_2\text{O} + 8\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 4\text{H}_4\text{SiO}_4^0$	--- ²	--- ²	-30.96	54
129	kSrOH +	$\text{Sr}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{SrOH}^+ + \text{H}^+$	--- ²	--- ²	-13.29	47
130	kBaOH +	$\text{Ba}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{BaOH}^+ + \text{H}^+$	--- ²	--- ²	-13.47	47
131	kNH4SO4 -	$\text{NH}_4^+ + \text{SO}_4^{2-} \rightleftharpoons \text{NH}_4\text{SO}_4^-$	--- ²	--- ²	1.110	67
132	Blank		--- ⁹	--- ⁹	--- ⁹	--- ⁹
133	Jarosite(ss)	$[\text{K}_{0.77}\text{Na}_{0.03}(\text{H}_3\text{O})_{0.2}]\text{Fe}_3(\text{SO}_4)_2(\text{OH})_6 + 5.8\text{H}^+ \rightleftharpoons 0.77\text{K}^+ + 0.03\text{Na}^+ + 3\text{Fe}^{3+} + 2\text{SO}_4^{2-} + 6.2\text{H}_2\text{O}$	--- ²	--- ²	-9.83	2
134	Mn2(SO4)3	$\text{Mn}_2(\text{SO}_4)_3 \rightleftharpoons 2\text{Mn}^{3+} + 3\text{SO}_4^{2-}$	-39.06	54	-5.711	54
135	kSrCO3 aq	$\text{Sr}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{SrCO}_3^0$	5.217 ⁴	11	2.81	11
		$\log K_f = -1.019 + 0.012826T$				
136	kO2 Sato	$0.5\text{H}_2\text{O} \rightleftharpoons 0.25\text{O}_2(\text{aq}) + \text{H}^+ + \text{e}^-$	--- ²	--- ²	-11.748	27
137	kCO2 aq	$\text{CO}_2(\text{g}) + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{CO}_3^0$	-4.776 ⁴	47	-1.468	47
		$\log K_f = 108.3865 + 0.01985076T - 6919.53/T - 6.69365 \cdot 10^5/T^2 - 40.45154\text{Log}_{10}T$				
138	kFeHPO4 aq	$\text{Fe}^{2+} + \text{HPO}_4^{2-} \rightleftharpoons \text{FeHPO}_4^0$	--- ²	--- ²	3.600	50
139	kFeHPO4 +	$\text{Fe}^{3+} + \text{HPO}_4^{2-} \rightleftharpoons \text{FeHPO}_4^+$	5.76	43	5.43	48
140	Al(OH)3 (a)	$\text{Al}(\text{OH})_3 + 3\text{H}^+ \rightleftharpoons \text{Al}^{3+} + 3\text{H}_2\text{O}$	-26.5	47	10.8	47
141	Prehnite	$\text{Ca}_2\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_2 + 8\text{H}_2\text{O} + 2\text{H}^+ \rightleftharpoons 2\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 3\text{H}_4\text{SiO}_4^0$	10.39	80	-11.695	80
142	Strontianite	$\text{SrCO}_3 \rightleftharpoons \text{Sr}^{2+} + \text{CO}_3^{2-}$	-0.401 ⁴	11	-9.271±0.02	11
		$\log K_f = 155.0305 - 7239.594/T - 56.58638\text{Log}_{10}T$				
143	Celestite	$\text{SrSO}_4 \rightleftharpoons \text{Sr}^{2+} + \text{SO}_4^{2-}$	-1.037 ⁴	47	-6.63	47
		$\log K_f = -14805.9622 - 2.4660924T + 756968.533/T - 4.05536 \cdot 10^7/T^2 + 5436.3588\text{Log}_{10}T$				
144	Barite	$\text{BaSO}_4 \rightleftharpoons \text{Ba}^{2+} + \text{SO}_4^{2-}$	6.35 ⁴	47	-9.97±0.02	47
		$\log K_f = 136.035 - 7680.41/T - 48.595\text{Log}_{10}T$				

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f \pm 1F$	Source
145	Witherite	$BaCO_3 \rightleftharpoons Ba^{2+} + CO_3^{2-}$	0.703 ⁴	47	-8.562	47
		$\log K_f = 607.642 + 0.121098T - 20011.25/T - 236.4948 \log_{10} T$				
146	Strengite	$FePO_4 \cdot 2H_2O \rightleftharpoons Fe^{3+} + PO_4^{3-} + 2H_2O$	-2.030	64	-26.400	49
147	Leonhardite	$Ca_2Al_4Si_8O_{24} \cdot 7H_2O + 17H_2O \rightleftharpoons 2Ca^{2+} + 4Al(OH)_4^- + 8H_4SiO_4^0$	90.070	64	-69.756	64
148	kFeHSO4 +	$Fe^{2+} + HSO_4^- \rightleftharpoons FeHSO_4^+$	--- ²	--- ²	1.08	37
149	Nesquehonite	$MgCO_3 \cdot 3H_2O \rightleftharpoons Mg^{2+} + CO_3^{2-} + 3H_2O$	-5.789	29	-5.621	44
150	Artinite	$MgCO_3 \cdot Mg(OH)_2 \cdot 3H_2O + 2H^+ \rightleftharpoons 2Mg^{2+} + CO_3^{2-} + 5H_2O$	-28.742	29	9.6 ⁵	54
151	kO2 calc	$0.5H_2O \rightleftharpoons 0.25O_2(aq) + H^+ + e^-$	33.457	44	-20.775	27
152	kw	$H_2O \rightleftharpoons H^+ + OH^-$	13.362 ⁴	47	-14.000	47
		$\log K_f = -283.971 - 0.05069842T + 13323/T - 1.119669 \cdot 10^6/T^2 + 102.24447 \log_{10} T$				
153	Sepiolite(d)	$Mg_2Si_3O_7 \cdot 5OH \cdot 3H_2O + 0.5H_2O + 4H^+ \rightleftharpoons 2Mg^{2+} + 3H_4SiO_4^0$	--- ²	--- ²	18.66	78
154	Diaspore	$AlOOH + 3H^+ \rightleftharpoons Al^{3+} + 2H_2O$	-24.681 ⁵	44	6.879 ⁵	44
155	Wairakite	$CaAl_2Si_4O_{12} \cdot 2H_2O + 10H_2O \rightleftharpoons Ca^{2+} + 2Al(OH)_4^- + 4H_4SiO_4^0$	26.140	80	-26.708	80
156	kFeH2PO4 +2	$Fe^{3+} + H_2PO_4^- \rightleftharpoons FeH_2PO_4^+$	--- ²	--- ²	5.43	50
157	Allophane(a)	$[Al(OH)_3]_{(1-x)}[SiO_2]_x + (3-3x)H^+ \rightleftharpoons (1-x)Al^{3+} + xH_4SiO_4^0 + (3-5x)H_2O$	--- ²	--- ²	6.06 ¹⁰	52
		$\log K_f = -5.7 + 1.68pH$				
158	Allophane(P)	$[Al(OH)_3]_{(1-x)}[SiO_2]_x + (3-3x)H^+ \rightleftharpoons (1-x)Al^{3+} + xH_4SiO_4^0 + (3-5x)H_2O$	--- ²	--- ²	5.24 ¹⁰	52
		$\log K_f = -5.4 + 1.52pH$				
159	kFeHSO4 +2	$Fe^{3+} + HSO_4^- \rightleftharpoons FeHSO_4^+$	--- ²	--- ²	2.48	37
160	kCaF +	$Ca^{2+} + F^- \rightleftharpoons CaF^+$	4.12	47	0.94	47
161	kBF(OH)3 -	$H_3BO_3^0 + F^- \rightleftharpoons BF(OH)_3^-$	1.85	46	-0.4	46
162	kBF2(OH)2 -	$H_3BO_3^0 + H^+ + 2F^- \rightleftharpoons BF_2(OH)_2^- + H_2O$	1.618 ⁵	46	7.63 ⁵	46
163	kBF3OH -	$H_3BO_3^0 + 2H^+ + 3F^- \rightleftharpoons BF_3OH^- + 2H_2O$	-1.614 ⁵	46	13.67 ⁵	46
164	kBF4 -	$H_3BO_3^0 + 3H^+ + 4F^- \rightleftharpoons BF_4^- + 3H_2O$	-1.846 ⁵	46	20.28 ⁵	46
165	kFeF +2	$Fe^{3+} + F^- \rightleftharpoons FeF^{2+}$	2.7	46	6.2	46
166	kFeF2 +	$Fe^{3+} + 2F^- \rightleftharpoons FeF_2^+$	4.8	46	10.8	46
167	kFeF3 aq	$Fe^{3+} + 3F^- \rightleftharpoons FeF_3^0$	5.4	46	14.0	46
168	kCaHSO4 +	$Ca^{2+} + HSO_4^- \rightleftharpoons CaHSO_4^+$	--- ²	--- ²	1.08	--- ¹¹
169	kMn +3	$Mn^{2+} \rightleftharpoons Mn^{3+} + e^-$	25.8	47	-25.51	47
170	kMnCl +	$Mn^{2+} + Cl^- \rightleftharpoons MnCl^+$	--- ²	--- ²	0.61	47

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta_f H^\circ_{298.15}$ (kcal/mol)	Source	$\log K^\circ_{298.15}$	Source
171	kMnCl2 aq	$\text{Mn}^{2+} + 2\text{Cl}^- \text{ W } \text{MnCl}_2^0$	--- ²	---	0.25	47
172	kMnCl3 -	$\text{Mn}^{2+} + 3\text{Cl}^- \text{ W } \text{MnCl}_3^-$	--- ²	---	-0.31	47
173	kMnOH +	$\text{Mn}^{2+} + \text{H}_2\text{O} \text{ W } \text{MnOH}^+ + \text{H}^+$	14.4	3	-10.59±0.04	3
174	kMn(OH)3 -	$\text{Mn}^{2+} + 3\text{H}_2\text{O} \text{ W } \text{Mn(OH)}_3 + 3\text{H}^+$	--- ²	---	-34.8	3
175	kMnF +	$\text{Mn}^{2+} + \text{F}^- \text{ W } \text{MnF}^+$	--- ²	---	0.84	47
176	kMnSO4 aq	$\text{Mn}^{2+} + \text{SO}_4^{2-} \text{ W } \text{MnSO}_4^0$	3.37	47	2.25	47
177	kMn(NO3)2 aq	$\text{Mn}^{2+} + 2\text{NO}_3^- \text{ W } \text{Mn(NO}_3)_2^0$	-0.396	54	0.6	69
178	kMnHCO3 +	$\text{Mn}^{2+} + \text{HCO}_3^- \text{ W } \text{MnHCO}_3^+$	--- ²	---	1.95	47
179	kMnO4 -	$\text{Mn}^{2+} + 4\text{H}_2\text{O} \text{ W } \text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^-$	176.62	54	-127.824	54
180	kMnO4 -2	$\text{Mn}^{2+} + 4\text{H}_2\text{O} \text{ W } \text{MnO}_4^{2-} + 8\text{H}^+ + 4\text{e}^-$	150.02	54	-118.44	54
181	Fe(OH)2.7Cl3	$\text{Fe(OH)}_{2.7}\text{Cl}_{0.3} + 2.7\text{H}^+ \text{ W } \text{Fe}^{3+} + 2.7\text{H}_2\text{O} + 0.3 \text{Cl}^-$	--- ²	---	-3.04	6
182	MnSO4	$\text{MnSO}_4 \text{ W } \text{Mn}^{2+} + \text{SO}_4^{2-}$	-15.48	54	2.669	54
183	Pyrolusite	$\text{MnO}_2 + 4\text{H}^+ + 2\text{e}^- \text{ W } \text{Mn}^{2+} + 2\text{H}_2\text{O}$	-65.11	47	41.38	47
184	Birnessite	$\text{MnO}_2 + 4\text{H}^+ + 2\text{e}^- \text{ W } \text{Mn}^{2+} + 2\text{H}_2\text{O}$	--- ²	---	43.601	47
185	Nsutite	$\text{MnO}_2 + 4\text{H}^+ + 2\text{e}^- \text{ W } \text{Mn}^{2+} + 2\text{H}_2\text{O}$	--- ²	---	42.564	47
186	Bixbyite	$\text{Mn}_2\text{O}_3 + 6\text{H}^+ \text{ W } 2\text{Mn}^{3+} + 3\text{H}_2\text{O}$	-15.245	54	-0.611	54
187	Hausmannite	$\text{Mn}_3\text{O}_4 + 8\text{H}^+ + 2\text{e}^- \text{ W } 3\text{Mn}^{2+} + 4\text{H}_2\text{O}$	-100.64	47	61.03	47
188	Pyrochroite	$\text{Mn(OH)}_2 + 2\text{H}^+ \text{ W } \text{Mn}^{2+} + 2\text{H}_2\text{O}$	--- ²	---	15.2	47
189	Manganite	$\text{MnOOH} + 3\text{H}^+ + \text{e}^- \text{ W } \text{Mn}^{2+} + 2\text{H}_2\text{O}$	--- ²	---	25.34	47
190	Rhodochrosite (d)	$\text{MnCO}_{3(\text{synthetic})} \text{ W } \text{Mn}^{2+} + \text{CO}_3^{2-}$	--- ²	---	-10.39	47
191	MnCl2, 4H2O	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O} \text{ W } \text{Mn}^{2+} + 2\text{Cl}^- + 4\text{H}_2\text{O}$	17.38	54	2.71	54
192	MnS Green	$\text{MnS}_{(\text{green})} + \text{H}^+ \text{ W } \text{Mn}^{2+} + \text{HS}^-$	-5.79	54	3.8	54
193	Mn3(PO4)2	$\text{Mn}_3(\text{PO}_4)_2 \text{ W } 3\text{Mn}^{2+} + 2\text{PO}_4^{3-}$	2.12	54	-23.827	54
194	MnHPO4	$\text{MnHPO}_4 \text{ W } \text{Mn}^{2+} + \text{HPO}_4^{2-}$	--- ²	---	-12.947	54
195	"-Cryptomelane	$\text{K}_{0.8}\text{Mn}_{0.6}^{2+}\text{Mn}_{0.8}^{4+}\text{O}_{17} + 34\text{H}^+ \text{ W } 16\text{Mn}^{3+} + 0.8\text{K}^+ + 17\text{H}_2\text{O} - 7.4\text{Mn}^{2+}$	--- ²	---	---	57,36 ²
196	Hollandite	$\text{Ba}_{0.82}\text{Fe}_{0.57}^{2+}\text{Mn}_{0.59}^{2+}\text{Mn}_{0.7}^{4+}\text{O}_{16} + 32\text{H}^+ \text{ W } 14\text{Mn}^{3+} + 0.82\text{Ba}^{2+} + 0.57\text{Fe}^{2+} + 16\text{H}_2\text{O} - 6.41\text{Mn}^{2+}$	--- ²	---	---	12 ²
197	Psilomelane	$\text{Ba}_{0.78}\text{Ca}_{0.19}\text{K}_{0.03}\text{Mn}^{2+}\text{Mn}_7^{4+}\text{O}_{16} + 2.5\text{H}_2\text{O} + 31.97\text{H}^+ \text{ W } 0.78\text{Ba}^{2+} + 0.19\text{Ca}^{2+} + 0.03\text{K}^+ + 14\text{Mn}^{3+} + 18.485\text{H}_2\text{O} - 6\text{Mn}^{2+}$	--- ²	---	---	8 ²
198	Todorokite	$\text{Ca}_{0.393}\text{Mg}_{0.473}\text{Mn}_{1.134}^{2+}\text{Mn}_3^{4+}\text{O}_{12} + 2\text{H}_2\text{O} + 24\text{H}^+ \text{ W } 14\text{Mn}^{3+} + 0.393\text{Ca}^{2+} + 0.473\text{Mg}^{2+} + 12\text{H}_2\text{O} - 6\text{Mn}^{2+}$	--- ²	---	---	73 ²

