

## APPENDIX A

### SITE CHARACTERIZATION PROGRAM BASELINE ACTIVITY NUMBERS AND NAMES

<u>ACTIVITY NO.</u>	<u>ACTIVITY NAME</u>
8.3.1.2.1.1.1	Precipitation and meteorological monitoring
8.3.1.2.1.2.1	Surface-water runoff monitoring
8.3.1.2.1.2.2	Transport of debris by severe runoff
8.3.1.2.1.3.1	Assessment of the regional hydrogeologic data needs in the saturated zones
8.3.1.2.1.3.2	Regional potentiometric-level distribution and hydrogeologic framework studies
8.3.1.2.1.3.3	Fortymile Wash recharge study
8.3.1.2.1.3.4	Evapotranspiration studies
8.3.1.2.1.4.1	Conceptualization of regional hydrologic flow models
8.3.1.2.1.4.2	Subregional two-dimensional area hydrologic modeling
8.3.1.2.2.1.1	Characterization of hydrological properties of surficial materials
8.3.1.2.2.1.2	Evaluation of natural infiltration
8.3.1.2.2.2.1	Chloride and chlorine-36 measurements of percolation at Yucca Mountain
8.3.1.2.2.3.1	Matrix hydrologic properties testing
8.3.1.2.2.3.2	Site vertical borehole studies
8.3.1.2.2.4.2	Percolation tests in the Exploratory Studies Facility
8.3.1.2.2.4.8	Hydrochemistry tests in the Exploratory Studies Facility
8.3.1.2.2.4.9	Multipurpose-borehole testing
8.3.1.2.2.6.1	Gaseous-phase circulation study

<b>ACTIVITY NO.</b>	<b>ACTIVITY NAME</b>
8.3.1.2.2.7.1	Gaseous - phase chemical investigations
8.3.1.2.2.7.2	Aqueous-phase chemical investigations
8.3.1.2.2.8.1	Development of conceptual and numerical models of fluid flow in unsaturated, fractured rock
8.3.1.2.2.9.1	Conceptualization of the unsaturated-zone hydrogeologic system
8.3.1.2.2.9.3	Simulation of the natural hydrogeologic system
8.3.1.2.3.1.2	Site potentiometric-level evaluation
8.3.1.2.3.1.3	Analysis of single- and multiple-well hydraulic-stress tests
8.3.1.2.3.1.4	Multiple-well interference testing
8.3.1.2.3.1.6	Well testing with conservative tracers throughout the site
8.3.1.2.3.1.7	Testing of the C-hole sites with conservative tracers
8.3.1.2.3.2.1	Assessment of saturated-zone hydrochemical data availability and needs
8.3.1.2.3.2.2	Hydrochemical characterization of water in the upper part of the saturated zone
8.3.1.2.3.2.3	Regional hydrochemical tests and analyses
8.3.1.2.3.3.1	Conceptualization of saturated-zone flow models within the boundaries of the accessible environment
8.3.1.2.3.3.2	Development of fracture network model
8.3.1.3.1.1	Ground-water chemistry model
8.3.1.3.2.1	Mineralogy, petrology, and chemistry of transport pathways
8.3.1.3.2.1.1	Petrologic stratigraphy of the Topopah Spring Member

<b>ACTIVITY NO.</b>	<b>ACTIVITY NAME</b>
8.3.1.3.2.1.2	Mineral distributions between the host rock and the accessible environment
8.3.1.3.2.1.3	Fracture mineralogy
8.3.1.3.2.2.1	History of mineralogic and geochemical alteration of Yucca Mountain
8.3.1.3.2.2.2	Smectite, zeolite, manganese minerals, glass dehydration, and transformation
8.3.1.3.4.1	Batch sorption studies
8.3.1.3.4.1.1	Batch sorption measurements as a function of solid phase composition
8.3.1.3.4.1.2	Sorption as a function of sorbing element concentrations (isotherms)
8.3.1.3.4.1.3	Sorption as a function of ground-water composition
8.3.1.3.4.2	Biological sorption and transport
8.3.1.3.5.1.1	Solubility measurements
8.3.1.3.6.1.1	Crushed tuff column experiments
8.3.1.3.6.2.1	Uptake of radionuclides on rock beakers in a saturated system
8.3.1.3.6.2.2	Diffusion through a saturated tuff slab
8.3.1.4.1.2	Integration of geophysical activities
8.3.1.4.2.1.1	Surface and subsurface stratigraphic studies of the host rock and surrounding units
8.3.1.4.2.1.2	Surface-based geophysical surveys
8.3.1.4.2.1.3	Borehole geophysical surveys
8.3.1.4.2.1.4	Petrophysical properties testing
8.3.1.4.2.1.5	Magnetic properties and stratigraphic correlations
8.3.1.4.2.1.6	Integration of geophysical activities

<b>ACTIVITY NO.</b>	<b>ACTIVITY NAME</b>
8.3.1.4.2.2	Characterization of the structural features within the site area
8.3.1.4.2.2.1	Geologic mapping of zonal features in the Paintbrush Tuff
8.3.1.4.2.2.2	Surface-fracture network studies
8.3.1.4.2.2.3	Borehole evaluation