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	) H _f ^o ±1F (kcal/mol)	Source	Log K _f ^o ±1F	Source
		0.393Ca ²⁺ + 0.473Mg ²⁺ + 10Mn ³⁺ + 14H ₂ O - 6Mn ²⁺				
199	Lithiophorite	Li ₂ Al ₈ Mn ₂ ²⁺ Mn ₁₀ ⁴⁺ O ₃₅ "14H ₂ O + 70H ⁺ W	--- ²	---	---	76 ²
		2Li ⁺ + 8Al ³⁺ + 20Mn ³⁺ 49H ₂ O - 8Mn ²⁺				
200	Rancieite	Ca _{0.44} Mn _{0.56} ²⁺ Mn ₄ ⁴⁺ O ₉ "3H ₂ O + 18H ⁺ W	--- ²	---	---	60 ²
		0.44Ca ²⁺ + 8Mn ³⁺ + 12H ₂ O - 3.44Mn ²⁺				
201	kSiF6 -2	H ₄ SiO ₄ ⁰ + 4H ⁺ + 6F ⁻ W SiF ₆ ²⁻ + 4H ₂ O	-16.26	61	30.18	61
202	kHF aq	H ⁺ + F ⁻ W HF ⁰	3.18 ⁴	47	3.18±0.01	47
		log K _f = -2.033+0.012645T+429.01/T				
203	kHF2 -	H ⁺ + 2F ⁻ W HF ₂ ⁻	4.55	47	3.76±0.06	47
204	Jarosite Na	NaFe ₃ (SO ₄) ₂ (OH) ₆ + 6H ⁺ W Na ⁺ + 3Fe ³⁺ + 2SO ₄ ²⁻ + 6H ₂ O	-36.18	4	-5.28±1.0	2
205	Jarosite K	KFe ₃ (SO ₄) ₂ (OH) ₆ + 6H ⁺ W K ⁺ + 3Fe ³⁺ + 2SO ₄ ²⁻ + 6H ₂ O	-45.0	4	-11.0±0.3	2
206	kCuCl2 -	Cu ²⁺ + 2Cl ⁻ + e ⁻ W CuCl ₂ ⁻	1.23	22,44	8.22	69
207	kCuCl3 -2	Cu ²⁺ + 3Cl ⁻ + e ⁻ W CuCl ₃ ²⁻	1.91	22,44	8.42	69
208	kCu +	Cu ²⁺ + e ⁻ W Cu ⁺	1.65	44	2.72	44
209	kCuCO3 aq	Cu ²⁺ + CO ₃ ²⁻ W CuCO ₃ ⁰	---	---	6.73±0.05	3
210	kCu(CO3)2 -2	Cu ²⁺ + 2CO ₃ ²⁻ W Cu(CO ₃) ₂ ²⁻	---	---	9.83±0.04	3
211	kCuCl +	Cu ²⁺ + Cl ⁻ W CuCl ⁺	8.65	22	0.43	44
212	kCuCl2 aq	Cu ²⁺ + 2Cl ⁻ W CuCl ₂ ⁰	10.56	22	0.16	44
213	kCuCl3 -	Cu ²⁺ + 3Cl ⁻ W CuCl ₃ ⁻	13.69	22	-2.29	22
214	kCuCl4 -2	Cu ²⁺ + 4Cl ⁻ W CuCl ₄ ²⁻	17.78	22	-4.59	22
215	kCuF +	Cu ²⁺ F ⁻ W CuF ⁺	1.62	44	1.26	44
216	kCuOH +	Cu ²⁺ H ₂ O W CuOH ⁺ + H ⁺	---	---	-8.0	3
217	kCu(OH)2 aq	Cu ²⁺ + 2H ₂ O W Cu(OH) ₂ ⁰ + 2H ⁺	---	---	-13.68	75
218	kCu(OH)3 -	Cu ²⁺ + 3H ₂ O W Cu(OH) ₃ ⁻ + 3H ⁺	---	---	-26.9	75
219	kCu(OH)4 -2	Cu ²⁺ + 4H ₂ O W Cu(OH) ₄ ²⁻ + 4H ⁺	---	---	-39.6	3
220	kCu2(OH)2 +2	2Cu ²⁺ + 2H ₂ O W Cu ₂ (OH) ₂ ²⁺ + 2H ⁺	17.539 ⁴	3	-10.359	3
		log K _f = 2.497-3833/T				
221	kCuSO4 aq	Cu ²⁺ + SO ₄ ²⁻ W CuSO ₄ ⁰	1.22	45	2.31	3
222	kCu(HS)3 -	Cu ²⁺ + 3HS ⁻ W Cu(HS) ₃ ⁻	---	---	25.9	43
223	Cu Metal	Cu W Cu ⁺ + e ⁻	17.13	44	-8.76	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f^\circ \pm 1F$	Source
224	Nantokite	$\text{CuCl} \rightleftharpoons \text{Cu}^+ + \text{Cl}^-$	9.98	44	-6.76	44
225	CuF	$\text{CuF} \rightleftharpoons \text{Cu}^+ + \text{F}^-$	-12.37	41	7.08	41
226	Cuprite	$\text{Cu}_2\text{O} + 2\text{H}^+ \rightleftharpoons 2\text{Cu}^+ + \text{H}_2\text{O}$	6.245	44	-1.55	44
227	Chalcocite	$\text{Cu}_2\text{S} + \text{H}^+ \rightleftharpoons 2\text{Cu}^+ + \text{HS}^-$	49.35	56	-34.619±0.16	56
228	Cu ₂ SO ₄	$\text{Cu}_2\text{SO}_4 \rightleftharpoons 2\text{Cu}^+ + \text{SO}_4^{2-}$	-4.56	41	-1.95	19
229	Cuprous Ferrite	$\text{CuFeO}_2 + 4\text{H}^+ \rightleftharpoons \text{Cu}^+ + \text{Fe}^{3+} + 2\text{H}_2\text{O}$	-3.80	44	-8.92	44
230	Melanothallite	$\text{CuCl}_2 \rightleftharpoons \text{Cu}^{2+} + 2\text{Cl}^-$	-12.32	41	3.73	44
231	CuCO ₃	$\text{CuCO}_3 \rightleftharpoons \text{Cu}^{2+} + \text{CO}_3^{2-}$	--- ²	--- ²	-9.63	69
232	CuF ₂	$\text{CuF}_2 \rightleftharpoons \text{Cu}^{2+} + 2\text{F}^-$	-13.32	41	-0.62	41
233	CuF ₂ , 2H ₂ O	$\text{CuF}_2 \cdot 2\text{H}_2\text{O} \rightleftharpoons \text{Cu}^{2+} + 2\text{F}^- + 2\text{H}_2\text{O}$	-3.65	41	-4.55	41
234	Cu(OH) ₂	$\text{Cu(OH)}_2 + 2\text{H}^+ \rightleftharpoons \text{Cu}^{2+} + 2\text{H}_2\text{O}$	-15.25	41	8.64	3
235	Malachite	$\text{Cu}_2(\text{OH})_2\text{CO}_3 + 3\text{H}^+ \rightleftharpoons 2\text{Cu}^{2+} + 2\text{H}_2\text{O} + \text{HCO}_3^-$	-19.76	44	5.15±0.08	3
236	Azurite	$\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2 + 4\text{H}^+ \rightleftharpoons 3\text{Cu}^{2+} + 2\text{H}_2\text{O} + 2\text{HCO}_3^-$	-30.87	44	3.75±0.09	3
237	Atacamite	$\text{Cu}_2(\text{OH})_3\text{Cl} + 3\text{H}^+ \rightleftharpoons 2\text{Cu}^{2+} + 3\text{H}_2\text{O} + \text{Cl}^-$	-18.69	41	7.34	44
238	Cu ₂ (OH) ₃ NO ₃	$\text{Cu}_2(\text{OH})_3\text{NO}_3 + 3\text{H}^+ \rightleftharpoons 2\text{Cu}^{2+} + 3\text{H}_2\text{O} + \text{NO}_3^-$	-17.35	41	9.24	44
239	Antlerite	$\text{Cu}_3(\text{OH})_4\text{SO}_4 + 4\text{H}^+ \rightleftharpoons 3\text{Cu}^{2+} + 4\text{H}_2\text{O} + \text{SO}_4^{2-}$	--- ²	--- ²	8.29	44
240	Brochantite	$\text{Cu}_4(\text{OH})_6\text{SO}_4 + 6\text{H}^+ \rightleftharpoons 4\text{Cu}^{2+} + 6\text{H}_2\text{O} + \text{SO}_4^{2-}$	--- ²	--- ²	15.34±0.16	69
241	Langite	$\text{Cu}_4(\text{OH})_6\text{SO}_4 \cdot \text{H}_2\text{O} + 6\text{H}^+ \rightleftharpoons 4\text{Cu}^{2+} + 7\text{H}_2\text{O} + \text{SO}_4^{2-}$	-39.61	44	16.79	44
242	Tenorite	$\text{CuO} + 2\text{H}^+ \rightleftharpoons \text{Cu}^{2+} + \text{H}_2\text{O}$	-15.24	44	7.62	3
243	CuOCuSO ₄	$\text{CuO} \cdot \text{CuSO}_4 + 2\text{H}^+ \rightleftharpoons 2\text{Cu}^{2+} + \text{H}_2\text{O} + \text{SO}_4^{2-}$	-35.575	41	11.53	41
244	Cu ₃ (PO ₄) ₂	$\text{Cu}_3(\text{PO}_4)_2 \rightleftharpoons 3\text{Cu}^{2+} + 2\text{PO}_4^{3-}$	--- ²	--- ²	-36.85	44
245	Cu ₃ (PO ₄) ₂ , 3H ₂ O	$\text{Cu}_3(\text{PO}_4)_2 \cdot 3\text{H}_2\text{O} \rightleftharpoons 3\text{Cu}^{2+} + 2\text{PO}_4^{3-} + 3\text{H}_2\text{O}$	--- ²	--- ²	-35.12	41
246	Covellite	$\text{CuS} + \text{H}^+ \rightleftharpoons \text{Cu}^{2+} + \text{HS}^-$	24.01	56	-22.27±0.03	66
247	CuSO ₄	$\text{CuSO}_4 \rightleftharpoons \text{Cu}^{2+} + \text{SO}_4^{2-}$	-18.14	41	3.01	44
248	Chalcanthite	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O} \rightleftharpoons \text{Cu}^{2+} + \text{SO}_4^{2-} + 5\text{H}_2\text{O}$	1.44	44	-2.64	44
249	Cupric Ferrite	$\text{CuFe}_2\text{O}_4 + 8\text{H}^+ \rightleftharpoons \text{Cu}^{2+} + 2\text{Fe}^{3+} + 4\text{H}_2\text{O}$	-38.69	44	5.88	44
250	Chalcopyrite	$\text{CuFeS}_2 + 2\text{H}^+ \rightleftharpoons \text{Cu}^{2+} + \text{Fe}^{2+} + 2\text{HS}^-$	35.48	41	-35.27	41
251	kZnCl +	$\text{Zn}^{2+} + \text{Cl}^- \rightleftharpoons \text{ZnCl}^+$	7.79	22	0.43	69
252	kZnCl ₂ aq	$\text{Zn}^{2+} + 2\text{Cl}^- \rightleftharpoons \text{ZnCl}_2^0$	8.5	22	0.45	-- ¹²
253	kZnCl ₃ -	$\text{Zn}^{2+} + 3\text{Cl}^- \rightleftharpoons \text{ZnCl}_3^-$	9.56	22	0.5	69

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
254	kZnCl4 -2	$Zn^{2+} + 4Cl^- \rightleftharpoons ZnCl_4^{2-}$	10.96	22	0.2	69
255	kZnF +	$Zn^{2+} + F^- \rightleftharpoons ZnF^+$	2.22	43	1.15	69
256	kZnOH +	$Zn^{2+} + H_2O \rightleftharpoons ZnOH^+ + H^+$	13.4	3	-8.96±0.05	3
257	kZn(OH)2 aq	$Zn^{2+} + 2H_2O \rightleftharpoons Zn(OH)_2^0 + 2H^+$	--- ²	---2	-16.9	3
258	kZn(OH)3 -	$Zn^{2+} + 3H_2O \rightleftharpoons Zn(OH)_3^- + 3H^+$	--- ²	---2	-28.4±0.2	3
259	kZn(OH)4 -2	$Zn^{2+} + 4H_2O \rightleftharpoons Zn(OH)_4^{2-} + 4H^+$	--- ²	---2	-41.2±0.1	3
260	kZnOHCl aq	$Zn^{2+} + H_2O + Cl^- \rightleftharpoons ZnOHCl^0 + H^+$	--- ²	---2	-7.48	44
261	kZn(HS)2 aq	$Zn^{2+} + 2HS^- \rightleftharpoons Zn(HS)_2^0$	--- ²	---2	14.94	43
262	kZn(HS)3 -	$Zn^{2+} + 3HS^- \rightleftharpoons Zn(HS)_3^-$	--- ²	---2	16.10	43
263	kZnSO4 aq	$Zn^{2+} + SO_4^{2-} \rightleftharpoons ZnSO_4^0$	1.36	14	2.37	45
264	kZn(SO4)2 -2	$Zn^{2+} + 2SO_4^{2-} \rightleftharpoons Zn(SO_4)_2^{2-}$	--- ²	---2	3.28	45
265	Zn Metal	$Zn \rightleftharpoons Zn^{2+} + 2e^-$	-36.78	44	25.757	44
266	Zn(BO2)2	$Zn(BO_2)_2 + 2H_2O + 2H^+ \rightleftharpoons Zn^{2+} + 2H_3BO_3^0$	--- ²	---2	8.29	44
267	ZnCl2	$ZnCl_2 \rightleftharpoons Zn^{2+} + 2Cl^-$	-17.48	44	7.03	44
268	Smithsonite	$ZnCO_3 \rightleftharpoons Zn^{2+} + CO_3^{2-}$	-4.36	44	-10.00	69
269	ZnCO3, H2O	$ZnCO_3 \cdot H_2O \rightleftharpoons Zn^{2+} + CO_3^{2-} + H_2O$	--- ²	---2	-10.26	44
270	ZnF2	$ZnF_2 \rightleftharpoons Zn^{2+} + 2F^-$	-13.08	44	-1.52	44
271	Zn(OH)2 (a)	$Zn(OH)_{2(amorph)} + 2H^+ \rightleftharpoons Zn^{2+} + 2H_2O$	--- ²	---2	12.45	3
272	Zn(OH)2 (c)	$Zn(OH)_{2(cryst)} + 2H^+ \rightleftharpoons Zn^{2+} + 2H_2O$	--- ²	---2	12.2	65
273	Zn(OH)2 (b)	$Zn(OH)_{2(s)} + 2H^+ \rightleftharpoons Zn^{2+} + 2H_2O$	--- ²	---2	11.75±0.02	3
274	Zn(OH)2 (g)	$Zn(OH)_{2(l)} + 2H^+ \rightleftharpoons Zn^{2+} + 2H_2O$	--- ²	---2	11.71	3
275	Zn(OH)2 (e)	$Zn(OH)_{2(l)} + 2H^+ \rightleftharpoons Zn^{2+} + 2H_2O$	--- ²	---2	11.50±0.03	3
276	Zn2(OH)3Cl	$Zn_2(OH)_3Cl + 3H^+ \rightleftharpoons 2Zn^{2+} + 3H_2O + Cl^-$	--- ²	---2	15.2	44
277	Zn5(OH)8Cl2	$Zn_5(OH)_8Cl_2 + 8H^+ \rightleftharpoons 5Zn^{2+} + 8H_2O + 2Cl^-$	--- ²	---2	38.5	28
278	Zn2(OH)2SO4	$Zn_2(OH)_2SO_4 + 2H^+ \rightleftharpoons 2Zn^{2+} + 2H_2O + SO_4^{2-}$	--- ²	---2	7.5	44
279	Zn4(OH)6SO4	$Zn_4(OH)_6SO_4 + 6H^+ \rightleftharpoons 4Zn^{2+} + 6H_2O + SO_4^{2-}$	--- ²	---2	28.4	28
280	Zn(NO3)2, 6H2O	$Zn(NO_3)_2 \cdot 6H_2O \rightleftharpoons Zn^{2+} + 2NO_3^- + 6H_2O$	5.51	44	3.44	44
281	ZnO (a)	$ZnO_{(active)} + 2H^+ \rightleftharpoons Zn^{2+} + H_2O$	--- ²	---2	11.31	3
282	Zincite (c)	$ZnO_{(cryst)} + 2H^+ \rightleftharpoons Zn^{2+} + H_2O$	-21.86	44	11.14	3
283	Zn3O(SO4)2	$ZnO \cdot 2ZnSO_4 + 2H^+ \rightleftharpoons 3Zn^{2+} + 2SO_4^{2-} + H_2O$	-62.0	44	19.02	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
284	Zn ₃ (PO ₄) ₂ ,4w	$Zn_3(PO_4)_2 + 4H_2O \rightleftharpoons 3Zn^{2+} + 2PO_4^{3-} + 4H_2O$	--- ²	---	-32.04	43
285	ZnS (a)	$ZnS_{(amorph)} + H^+ \rightleftharpoons Zn^{2+} + HS^-$	3.67	19	-9.052	19
286	Sphalerite (c)	$ZnS_{(sphaler)} + H^+ \rightleftharpoons Zn^{2+} + HS^-$	8.25	44	-11.618	44
287	Wurtzite	$ZnS_{(wurtz)} + H^+ \rightleftharpoons Zn^{2+} + HS^-$	5.06	44	-9.682	28
288	ZnSiO ₃	$ZnSiO_3 + 2H^+ + H_2O \rightleftharpoons Zn^{2+} + H_4SiO_4^0$	-18.27	44	2.93	19
289	Willemite	$Zn_2SiO_4 + 4H^+ \rightleftharpoons 2Zn^{2+} + H_4SiO_4^0$	-33.37	44	15.33	44
290	Zincosite	$ZnSO_4 \rightleftharpoons Zn^{2+} + SO_4^{2-}$	-19.20	44	3.01	44
291	ZnSO ₄ , H ₂ O	$ZnSO_4 \cdot H_2O \rightleftharpoons Zn^{2+} + SO_4^{2-} + H_2O$	-10.64	44	-0.57	44
292	Bianchite	$ZnSO_4 \cdot 6H_2O \rightleftharpoons Zn^{2+} + SO_4^{2-} + 6H_2O$	-0.16	44	-1.765	44
293	Goslarite	$ZnSO_4 \cdot 7H_2O \rightleftharpoons Zn^{2+} + SO_4^{2-} + 7H_2O$	3.3	44	-1.96	44
294	kCdCl +	$Cd^{2+} + Cl^- \rightleftharpoons CdCl^+$	0.59	44	1.98±0.03	69
295	kCdCl ₂ aq	$Cd^{2+} + 2Cl^- \rightleftharpoons CdCl_2^0$	1.24	44	2.6±0.1	69
296	kCdCl ₃ -	$Cd^{2+} + 3Cl^- \rightleftharpoons CdCl_3^-$	3.90	44	2.4±0.1	69
297	kCdF +	$Cd^{2+} + F^- \rightleftharpoons CdF^+$	---	---	1.1	28
298	kCdF ₂ aq	$Cd^{2+} + 2F^- \rightleftharpoons CdF_2^0$	---	---	1.5	28
299	kCd(CO ₃) ₂ -2	$Cd^{2+} + 2CO_3^{2-} \rightleftharpoons Cd(CO_3)_2^{2-}$	---	---	6.4	72
300	kCdOH +	$Cd^{2+} + H_2O \rightleftharpoons CdOH^+ + H^+$	13.1	3	-10.08±0.1	3
301	kCd(OH) ₂ aq	$Cd^{2+} + 2H_2O \rightleftharpoons Cd(OH)_2^0 + 2H^+$	---	---	-20.35±0.2	3
302	kCd(OH) ₃ -	$Cd^{2+} + 3H_2O \rightleftharpoons Cd(OH)_3^- + 3H^+$	---	---	-33.3	3
303	kCd(OH) ₄ -2	$Cd^{2+} + 4H_2O \rightleftharpoons Cd(OH)_4^{2-} + 4H^+$	---	---	-47.35±0.1	3
304	kCd ₂ OH +3	$2Cd^{2+} + H_2O \rightleftharpoons Cd_2OH^{3+} + H^+$	10.9	3	-9.39±0.05	3
305	kCdOHCl aq	$Cd^{2+} + H_2O + Cl^- \rightleftharpoons CdOHCl^0 + H^+$	4.355	44	-7.404	44
306	kCdNO ₃ +	$Cd^{2+} + NO_3^- \rightleftharpoons CdNO_3^+$	-5.20	43	0.4	28
307	kCdSO ₄ aq	$Cd^{2+} + SO_4^{2-} \rightleftharpoons CdSO_4^0$	1.08	45	2.46	69
308	kCdHS +	$Cd^{2+} + HS^- \rightleftharpoons CdHS^+$	---	---	10.17	43
309	kCd(HS) ₂ aq	$Cd^{2+} + 2HS^- \rightleftharpoons Cd(HS)_2^0$	---	---	16.53	43
310	kCd(HS) ₃ -	$Cd^{2+} + 3HS^- \rightleftharpoons Cd(HS)_3^-$	---	---	18.71	43
311	kCd(HS) ₄ -2	$Cd^{2+} + 4HS^- \rightleftharpoons Cd(HS)_4^{2-}$	---	---	20.90	43
312	Cd Metal	$Cd \rightleftharpoons Cd^{2+} + 2e^-$	-18.0	44	13.49	44
313	Gamma Cd	$Cd_{(l)} \rightleftharpoons Cd^{2+} + 2e^-$	-18.14	44	13.59	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f^\circ \pm 1F$	Source
314	Cd(BO ₂) ₂	$\text{Cd(BO}_2)_2 + 2\text{H}_2\text{O} + 2\text{H}^+ \rightleftharpoons \text{Cd}^{2+} + 2\text{H}_3\text{BO}_3^0$	--- ²	---	9.84	44
315	Otavite	$\text{CdCO}_3 \rightleftharpoons \text{Cd}^{2+} + \text{CO}_3^{2-}$	-0.019	72	-12.1±0.1	72
316	CdCl ₂	$\text{CdCl}_2 \rightleftharpoons \text{Cd}^{2+} + 2\text{Cl}^-$	-4.47	44	-0.68	44
317	CdCl ₂ , H ₂ O	$\text{CdCl}_2 \cdot \text{H}_2\text{O} \rightleftharpoons \text{Cd}^{2+} + 2\text{Cl}^- + \text{H}_2\text{O}$	-1.82	44	-1.71	44
318	CdCl ₂ , 2.5H ₂ O	$\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O} \rightleftharpoons \text{Cd}^{2+} + 2\text{Cl}^- + 2.5\text{H}_2\text{O}$	1.71	44	-1.94	44
319	CdF ₂	$\text{CdF}_2 \rightleftharpoons \text{Cd}^{2+} + 2\text{F}^-$	-9.72	19	-2.98	19
320	Cd(OH) ₂ (a)	$\text{Cd(OH)}_{2(\text{amorph})} + 2\text{H}^+ \rightleftharpoons \text{Cd}^{2+} + 2\text{H}_2\text{O}$	-20.77	44	13.73	44
321	Cd(OH) ₂ (c)	$\text{Cd(OH)}_{2(\text{cryst})} + 2\text{H}^+ \rightleftharpoons \text{Cd}^{2+} + 2\text{H}_2\text{O}$	---	---	13.65±0.04	3
322	CdOHCl	$\text{CdOHCl} + \text{H}^+ \rightleftharpoons \text{Cd}^{2+} + \text{H}_2\text{O} + \text{Cl}^-$	-7.407	44	3.52	44
323	Cd ₃ (OH) ₄ SO ₄	$\text{Cd}_3(\text{OH})_4\text{SO}_4 + 4\text{H}^+ \rightleftharpoons 3\text{Cd}^{2+} + 4\text{H}_2\text{O} + \text{SO}_4^{2-}$	---	---	22.56	44
324	Cd ₃ (OH) ₂ (SO ₄) ₂	$\text{Cd}_3(\text{OH})_2(\text{SO}_4)_2 + 2\text{H}^+ \rightleftharpoons 3\text{Cd}^{2+} + 2\text{H}_2\text{O} + 2\text{SO}_4^{2-}$	---	---	6.71	44
325	Cd ₄ (OH) ₆ SO ₄	$\text{Cd}_4(\text{OH})_6\text{SO}_4 + 6\text{H}^+ \rightleftharpoons 4\text{Cd}^{2+} + 6\text{H}_2\text{O} + \text{SO}_4^{2-}$	---	---	28.4	28
326	Monteponite	$\text{CdO} + 2\text{H}^+ \rightleftharpoons \text{Cd}^{2+} + \text{H}_2\text{O}$	-24.76	44	13.77	18
327	Cd ₃ (PO ₄) ₂	$\text{Cd}_3(\text{PO}_4)_2 \rightleftharpoons 3\text{Cd}^{2+} + 2\text{PO}_4^{3-}$	---	---	-32.6	44
328	CdSiO ₃	$\text{CdSiO}_3 + \text{H}_2\text{O} + 2\text{H}^+ \rightleftharpoons \text{Cd}^{2+} + \text{H}_4\text{SiO}_4^0$	-16.63	44	9.06	44
329	CdSO ₄	$\text{CdSO}_4 \rightleftharpoons \text{Cd}^{2+} + \text{SO}_4^{2-}$	-14.74	44	-0.10	44
330	CdSO ₄ , H ₂ O	$\text{CdSO}_4 \cdot \text{H}_2\text{O} \rightleftharpoons \text{Cd}^{2+} + \text{SO}_4^{2-} + \text{H}_2\text{O}$ -7.52	44	-1.657	44	
331	CdSO ₄ , 2.7H ₂ O	$\text{CdSO}_4 \cdot 2.67\text{H}_2\text{O} \rightleftharpoons \text{Cd}^{2+} + \text{SO}_4^{2-} + 2.67\text{H}_2\text{O}$	-4.30	44	-1.873	44
332	Greenockite	$\text{CdS} + \text{H}^+ \rightleftharpoons \text{Cd}^{2+} + \text{HS}^-$	16.36	44	-15.93	44
333	kFe(SO ₄) ₂ -	$\text{Fe}^{3+} + 2\text{SO}_4^{2-} \rightleftharpoons \text{Fe(SO}_4)_2^-$	4.60	47	5.38	47
334	kFe ₂ (OH) ₂ +4	$2\text{Fe}^{3+} + 2\text{H}_2\text{O} \rightleftharpoons \text{Fe}_2(\text{OH})_2^{4+} + 2\text{H}^+$	13.5	3	-2.95±0.05	3
335	kFe ₃ (OH) ₄ +5	$3\text{Fe}^{3+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Fe}_3(\text{OH})_4^{5+} + 4\text{H}^+$	14.3	3	-6.3±0.1	3
336	kAl(OH) ₃ aq	$\text{Al}^{3+} + 3\text{H}_2\text{O} \rightleftharpoons \text{Al(OH)}_3^0 + 3\text{H}^+$	39.89 ⁴	47	-16.9	47
$\log K_f = 226.374 - 18247.8/T - 73.597 \log_{10} T$						
337	Jarosite H	$(\text{H}_3\text{O})\text{Fe}_3(\text{SO}_4)_2(\text{OH})_6 + 5\text{H}^+ \rightleftharpoons 3\text{Fe}^{3+} + 2\text{SO}_4^{2-} + 7\text{H}_2\text{O}$	-55.15	4	-5.39	4
338	Alum K	$\text{KAl(SO}_4)_2 \cdot 12\text{H}_2\text{O} \rightleftharpoons \text{K}^+ + \text{Al}^{3+} + 2\text{SO}_4^{2-} + 12\text{H}_2\text{O}$	7.22	4	-5.17	4
339	Melanterite	$\text{FeSO}_4 \cdot 7\text{H}_2\text{O} \rightleftharpoons \text{Fe}^{2+} + \text{SO}_4^{2-} + 7\text{H}_2\text{O}$	4.91 ⁴	47	-2.209	47
$\log K_f = 1.447 - 0.004153T - 2.14949 \cdot 10^5/T^2$						
340	Epsomite	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O} \rightleftharpoons \text{Mg}^{2+} + \text{SO}_4^{2-} + 7\text{H}_2\text{O}$	2.82	45	-2.14	45
341	kPbCl +	$\text{Pb}^{2+} + \text{Cl}^- \rightleftharpoons \text{PbCl}^+$	4.38	14	1.60	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
342	kPbCl2 aq	$Pb^{2+} + 2Cl^- \rightleftharpoons PbCl_2^0$	1.08	22	1.80	44
343	kPbCl3 -	$Pb^{2+} + 3Cl^- \rightleftharpoons PbCl_3^-$	2.17	22	1.7	69
344	kPbCl4 -2	$Pb^{2+} + 4Cl^- \rightleftharpoons PbCl_4^{2-}$	3.53	22	1.38	22
345	kPb(CO3)2 -2	$Pb^{2+} + 2CO_3^{2-} \rightleftharpoons Pb(CO_3)_2^{2-}$	--- ²	---2	10.64	24
346	kPbF +	$Pb^{2+} + F^- \rightleftharpoons PbF^+$	--- ²	---2	1.25	44
347	kPbF2 aq	$Pb^{2+} + 2F^- \rightleftharpoons PbF_2^0$	--- ²	---2	2.56	44
348	kPbF3 -	$Pb^{2+} + 3F^- \rightleftharpoons PbF_3^-$	--- ²	---2	3.42	67
349	kPbF4 -2	$Pb^{2+} + 4F^- \rightleftharpoons PbF_4^{2-}$	--- ²	---2	3.1	67
350	kPbOH +	$Pb^{2+} + H_2O \rightleftharpoons PbOH^+ + H^+$	--- ²	---2	-7.71±0.1	3
351	kPb(OH)2 aq	$Pb^{2+} + 2H_2O \rightleftharpoons Pb(OH)_2^0 + 2H^+$	--- ²	---2	-17.12±0.1	3
352	kPb(OH)3 -	$Pb^{2+} + 3H_2O \rightleftharpoons Pb(OH)_3^- + 3H^+$	--- ²	---2	-28.06±0.05	3
353	kPb2OH +3	$2Pb^{2+} + H_2O \rightleftharpoons Pb_2OH^{3+} + H^+$	--- ²	---2	-6.36±0.1	3
354	kPbNO3 +	$Pb^{2+} + NO_3^- \rightleftharpoons PbNO_3^+$	--- ²	---2	1.17±0.02	69
355	kPbSO4 aq	$Pb^{2+} + SO_4^{2-} \rightleftharpoons PbSO_4^0$	--- ²	---2	2.75±0.1	69
356	kPb(HS)2 aq	$Pb^{2+} + 2HS^- \rightleftharpoons Pb(HS)_2^0$	--- ²	---2	15.27	43
357	kPb(HS)3 -	$Pb^{2+} + 3HS^- \rightleftharpoons Pb(HS)_3^-$	--- ²	---2	16.57	43
358	kPb3(OH)4 +2	$3Pb^{2+} + 4H_2O \rightleftharpoons Pb_3(OH)_4^{2+} + 4H^+$	26.5	3	-23.88±0.2	3
359	kFeF +	$Fe^{2+} + F^- \rightleftharpoons FeF^+$	--- ²	---2	1.0	47
360	Pb Metal	$Pb \rightleftharpoons Pb^{2+} + 2e^-$	0.4	44	4.27	44
361	Pb(BO2)2	$Pb(BO_2)_2 + 2H_2O + 2H^+ \rightleftharpoons Pb^{2+} + 2H_3BO_3^0$	-5.80	43	7.61	43
362	Cotunnite	$PbCl_2 \rightleftharpoons Pb^{2+} + 2Cl^-$	5.60	44	-4.77	44
363	Matlockite	$PbClF \rightleftharpoons Pb^{2+} + Cl^- + F^-$	7.95	44	-9.43	44
364	Phosgenite	$PbCl_2 \rightleftharpoons PbCO_3 \rightleftharpoons 2Pb^{2+} + 2Cl^- + CO_3^{2-}$	--- ²	---2	-19.81	44
365	Cerrusite	$PbCO_3 \rightleftharpoons Pb^{2+} + CO_3^{2-}$	4.86	44	-13.13	24
366	PbF2	$PbF_2 \rightleftharpoons Pb^{2+} + 2F^-$	-0.7	44	-7.44	69
367	Massicot	$PbO + 2H^+ \rightleftharpoons Pb^{2+} + H_2O$	-16.78	44	12.91	24
368	Litharge	$PbO + 2H^+ \rightleftharpoons Pb^{2+} + H_2O$	-16.38	44	12.72	3
369	PbO, 0.3H2O	$PbO \cdot 0.33H_2O + 2H^+ \rightleftharpoons Pb^{2+} + 1.33H_2O$	--	--	12.98	44
370	Pb2OCO3	$PbO \rightleftharpoons PbCO_3 + 2H^+ \rightleftharpoons 2Pb^{2+} + CO_3^{2-} + H_2O$	-11.46	44	-0.5	44
371	Larnakite	$PbO \rightleftharpoons PbSO_4 + 2H^+ \rightleftharpoons 2Pb^{2+} + SO_4^{2-} + H_2O$	-6.44	44	-0.28	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	$\log K_f^\circ \pm 1F$	Source
372	Pb3O2SO4	$2PbO \cdot PbSO_4 + 4H^+ \rightleftharpoons 3Pb^{2+} + SO_4^{2-} + 2H_2O$	-20.75	44	10.4	44
373	Pb4O3SO4	$3PbO \cdot PbSO_4 + 6H^+ \rightleftharpoons 4Pb^{2+} + SO_4^{2-} + 3H_2O$	-35.07	44	22.1	44
374	PbHPO4	$PbHPO_4 \rightleftharpoons Pb^{2+} + HPO_4^{2-}$	7.04	51	-11.46	51
375	Pb3(PO4)2	$Pb_3(PO_4)_2 + 2H^+ \rightleftharpoons 3Pb^{2+} + 2HPO_4^{2-}$	-1.67	51	-19.67	51
376	Clpyromorphite	$Pb_3(PO_4)_3Cl \rightleftharpoons 5Pb^{2+} + 3PO_4^{3-} + Cl^-$	---2	---2	-84.43	51
377	Hxypyromorphite	$Pb_3(PO_4)_3OH + H^+ \rightleftharpoons 5Pb^{2+} + 3PO_4^{3-} + H_2O$	---2	---2	-62.79	51
378	Pb3O2CO3	$2PbO \cdot PbCO_3 + 4H^+ \rightleftharpoons 3Pb^{2+} + CO_3^{2-} + 2H_2O$	-26.43	19	11.02	19
379	Plumbogummite	$PbAl_3(PO_4)_2(OH)_5 \cdot H_2O + 5H^+ \rightleftharpoons Pb^{2+} + 3Al^{3+} + 2PO_4^{3-} + 6H_2O$	---2	---2	-32.79	51
380	Hinsdalite	$PbAl_3PO_4SO_4(OH)_6 + 6H^+ \rightleftharpoons Pb^{2+} + 3Al^{3+} + PO_4^{3-} + SO_4^{2-} + 6H_2O$	---2	---2	-2.5	51
381	Tsumebite	$Pb_2CuPO_4(OH)_3 \cdot 3H_2O + 3H^+ \rightleftharpoons 2Pb^{2+} + Cu^{2+} + PO_4^{3-} + 6H_2O$	---2	---2	-9.79	51
382	PbSiO3	$PbSiO_3 + H_2O + 2H^+ \rightleftharpoons Pb^{2+} + H_4SiO_4^0$	-9.26	44	7.32	44
383	Pb2SiO4	$Pb_2SiO_4 + 4H^+ \rightleftharpoons 2Pb^{2+} + H_4SiO_4^0$	-26.0	44	19.76	44
384	Anglesite	$PbSO_4 \rightleftharpoons Pb^{2+} + SO_4^{2-}$	2.15	44	-7.79±0.02	69
385	Galena	$PbS + H^+ \rightleftharpoons Pb^{2+} + HS^-$	19.4	44	-12.78	66
386	Plattnerite	$PbO_2 + 4H^+ + 2e^- \rightleftharpoons Pb^{2+} + 2H_2O$	-70.73	44	49.3	44
387	Pb2O3	$Pb_2O_3 + 6H^+ + 2e^- \rightleftharpoons 2Pb^{2+} + 3H_2O$	---2	---2	61.04	19
388	Minium	$Pb_3O_4 + 8H^+ + 2e^- \rightleftharpoons 3Pb^{2+} + 4H_2O$	-102.76	44	73.69	44
389	Pb(OH)2 (c)	$Pb(OH)_2 + 2H^+ \rightleftharpoons Pb^{2+} + 2H_2O$	-13.99	19	8.15	44
390	Laurionite	$PbOHC1 + H^+ \rightleftharpoons Pb^{2+} + Cl^- + H_2O$	---2	---2	0.623	71
391	Pb2(OH)3Cl	$Pb_2(OH)_3Cl + 3H^+ \rightleftharpoons 2Pb^{2+} + 3H_2O + Cl^-$	---2	---2	8.793	71
392	Hydrocerrusite	$2PbCO_3 \cdot Pb(OH)_2 + 2H^+ \rightleftharpoons 3Pb^{2+} + 2CO_3^{2-} + 2H_2O$	---2	---2	-17.46	67
393	Pb2O(OH)2	$PbO \cdot Pb(OH)_2 + 4H^+ \rightleftharpoons 2Pb^{2+} + 3H_2O$	---2	---2	26.2	67
394	Pb4(OH)6SO4	$Pb_4(OH)_6SO_4 + 6H^+ \rightleftharpoons 4Pb^{2+} + SO_4^{2-} + 6H_2O$	---2	---2	21.1	67
395	SiO2 (a)	$SiO_2 + 2H_2O \rightleftharpoons H_4SiO_4^0$	3.34 ⁴	47	-2.71	47
$\log K_f = -0.26-731/T$						
396	FCO3Apatite	$Ca_{9.496}Na_{0.36}Mg_{0.144}(PO_4)_4.8(CO_3)_{1.2}F_{2.48} \rightleftharpoons 9.496Ca^{2+} + 0.36Na^+ + 0.144Mg^{2+} + 4.8PO_4^{3-} + 1.2CO_3^{2-} + 2.48F^-$	39.39	13	-114.4	13
397	kAlHSO4 +2	$Al^{3+} + HSO_4^- \rightleftharpoons AlHSO_4^+$	---2	---2	0.46	1
398	BaF2	$BaF_2 \rightleftharpoons Ba^{2+} + 2F^-$	1.0	44	-5.76	44
399	SrF2	$SrF_2 \rightleftharpoons Sr^{2+} + 2F^-$	1.25	44	-8.54	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
400	kNO3/NO2	$\text{NO}_3^- + 2\text{H}^+ + 2e^- \rightleftharpoons \text{NO}_2 + \text{H}_2\text{O}$	-43.76	44	28.57	44
401	Dolomite (c)	$\text{CaMg}(\text{CO}_3)_2 \rightleftharpoons \text{Ca}^{2+} + \text{Mg}^{2+} + 2\text{CO}_3^{2-}$	-9.436	47	-17.09	47
402	Sulfur	$\text{S} + 2e^- \rightleftharpoons \text{S}^{2-}$	7.9	44	-15.026	44
403	kNiBr +	$\text{Ni}^{2+} + \text{Br}^- \rightleftharpoons \text{NiBr}^+$	--- ²	--- ²	0.5	67
404	kNiCl +	$\text{Ni}^{2+} + \text{Cl}^- \rightleftharpoons \text{NiCl}^+$	--- ²	--- ²	0.4	67
405	kNiF +	$\text{Ni}^{2+} + \text{F}^- \rightleftharpoons \text{NiF}^+$	--- ²	--- ²	1.3	67
406	kNiOH +	$\text{Ni}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{NiOH}^+ + \text{H}^+$	12.42	44	-9.86±0.03	3
407	kNi(OH)2 aq	$\text{Ni}^{2+} + 2\text{H}_2\text{O} \rightleftharpoons \text{Ni(OH)}_2^0 + 2\text{H}^+$	--- ²	--- ²	-19.0±1.0	3
408	kNi(OH)3 -	$\text{Ni}^{2+} + 3\text{H}_2\text{O} \rightleftharpoons \text{Ni(OH)}_3^- + 3\text{H}^+$	--- ²	--- ²	-30.0±0.5	3
409	kNiSO4 aq	$\text{Ni}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{NiSO}_4^0$	1.52	14	2.29	44
410	NiCO3	$\text{NiCO}_3 \rightleftharpoons \text{Ni}^{2+} + \text{CO}_3^{2-}$	-9.94	43	-6.84	44
411	Ni(OH)2	$\text{Ni(OH)}_2 + 2\text{H}^+ \rightleftharpoons \text{Ni}^{2+} + 2\text{H}_2\text{O}$	30.45	44	10.8±0.1	3
412	Ni4(OH)6SO4	$\text{Ni}_4(\text{OH})_6\text{SO}_4 + 6\text{H}^+ \rightleftharpoons 4\text{Ni}^{2+} + \text{SO}_4^{2-} + 6\text{H}_2\text{O}$	--- ²	--- ²	32.0	67
413	Bunsenite	$\text{NiO} + 2\text{H}^+ \rightleftharpoons \text{Ni}^{2+} + \text{H}_2\text{O}$	-23.92	44	12.45	44
414	Ni3(PO4)2	$\text{Ni}_3(\text{PO}_4)_2 \rightleftharpoons 3\text{Ni}^{2+} + 2\text{PO}_4^{3-}$	--- ²	--- ²	-31.3	44
415	Millerite	$\text{NiS} + \text{H}^+ \rightleftharpoons \text{Ni}^{2+} + \text{HS}^-$	2.5	44	-8.042	44
416	Retgersite	$\text{NiSO}_4 \cdot 6\text{H}_2\text{O} \rightleftharpoons \text{Ni}^{2+} + \text{SO}_4^{2-} + 6\text{H}_2\text{O}$	1.1	44	-2.04	44
417	Morenosite	$\text{NiSO}_4 \cdot 7\text{H}_2\text{O} \rightleftharpoons \text{Ni}^{2+} + \text{SO}_4^{2-} + 7\text{H}_2\text{O}$	2.94	44	-2.36	44
418	Ni2SiO4	$\text{Ni}_2\text{SiO}_4 + 4\text{H}^+ \rightleftharpoons 2\text{Ni}^{2+} + \text{H}_4\text{SiO}_4^0$	-33.36	43	14.54	43
419	Fe3(OH)8	$\text{Fe}_3(\text{OH})_8 + 8\text{H}^+ \rightleftharpoons 2\text{Fe}^{3+} + \text{Fe}^{2+} + 8\text{H}_2\text{O}$	--- ²	--- ²	20.222	55
420	Diopside	$\text{CuSiO}_3 \cdot \text{H}_2\text{O} + 2\text{H}^+ \rightleftharpoons \text{Cu}^{2+} + \text{H}_4\text{SiO}_4^0$	-8.96	43	6.50	43
421	kAgBr aq	$\text{Ag}^+ + \text{Br}^- \rightleftharpoons \text{AgBr}^0$	--- ²	--- ²	4.24	44
422	kAgBr2 -	$\text{Ag}^+ + 2\text{Br}^- \rightleftharpoons \text{AgBr}_2^-$	--- ²	--- ²	7.28	44
423	kAgCl aq	$\text{Ag}^+ + \text{Cl}^- \rightleftharpoons \text{AgCl}^0$	-2.68	44	3.27	44
424	kAgCl2 -	$\text{Ag}^+ + 2\text{Cl}^- \rightleftharpoons \text{AgCl}_2^-$	-3.93	44	5.27	44
425	kAgCl3 -2	$\text{Ag}^+ + 3\text{Cl}^- \rightleftharpoons \text{AgCl}_3^{2-}$	--- ²	--- ²	5.29	22
426	kAgCl4 -3	$\text{Ag}^+ + 4\text{Cl}^- \rightleftharpoons \text{AgCl}_4^{3-}$	--- ²	--- ²	5.51	22
427	kAgF aq	$\text{Ag}^+ + \text{F}^- \rightleftharpoons \text{AgF}^0$	-2.83	44	0.36	44
428	kAgHS aq	$\text{Ag}^+ + \text{HS}^- \rightleftharpoons \text{AgHS}^0$	--- ²	--- ²	14.05	43
429	kAg(HS)2 -	$\text{Ag}^+ + 2\text{HS}^- \rightleftharpoons \text{Ag(HS)}_2^-$	--- ²	--- ²	18.45	43

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
430	kAgI aq	$Ag^+ + I^- \rightleftharpoons AgI^0$	--- ²	---	6.6	44
431	kAgI2 -	$Ag^+ + 2I^- \rightleftharpoons AgI_2^-$	--- ²	---	10.68	44
432	kAgOH aq	$Ag^+ + H_2O \rightleftharpoons AgOH^0 + H^+$	--- ²	---	-12.0±0.3	3
433	kAg(OH)2 -	$Ag^+ + 2H_2O \rightleftharpoons Ag(OH)_2^- + 2H^+$	--- ²	---	-24.0±0.05	3
434	kAgSO4 -	$Ag^+ + SO_4^{2-} \rightleftharpoons AgSO_4^-$	1.49	44	1.29	44
435	kAgNO3 aq	$Ag^+ + NO_3^- \rightleftharpoons AgNO_3^0$	--- ²	---	-0.29	44
436	kAg(NO2)2 -	$Ag^+ + 2NO_2^- \rightleftharpoons Ag(NO_2)_2^-$	--- ²	---	2.22	44
437	Ag Metal	$Ag \rightleftharpoons Ag^+ + e^-$	25.234	44	-13.51	44
438	Bromyrite	$AgBr \rightleftharpoons Ag^+ + Br^-$	20.17	44	-12.27	44
439	Cerargyrite	$AgCl \rightleftharpoons Ag^+ + Cl^-$	15.652	44	-9.75	44
440	Ag2CO3	$Ag_2CO_3 \rightleftharpoons 2Ag^+ + CO_3^{2-}$	9.53	44	-11.07	44
441	AgF, 4H2O	$AgF \cdot 4H_2O \rightleftharpoons Ag^+ + F^- + 4H_2O$	4.27	44	0.55	44
442	Iodyrite	$AgI \rightleftharpoons Ag^+ + I^-$	26.82	44	-16.07	44
443	Ag2O	$Ag_2O + 2H^+ \rightleftharpoons 2Ag^+ + H_2O$	-10.43	44	12.58±0.1	3
444	Ag3PO4	$Ag_3PO_4 \rightleftharpoons 3Ag^+ + PO_4^{3-}$	--- ²	---	-17.55	69
445	Acanthite	$Ag_2S + H^+ \rightleftharpoons 2Ag^+ + HS^-$	53.3	44	-36.05	44
446	Ag2SO4	$Ag_2SO_4 \rightleftharpoons 2Ag^+ + SO_4^{2-}$	4.25	44	-4.92	44
447	kZnBr +	$Zn^{2+} + Br^- \rightleftharpoons ZnBr^+$	--- ²	---	-0.58	44
448	kZnBr2 aq	$Zn^{2+} + 2Br^- \rightleftharpoons ZnBr_2^0$	--- ²	---	-0.98	44
449	kZnI +	$Zn^{2+} + I^- \rightleftharpoons ZnI^+$	--- ²	---	-2.91	44
450	kZnI2 aq	$Zn^{2+} + 2I^- \rightleftharpoons ZnI_2^0$	--- ²	---	-1.69	44
451	kCdBr +	$Cd^{2+} + Br^- \rightleftharpoons CdBr^+$	-0.81	44	2.17	44
452	kCdBr2 aq	$Cd^{2+} + 2Br^- \rightleftharpoons CdBr_2^0$	--- ²	---	2.9	44
453	kCdI +	$Cd^{2+} + I^- \rightleftharpoons CdI^+$	-2.37	44	2.15	44
454	kCdI2 aq	$Cd^{2+} + 2I^- \rightleftharpoons CdI_2^0$	--- ²	---	3.59	44
455	kPbBr +	$Pb^{2+} + Br^- \rightleftharpoons PbBr^+$	2.88	44	1.77±0.1	69
456	kPbBr2 aq	$Pb^{2+} + 2Br^- \rightleftharpoons PbBr_2^0$	--- ²	---	1.44	44
457	kPbI +	$Pb^{2+} + I^- \rightleftharpoons PbI^+$	--- ²	---	1.94	44
458	kPbI2 aq	$Pb^{2+} + 2I^- \rightleftharpoons PbI_2^0$	--- ²	---	3.2	69
459	CuBr	$CuBr \rightleftharpoons Cu^+ + Br^-$	13.08	44	-8.21	44

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
460	CuI	$\text{CuI} \rightleftharpoons \text{Cu}^+ + \text{I}^-$	20.14	44	-11.89	44
461	ZnBr ₂ , 2H ₂ O	$\text{ZnBr}_2 \cdot 2\text{H}_2\text{O} \rightleftharpoons \text{Zn}^{2+} + 2\text{Br}^- + 2\text{H}_2\text{O}$	-7.51	44	5.21	44
462	ZnI ₂	$\text{ZnI}_2 \rightleftharpoons \text{Zn}^{2+} + 2\text{I}^-$	-13.44	44	7.23	44
463	CdBr ₂ , 4H ₂ O	$\text{CdBr}_2 \cdot 4\text{H}_2\text{O} \rightleftharpoons \text{Cd}^{2+} + 2\text{Br}^- + 4\text{H}_2\text{O}$	7.23	44	-2.42	44
464	CdI ₂	$\text{CdI}_2 \rightleftharpoons \text{Cd}^{2+} + 2\text{I}^-$	4.08	44	-3.61	44
465	PbBr ₂	$\text{PbBr}_2 \rightleftharpoons \text{Pb}^{2+} + 2\text{Br}^-$	8.10	44	-5.18	44
466	PbBrF	$\text{PbBrF} \rightleftharpoons \text{Pb}^{2+} + \text{Br}^- + \text{F}^-$	--- ²	---	-8.49	44
467	PbI ₂	$\text{PbI}_2 \rightleftharpoons \text{Pb}^{2+} + 2\text{I}^-$	15.16	44	-8.07	44
468	kPbCO ₃ aq	$\text{Pb}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{PbCO}_3^\circ$	--- ²	---	7.24	24
469	kPb(OH) ₄ -2	$\text{Pb}^{2+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Pb(OH)}_4^{2-} + 4\text{H}^+$	--- ²	---	-39.7	24
470	kPb(SO ₄) ₂ -2	$\text{Pb}^{2+} + 2\text{SO}_4^{2-} \rightleftharpoons \text{Pb(SO}_4)_2^{2-}$	--- ²	---	3.47	24
471	Jurbanite	$\text{AlOHSO}_4 + \text{H}^+ \rightleftharpoons \text{Al}^{3+} + \text{SO}_4^{2-} + \text{H}_2\text{O}$	--- ²	---	-3.23	58
472	Basaluminite	$\text{Al}_4(\text{OH})_{10}\text{SO}_4 + 10\text{H}^+ \rightleftharpoons 4\text{Al}^{3+} + \text{SO}_4^{2-} + 10\text{H}_2\text{O}$	--- ²	---	22.7	68
473	kAgBr ₃ -2	$\text{Ag}^+ + 3\text{Br}^- \rightleftharpoons \text{AgBr}_3^{2-}$	--- ²	---	8.71	44
474	kAgI ₃ -2	$\text{Ag}^+ + 3\text{I}^- \rightleftharpoons \text{AgI}_3^{2-}$	-27.03	44	13.37	44
475	kAgI ₄ -3	$\text{Ag}^+ + 4\text{I}^- \rightleftharpoons \text{AgI}_4^{3-}$	--- ²	---	14.08	44
476	kFe(HS) ₂ aq	$\text{Fe}^{2+} + 2\text{HS}^- \rightleftharpoons \text{Fe(HS)}_2^\circ$	--- ²	---	8.95	43
477	kFe(HS) ₃ -	$\text{Fe}_2^{2+} + 3\text{HS}^- \rightleftharpoons \text{Fe(HS)}_3$	--- ²	---	10.987	43
478	kH ₂ AsO ₃ -	$\text{H}_3\text{AsO}_3^\circ \rightleftharpoons \text{H}^+ + \text{H}_2\text{AsO}_3^-$	6.56	44	-9.228	44
479	kHAsO ₃ -2	$\text{H}_3\text{AsO}_3^\circ \rightleftharpoons 2\text{H}^+ + \text{HAsO}_3^{2-}$	14.2	43	-21.33	43
480	KAsO ₃ -3	$\text{H}_3\text{AsO}_3^\circ \rightleftharpoons 3\text{H}^+ + \text{AsO}_3^{3-}$	20.25	43	-34.744	43
481	kH ₄ AsO ₃ +	$\text{H}_3\text{AsO}_3^\circ + \text{H}^+ \rightleftharpoons \text{H}_4\text{AsO}_3^+$	--- ²	---	-0.305	44
482	kH ₂ AsO ₄ -	$\text{H}_3\text{AsO}_4^\circ \rightleftharpoons \text{H}^+ + \text{H}_2\text{AsO}_4^-$	-1.69	44	-2.243	44
483	kHAsO ₄ -2	$\text{H}_3\text{AsO}_4^\circ \rightleftharpoons 2\text{H}^+ + \text{HAsO}_4^{2-}$	-0.92	44	-9.001	44
484	kAsO ₄ -3	$\text{H}_3\text{AsO}_4^\circ \rightleftharpoons 3\text{H}^+ + \text{AsO}_4^{3-}$	3.43	44	-20.597	44
485	kCu(S ₄) ₂ -3	$\text{Cu}^{2+} + 2\text{HS}^- + 6\text{S}^\circ + \text{e}^- \rightleftharpoons \text{Cu(S}_4)_2^{3-} + 2\text{H}^+$	--- ²	---	6.109	16
486	kCuS ₄ S ₅ -3	$\text{Cu}^{2+} + 2\text{HS}^- + 7\text{S}^\circ + \text{e}^- \rightleftharpoons \text{CuS}_4\text{S}_5^{3-} + 2\text{H}^+$	--- ²	---	5.382	16
487	kAs ₃ /As ₅	$\text{H}_3\text{AsO}_3^\circ + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{AsO}_4^\circ + 2\text{H}^+ + 2\text{e}^-$	30.015	44	-19.444	44
488	As ₂ O ₅	$\text{As}_2\text{O}_5 + 3\text{H}_2\text{O} \rightleftharpoons 2\text{H}_3\text{AsO}_4^\circ$	-5.405	44	6.699	44
489	AlAsO ₄ , 2H ₂ O	$\text{AlAsO}_4 \cdot 2\text{H}_2\text{O} \rightleftharpoons \text{Al}^{3+} + \text{AsO}_4^{3-} + 2\text{H}_2\text{O}$	--- ²	---	-15.837	43

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
490	Ca ₃ (AsO ₄) ₂ , 4w	Ca ₃ (AsO ₄) ₂ + 4H ₂ O = 3Ca ²⁺ + 2AsO ₄ ³⁻ + 4H ₂ O	--- ²	---	-18.905	43
491	Cu ₃ (AsO ₄) ₂ , 6w	Cu ₃ (AsO ₄) ₂ + 6H ₂ O = 3Cu ²⁺ + 2AsO ₄ ³⁻ + 6H ₂ O	--- ²	---	-35.123	43
492	Scorodite	FeAsO ₄ + 2H ₂ O = Fe ³⁺ + AsO ₄ ³⁻ + 2H ₂ O	--- ²	---	-20.249	43
493	Mn ₃ (AsO ₄) ₂ , 8H ₂ O	Mn ₃ (AsO ₄) ₂ + 8H ₂ O = 3Mn ²⁺ + 2AsO ₄ ³⁻ + 8H ₂ O	--- ²	---	-28.707	43
494	Ni ₃ (AsO ₄) ₂ , 8H ₂ O	Ni ₃ (AsO ₄) ₂ + 8H ₂ O = 3Ni ²⁺ + 2AsO ₄ ³⁻ + 8H ₂ O	--- ²	---	-25.511	43
495	Pb ₃ (AsO ₄) ₂	Pb ₃ (AsO ₄) ₂ = 3Pb ²⁺ + 2AsO ₄ ³⁻	--- ²	---	-35.403	43
496	Zn ₃ (AsO ₄) ₂ , 2.5w	Zn ₃ (AsO ₄) ₂ + 2.5H ₂ O = 3Zn ²⁺ + 2AsO ₄ ³⁻ + 2.5H ₂ O	--- ²	---	-27.546	44
497	Arsenolite	As ₄ O ₆ + 6H ₂ O = 4H ₃ AsO ₃ ⁰	14.33	44	-2.801	44
498	Claudetite	As ₄ O ₆ + 6H ₂ O = 4H ₃ AsO ₃ ⁰	13.29	44	-3.065	44
499	AsI ₃	AsI ₃ + 3H ₂ O = H ₃ AsO ₃ ⁰ + 3I ⁻ + 3H ⁺	1.875	44	4.155	44
500	Orpiment	As ₂ S ₃ + 6H ₂ O = 2H ₃ AsO ₃ ⁰ + 3HS ⁻ + 3H ⁺	82.89	44	-60.971	44
501	Realgar	AsS + 3H ₂ O = H ₃ AsO ₃ ⁰ + HS ⁻ + 2H ⁺ + e ⁻	30.545	43	-19.747	43
502	kS2 -2	HS ⁻ + S ⁰ = S ₂ ²⁻ + H ⁺	11.4	44	-14.528	16
503	kS3 -2	HS ⁻ + 2S ⁰ = S ₃ ²⁻ + H ⁺	10.4	44	-13.282	16
504	kS4 -2	HS ⁻ + 3S ⁰ = S ₄ ²⁻ + H ⁺	9.7	44	-9.829	16
505	kS5 -2	HS ⁻ + 4S ⁰ = S ₅ ²⁻ + H ⁺	9.3	44	-9.595	16
506	kS6 -2	HS ⁻ + 5S ⁰ = S ₆ ²⁻ + H ⁺	--- ²	---	-9.881	16
507	kAg(S ₄) ₂ -3	Ag ⁺ + 2HS ⁻ + 6S ⁰ = Ag(S ₄) ₂ ³⁻ + 2H ⁺	--- ²	---	0.991	16
508	kAgS ₄ S ₅ -3	Ag ⁺ + 2HS ⁻ + 7S ⁰ = AgS ₄ S ₅ ³⁻ + 2H ⁺	--- ²	---	0.680	16
509	kAg(HS)S ₄ -2	Ag ⁺ + 2HS ⁻ + 3S ⁰ = Ag(HS)S ₄ ²⁻ + H ⁺	--- ²	---	10.431	16
510	kCuHCO ₃ +	Cu ²⁺ + HCO ₃ ⁻ = CuHCO ₃ ⁺	--- ²	---	2.7	81
511	kZnHCO ₃ +	Zn ²⁺ + HCO ₃ ⁻ = ZnHCO ₃ ⁺	--- ²	---	2.1	81
512	kZnCO ₃ aq	Zn ²⁺ + CO ₃ ²⁻ = ZnCO ₃ ⁰	--- ²	---	5.3	81
513	kZn(CO ₃) ₂ -2	Zn ²⁺ + 2CO ₃ ²⁻ = Zn(CO ₃) ₂ ²⁻	--- ²	---	9.63	37
514	kCdHCO ₃	Cd ²⁺ + HCO ₃ ⁻ = CdHCO ₃ ⁺	--- ²	---	1.5	72
515	kCdCO ₃ aq	Cd ²⁺ + CO ₃ ²⁻ = CdCO ₃ ⁰	--- ²	---	2.9±0.4	72
516	kCd(SO ₄) ₂ -2	Cd ²⁺ + 2SO ₄ ²⁻ = Cd(SO ₄) ₂ ²⁻	--- ²	---	3.5	81
517	kPbHCO ₃ +	Pb ²⁺ + HCO ₃ ⁻ = PbHCO ₃ ⁺	--- ²	---	2.9	81
518	kNiCl ₂ aq	Ni ²⁺ + 2Cl ⁻ = NiCl ₂ ⁰	--- ²	---	0.96	37
519	kNiHCO ₃ +	Ni ²⁺ + HCO ₃ ⁻ = NiHCO ₃ ⁺	--- ²	---	2.14	37

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
520	kNiCO ₃ aq	$Ni^{2+} + CO_3^{2-} \rightleftharpoons NiCO_3^0$	--- ²	--- ²	6.87	37
521	kNi(CO ₃) ₂ -2	$Ni^{2+} + 2CO_3^{2-} \rightleftharpoons Ni(CO_3)_2^{2-}$	--- ²	--- ²	10.11	37
522	kNi(SO ₄) ₂ -2	$Ni^{2+} + 2SO_4^{2-} \rightleftharpoons Ni(SO_4)_2^{2-}$	--- ²	--- ²	1.02	37
523	kH Fulvate	$H^+ + L^{2-} \rightleftharpoons HL^-$	--- ²	--- ²	4.27	70 ¹³
524	kH Humate	$H^+ + L^{2-} \rightleftharpoons HL^-$	--- ²	--- ²	4.27	70 ¹³
525	kFe Fulvate	$Fe^{3+} + L^{2-} \rightleftharpoons FeL^+$	--- ²	--- ²	9.4	70 ¹³
526	kFe Humate	$Fe^{3+} + L^{2-} \rightleftharpoons FeL^+$	--- ²	--- ²	9.4	70 ¹³
527	kCu Fulvate	$Cu^{2+} + L^{2-} \rightleftharpoons CuL^0$	--- ²	--- ²	6.2	70 ¹³
528	kCu Humate	$Cu^{2+} + L^{2-} \rightleftharpoons CuL^0$	--- ²	--- ²	6.2	70 ¹³
529	kCd Fulvate	$Cd^{2+} + L^{2-} \rightleftharpoons CdL^0$	--- ²	--- ²	3.5	70 ¹³
530	kCd Humate	$Cd^{2+} + L^{2-} \rightleftharpoons CdL^0$	--- ²	--- ²	3.5	70 ¹³
531	kAg Fulvate	$Ag^+ + L^{2-} \rightleftharpoons AgL^-$	--- ²	--- ²	2.4	70 ¹³
532	kAg Humate	$Ag^+ + L^{2-} \rightleftharpoons AgL^-$	--- ²	--- ²	2.4	70 ¹³
533	Blaublei I	$Cu_{0.9}^{2+}Cu_{0.2}^{+}S + H^+ \rightleftharpoons 0.9Cu^{2+} + 0.2Cu^+ + HS^-$	--- ²	--- ²	-24.162±0.15	56
534	Blaublei II	$Cu_{0.6}^{2+}Cu_{0.8}^{+}S + H^+ \rightleftharpoons 0.6Cu^{2+} + 0.8Cu^+ + HS^-$	--- ²	--- ²	-27.279±0.15	56
535	Anilite	$Cu_{0.25}^{2+}Cu_{1.5}^{+}S + H^+ \rightleftharpoons 0.25Cu^{2+} + 1.5Cu^+ + HS^-$	43.535	56	-31.878±0.15	56
536	Djurleite	$Cu_{0.066}^{2+}Cu_{1.868}^{+}S + H^+ \rightleftharpoons 0.066Cu^{2+} + 1.868Cu^+ + HS^-$	47.881	56	-33.920±0.15	56
537	kH ₂ F ₂ aq	$2H^+ + 2F^- \rightleftharpoons H_2F_2$	--- ²	--- ²	6.768	4
538	kpeS/H ₂ S	$S_8 + 2H^+ + 2e^- \rightleftharpoons H_2S^0$	-9.5	67	4.882	67
539	Portlandite	$Ca(OH)_2 + 2H^+ \rightleftharpoons Ca^{2+} + 2H_2O$	-31.0	47	22.8	47
540	kNaF aq	$Na^+ + F^- \rightleftharpoons NaF^0$	--- ²	--- ²	-0.24±0.05	47
541	Ba ₃ (AsO ₄) ₂	$Ba_3(AsO_4)_2 \rightleftharpoons 3Ba^{2+} + 2AsO_4^{3-}$	9.5	44	-50.11	67
542	kFeCl +	$Fe^{2+} + Cl^- \rightleftharpoons FeCl^+$	--- ²	--- ²	0.14	47
543	kBaSO ₄ aq	$Ba^{2+} + SO_4^{2-} \rightleftharpoons BaSO_4^0$	--- ²	--- ²	2.7	69
544	kH ₂ Se aq	$H_2Se^0 \rightleftharpoons H^+ + HSe^-$	5.3	--- ¹⁴	-3.8	--- ¹⁴
545	kH ₂ SeO ₃ aq	$SeO_3^{2-} + 2H^+ \rightleftharpoons H_2SeO_3^0$	--- ²	--- ²	11.25	--- ¹⁴
546	kHSeO ₃ -	$SeO_3^{2-} + H^+ \rightleftharpoons HSeO_3^-$	--- ²	--- ²	8.5	--- ¹⁴
547	kHSeO ₄ -	$SeO_4^{2-} + H^+ \rightleftharpoons HSeO_4^-$	4.91	--- ¹⁴	1.66	--- ¹⁴
548	kSe ₄ /Se ₆	$SeO_3^{2-} + H_2O \rightleftharpoons SeO_4^{2-} + 2H^+ + 2e^-$	--- ²	--- ²	-30.256	--- ¹⁴
549	kSe ₄ /Se-2	$SeO_3^{2-} + 7H^+ + 6e^- \rightleftharpoons HSe^- + 3H_2O$	--- ²	--- ²	42.514	--- ¹⁴

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
550	Se metal<Se=	$\text{Se}_8 + \text{H}^+ + 2\text{e}^- \rightleftharpoons \text{HSe}^-$	--- ²	--- ²	-17.322	--- ¹⁴
551	Se metal<Se4	$\text{Se}_8 + 3\text{H}_2\text{O} \rightleftharpoons \text{SeO}_3^{2-} + 6\text{H}^+ + 4\text{e}^-$	--- ²	--- ²	-59.836	--- ¹⁴
552	FeSe2	$\text{FeSe}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Fe}^{2+} + 2\text{HSe}^-$	--- ²	--- ²	-18.58	--- ¹⁴
553	SeO2	$\text{SeO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{SeO}_3^{2-} + 2\text{H}^+$	--- ²	--- ²	-8.38	--- ¹⁴
554	CaSeO3	$\text{CaSeO}_3 \rightleftharpoons \text{Ca}^{2+} + \text{SeO}_3^{2-}$	--- ²	--- ²	-5.6	--- ¹⁴
555	BaSeO3	$\text{BaSeO}_3 \rightleftharpoons \text{Ba}^{2+} + \text{SeO}_3^{2-}$	--- ²	--- ²	-6.39	--- ¹⁴
556	Fe2(SeO3)3	$\text{Fe}_2(\text{SeO}_3)_3 \rightleftharpoons 2\text{Fe}^{2+} + 3\text{SeO}_3^{2-}$	--- ²	--- ²	-35.43	--- ¹⁴
557	kAs3/As	$\text{H}_3\text{AsO}_3^\circ + 3\text{H}^+ + 3\text{e}^- \rightleftharpoons \text{As}_8 + 3\text{H}_2\text{O}$	--- ²	--- ²	12.17	--- ¹⁴
558	kFeHCO3 +	$\text{Fe}^{2+} + \text{HCO}_3^- \rightleftharpoons \text{FeHCO}_3^\circ$	--- ²	--- ²	2.0	47
559	kFeCO3 aq	$\text{Fe}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{FeCO}_3^\circ$	--- ²	--- ²	4.38	47
560	kMnCO3 aq	$\text{Mn}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{MnCO}_3^\circ$	--- ²	--- ²	4.90	47
561	kBaHCO3 +	$\text{Ba}^{2+} + \text{HCO}_3^- \rightleftharpoons \text{BaHCO}_3^\circ$	5.56 ⁴	47	0.982	47
log $K_f = -3.0938 + 0.013669T$						
562	kBaCO3 aq	$\text{Ba}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{BaCO}_3^\circ$	3.55 ⁴	47	2.71	47
log $K_f = 0.113 + 0.008721T$						
563	kSrSO4 aq	$\text{Sr}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{SrSO}_4^\circ$	2.08	47	2.29	47
564	Rhodochrosite (c)	$\text{MnCO}_{3(\text{crystal})} \rightleftharpoons \text{Mn}^{2+} + \text{CO}_3^{2-}$	-1.43	47	-11.13	47
565	kU +4	$\text{UO}_2^{2+} + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{U}^{4+} + 2\text{H}_2\text{O}$	-34.38	21	9.04±0.44	21
566	kU +3	$\text{U}^{4+} + \text{e}^- \rightleftharpoons \text{U}^{3+}$	24.4±0.4	21	-9.35±0.07	21
567	kUOH +3	$\text{U}^{4+} + \text{H}_2\text{O} \rightleftharpoons \text{UOH}^{3+} + \text{H}^+$	11.21±2.16	21	-0.54±0.06	21
568	kU(OH)2 +2	$\text{U}^{4+} + 2\text{H}_2\text{O} \rightleftharpoons \text{U(OH)}_2^{2+} + 2\text{H}^+$	17.73	33	-2.27	33
569	kU(OH)3 +	$\text{U}^{4+} + 3\text{H}_2\text{O} \rightleftharpoons \text{U(OH)}_3^+ + 3\text{H}^+$	22.645	33	-4.935	33
570	kU(OH)4 aq	$\text{U}^{4+} + 4\text{H}_2\text{O} \rightleftharpoons \text{U(OH)}_4^+ + 4\text{H}^+$	24.76	33	-8.498	33
571	Na4UO2(CO3)3	$\text{Na}_4\text{UO}_2(\text{CO}_3)_3 \rightleftharpoons 4\text{Na}^+ + \text{UO}_2^{2+} + 3\text{CO}_3^{2-}$	--- ²	--- ²	-21.68±0.56	21
572	kU6(OH)15 +9	$6\text{U}^{4+} + 15\text{H}_2\text{O} \rightleftharpoons \text{U}_6(\text{OH})_{15}^{9+} + 15\text{H}^+$	--- ²	--- ²	-16.9±0.6	21
573	Uraninite (c)	$\text{UO}_2 + 4\text{H}^+ \rightleftharpoons \text{U}^{4+} + 2\text{H}_2\text{O}$	-18.61±0.96	21	-4.85±0.36	21
574	UO2 (a)	$\text{UO}_2 + 4\text{H}^+ \rightleftharpoons \text{U}^{4+} + 2\text{H}_2\text{O}$	--- ²	--- ²	0.1±0.7	21
575	U4O9 (c)	$\text{U}_4\text{O}_9 + 18\text{H}^+ + 2\text{e}^- \rightleftharpoons 4\text{U}^{4+} + 9\text{H}_2\text{O}$	-101.64	21	-3.99±1.72	21
576	U3O8 (c)	$\text{U}_3\text{O}_8 + 16\text{H}^+ + 4\text{e}^- \rightleftharpoons 3\text{U}^{4+} + 8\text{H}_2\text{O}$	-116.02±1.4	21	20.54±1.02	21
577	Coffinite	$\text{USiO}_4 + 4\text{H}^+ \rightleftharpoons \text{U}^{4+} + \text{H}_4\text{SiO}_4^\circ$	-13.58	21	-8.06±0.79	21

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
578	kUF +3	$U^{4+} + F^- \rightleftharpoons UF^{3+}$	-1.34±0.1	21	9.28±0.09	21
579	kUF2 +2	$U^{4+} + 2F^- \rightleftharpoons UF_2^{2+}$	-0.84±0.1	21	16.23±0.15	21
580	kUF3 +	$U^{4+} + 3F^- \rightleftharpoons UF_3^+$	0.1±1.0	21	21.6±1.0	21
581	kUF4 aq	$U^{4+} + 4F^- \rightleftharpoons UF_4^0$	-1.01±1.82	21	25.6±1.0	21
582	kUF5 -	$U^{4+} + 5F^- \rightleftharpoons UF_5^-$	4.85	33	27.01±0.3	21
583	kUF6 -2	$U^{4+} + 6F^- \rightleftharpoons UF_6^{2-}$	3.3	33	29.08±0.18	21
584	UF4 (c)	$UF_4 \rightleftharpoons U^{4+} + 4F^-$	-4.4	21	-29.36±0.93	21
585	UF4, 2.5H2O	$UF_4 \cdot 2.5H_2O \rightleftharpoons U^{4+} + 4F^- + 2.5H_2O$	5.81	21	-33.55±1.23	21
586	kUCl +3	$U^{4+} + Cl^- \rightleftharpoons UCl^{3+}$	-4.54±2.15	21	1.72±0.13	21
587	kUSO4 +2	$U^{4+} + SO_4^{2-} \rightleftharpoons USO_4^{2+}$	1.91±0.7	21	6.58±0.19	21
588	kU(SO4)2 aq	$U^{4+} + 2SO_4^{2-} \rightleftharpoons U(SO_4)_2^0$	7.82±0.7	21	10.51±0.2	21
589	kU(CO3)4 -4	$U^{4+} + 4CO_3^{2-} \rightleftharpoons U(CO_3)_4^{4-}$	---2	---2	35.12±0.9	21
590	kU(CO3)5 -6	$U^{4+} + 5CO_3^{2-} \rightleftharpoons U(CO_3)_5^{6-}$	-4.8	21	33.9±1.0	21
591	U(OH)2SO4	$U(OH)_2SO_4 + 2H^+ \rightleftharpoons U^{4+} + SO_4^{2-} + 2H_2O$	---2	---2	-3.17±0.5	21
592	UO2HPO4, 4H2O	$UO_2HPO_4 \cdot 4H_2O \rightleftharpoons UO_2^{2+} + HPO_4^{2-} + 4H_2O$	2.07	21	-11.85±0.59	21
593	U(HPO4)2, 4H2O	$U(HPO_4)_2 \cdot 4H_2O \rightleftharpoons U^{4+} + 2PO_4^{3-} + 2H^+ + 4H_2O$	0.55	21	-30.49±0.91	21
594	Ningyosite	$CaU(PO_4)_2 \cdot 2H_2O \rightleftharpoons U^{4+} + Ca^{2+} + 2PO_4^{3-} + 2H_2O$	-2.27	33	-53.91	33
595	kUO2 +	$UO_2^{2+} + e^- \rightleftharpoons UO_2^+$	-3.3	33	1.48±0.02	21
596	kUO2OH +	$UO_2^{2+} + H_2O \rightleftharpoons UO_2OH^+ + H^+$	11.015	33	-5.2±0.3	21
597	k(UO2)2(OH)2+2	$2UO_2^{2+} + 2H_2O \rightleftharpoons (UO_2)_2(OH)_2^{2+} + 2H^+$	10.23	33	-5.62±0.04	21
598	k(UO2)3(OH)5 +	$3UO_2^{2+} + 5H_2O \rightleftharpoons (UO_2)_3(OH)_5^+ + 5H^+$	25.075	33	-15.55±0.12	21
599	UO3 (c)	$UO_3 + 2H^+ \rightleftharpoons UO_2^{2+} + H_2O$	-19.37	21	7.70±0.37	21
600	Gummite	$UO_3 + 2H^+ \rightleftharpoons UO_2^{2+} + H_2O$	-23.02	33	10.40	33
601	β-UO2(OH)2	$UO_2(OH)_2 + 2H^+ \rightleftharpoons UO_2^{2+} + 2H_2O$	-13.59	21	4.93±0.44	21
602	Schoepite	$UO_2(OH)_2 \cdot H_2O + 2H^+ \rightleftharpoons UO_2^{2+} + 3H_2O$	-12.04	21	4.81±0.43	21
603	kUO2CO3 aq	$UO_2^{2+} + CO_3^{2-} \rightleftharpoons UO_2CO_3^0$	1.20±0.48	21	9.67±0.45	21
604	kUO2(CO3)2 -2	$UO_2^{2+} + 2CO_3^{2-} \rightleftharpoons UO_2(CO_3)_2^{2-}$	4.42±0.96	21	16.94±0.12	21
605	kUO2(CO3)3 -4	$UO_2^{2+} + 3CO_3^{2-} \rightleftharpoons UO_2(CO_3)_3^{4-}$	-9.37±0.74	21	21.60±0.05	21
606	Rutherfordine	$UO_2CO_3 \rightleftharpoons UO_2^{2+} + CO_3^{2-}$	-1.44	33	-14.49±0.04	21
607	kUO2F +	$UO_2^{2+} + F^- \rightleftharpoons UO_2F^+$	0.41±0.02	21	5.09±0.13	21

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	ΔH_f° (kcal/mol)	Source	Log K _f ^o	Source
608	kUO2F2 aq	$\text{UO}_2^{2+} + 2\text{F}^- \text{W } \text{UO}_2\text{F}_2^\circ$	0.50±0.05	21	8.62±0.04	21
609	kUO2F3 -	$\text{UO}_2^{2+} + 3\text{F}^- \text{W } \text{UO}_2\text{F}_3^-$	0.56±0.07	21	10.9±0.4	21
610	kUO2F4 -2	$\text{UO}_2^{2+} + 4\text{F}^- \text{W } \text{UO}_2\text{F}_4^{2-}$	0.07±0.11	21	11.7±0.7	21
611	kUO2Cl +	$\text{UO}_2^{2+} + \text{Cl}^- \text{W } \text{UO}_2\text{Cl}^+$	1.9±0.5	21	0.17±0.02	21
612	kUO2SO4 aq	$\text{UO}_2^{2+} + \text{SO}_4^{2-} \text{W } \text{UO}_2\text{SO}_4^\circ$	4.66±0.4	21	3.15±0.02	21
613	kUO2(SO4)2 -2	$\text{UO}_2^{2+} + 2\text{SO}_4^{2-} \text{W } \text{UO}_2(\text{SO}_4)_2^{2-}$	8.39±0.2	21	4.14±0.07	21
614	kUO2HPO4 aq	$\text{UO}_2^{2+} + \text{PO}_4^{3-} + \text{H}^+ \text{W } \text{UO}_2\text{HPO}_4^\circ$	-13.37	21	19.59±0.64	21
615	kUO2HPO4)2 -2	$\text{UO}_2^{2+} + 2\text{PO}_4^{3-} + 2\text{H}^+ \text{W } \text{UO}_2(\text{HPO}_4)_2^{2-}$	-11.8	33	43.141	33
616	kUO2H2PO4 +	$\text{UO}_2^{2+} + \text{PO}_4^{3-} + 2\text{H}^+ \text{W } \text{UO}_2\text{H}_2\text{PO}_4^+$	-3.7	33	22.82±0.59	21
617	kUO2H2PO4)2 aq	$\text{UO}_2^{2+} + 2\text{PO}_4^{3-} + 4\text{H}^+ \text{W } \text{UO}_2(\text{H}_2\text{PO}_4)_2^\circ$	-16.5	33	44.05±0.76	21
618	kUO2H2PO4)3 -	$\text{UO}_2^{2+} + 3\text{PO}_4^{3-} + 6\text{H}^+ \text{W } \text{UO}_2(\text{H}_2\text{PO}_4)_3^-$	-28.6	33	66.245	33
619	(UO2)3(PO4)2,4w	$(\text{UO}_2)_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O} \text{W } 3\text{UO}_2^{2+} + 2\text{PO}_4^{3-} + 4\text{H}_2\text{O}$	-7.17	21	-49.37±1.55	21
620	H-Autunite	$\text{H}_2(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } 2\text{H}^+ + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-3.6	33	-47.931	33
621	Na-Autunite	$\text{Na}_2(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } 2\text{Na}^+ + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-0.46	33	-47.409	33
622	K-Autunite	$\text{K}_2(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } 2\text{K}^+ + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	5.86	33	-48.244	33
623	Uramphite	$(\text{NH}_4)_2(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } 2\text{NH}_4^+ + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	9.70	33	-51.749	33
624	Salceite	$\text{Mg}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Mg}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-20.18	33	-43.646	33
625	Autunite	$\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Ca}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-14.34	33	-43.927	33
626	Sr-Autunite	$\text{Sr}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Sr}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-13.05	33	-44.457	33
627	Uranocircite	$\text{Ba}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Ba}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-10.1	33	-44.631	33
628	Bassetite	$\text{Fe}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Fe}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-19.9	33	-44.485	33
629	Torbernite	$\text{Cu}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Cu}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-15.9	33	-45.279	33
630	Przhevalskite	$\text{Pb}(\text{UO}_2)_2(\text{PO}_4)_2 \text{W } \text{Pb}^{2+} + 2\text{UO}_2^{2+} + 2\text{PO}_4^{3-}$	-11.0	33	-44.365	33
631	Blank		--- ⁹	--- ⁹	--- ⁹	--- ⁹
632	Uranophane	$\text{Ca}(\text{UO}_2)_2(\text{SiO}_3\text{OH})_2 + 6\text{H}^+ \text{W } \text{Ca}^{2+} + 2\text{UO}_2^{2+} + 2\text{H}_4\text{SiO}_4^\circ$	--- ²	--- ²	11.7±0.6	82
633	kUBr +3	$\text{U}^{4+} + \text{Br}^- \text{W } \text{UBr}^{3+}$	--- ²	--- ²	1.46±0.2	21
634	kUI +3	$\text{U}^{4+} + \text{I}^- \text{W } \text{UI}^{3+}$	--- ²	--- ²	1.25±0.3	21
635	kUNO3 +3	$\text{U}^{4+} + \text{NO}_3^- \text{W } \text{UNO}_3^{3+}$	--- ²	--- ²	1.47±0.13	21
636	kU(NO3)2 +2	$\text{U}^{4+} + 2\text{NO}_3^- \text{W } \text{U}(\text{NO}_3)_2^{2+}$	--- ²	--- ²	2.30±0.35	21
637	Blank		--- ⁹	--- ⁹	--- ⁹	--- ⁹

Table 2. Thermodynamic Data (continued)

I ¹	Species	Reaction	$\Delta H_f^\circ \pm 1F$ (kcal/mol)	Source	Log $K_f^\circ \pm 1F$	Source
638	kUO ₂ (OH) ₃ -	UO ₂ ²⁺ + 3H ₂ O W UO ₂ (OH) ₃ ⁻ + 3H ⁺	--- ²	---	-19.2±0.4	21
639	kUO ₂ (OH) ₄ -2	UO ₂ ²⁺ + 4H ₂ O W UO ₂ (OH) ₄ ²⁻ + 4H ⁺	--- ²	---	-33.0±2.0	21
640	k(UO ₂) ₂ OH +3	2UO ₂ ²⁺ + H ₂ O W (UO ₂) ₂ OH ³⁺ + H ⁺	--- ²	---	-2.7±1.0	21
641	k(UO ₂) ₃ (OH) ₄ +2	3UO ₂ ²⁺ + 4H ₂ O W (UO ₂) ₃ (OH) ₄ ²⁺ + 4H ⁺	--- ²	---	-11.9±0.3	21
642	k(UO ₂) ₃ (OH) ₇ -	3UO ₂ ²⁺ + 7H ₂ O W (UO ₂) ₃ (OH) ₇ ⁺ + 7H ⁺	--- ²	---	-31.0±2.0	21
643	k(UO ₂) ₄ (OH) ₇ +	4UO ₂ ²⁺ + 7H ₂ O W (UO ₂) ₄ (OH) ₇ ⁺ + 7H ⁺	--- ²	---	-21.9±1.0	21
644	kUO ₂ Cl ₂ aq	UO ₂ ²⁺ + 2Cl ⁻ W UO ₂ Cl ₂	3.6±1.4	21	-1.1±0.4	21
645	kUO ₂ Br +	UO ₂ ²⁺ + Br ⁻ W UO ₂ Br ⁺	--- ²	---	0.22±0.02	21
646	kUO ₂ NO ₃ +	UO ₂ ²⁺ + NO ₃ ⁻ W UO ₂ NO ₃ ⁺	--- ²	---	0.30±0.15	21
647	kUO ₂ H ₃ PO ₄ +2	UO ₂ ²⁺ + PO ₄ ³⁻ + 3H ⁺ W UO ₂ H ₃ PO ₄ ²⁺	--- ²	---	22.46±0.60	21
648	k(UO ₂) ₃ (CO ₃) ₆ -6	3UO ₂ ²⁺ + 6CO ₃ ²⁻ W (UO ₂) ₃ (CO ₃) ₆ ⁶⁻	-15.0	21	54.0±1.0	21
649	kUO ₂ PO ₄ -	UO ₂ ²⁺ + PO ₄ ³⁻ W UO ₂ PO ₄ ⁻	--- ²	---	13.23±0.15	21
650	kUO ₂ (CO ₃) ₃ -5	UO ₂ ²⁺ + 3CO ₃ ²⁻ + e ⁻ W UO ₂ (CO ₃) ₃ ⁵⁻	--- ²	---	8.89±0.27	21
651	Blank		--- ⁹	---	---	---
652	Blank		--- ⁹	---	---	---
653	Blank		--- ⁹	---	---	---

Footnotes to Table 2

¹Reaction number.

²No thermodynamic data are presently available.

³Parenthetical letters after mineral names designate degree of crystallinity of phase:
a=amorphous; b=beta; c=crystalline; d=disordered; e=epsilon; g=gamma; AB=Aberdeen;
BF=Belle Fourche; Ca=calcium.

⁴Enthalpy derived from the temperature variation of log K using the vant Hoff relation.

⁵Changes in thermodynamic values reflect an alteration of the hydrolysis reaction from OH⁻ to H⁺ and H₂O.

⁶Phlogopite solubility product constant was calculated from the average free energy of formation for phlogopite (-1389 kcal mol⁻¹, Bird and Anderson, 1973; Munoz and Ludington, 1974), the most recent evaluation of the free energy of potassium ion (Giordano and others, 1977), magnesium ion (Parker and others, 1971), aluminum ion and silicic acid (Hemingway and others, 1978). The enthalpy of phlogopite dissolution was calculated from the free energies previously cited and the entropies listed in Robie and others (1978).

⁷Changes in thermodynamic values reflect an alteration of the sulfide dissolution from S²⁻ to HS⁻.

⁸Correction of error in sign in the original WATEQ.

⁹Not presently used.

¹⁰Calculated for 25°C and pH = 7.0.

¹¹Assumes that divalent metal bisulfate ion pair stability constants are approximately equivalent (see Mattigod and Sposito, 1977). No reliable data exist.

¹²Estimated (Ball and others, 1980).

¹³Thermodynamic data are for oxalic acid.

¹⁴Tentative, based on preliminary review of the literature.

Data Sources for Table 2

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Attachment A. Test Cases

Attachment B. Listing of WATEQ4F Data Base

Attachment C. Program Listing of WATEQ4F

Attachment D. Program Listing of BASIC version of WQ4FINPT

Attachment E. Program Listing of FORTRAN version of WQ4FINPT

Attachment F. Program Listing of WQ4F.BAT
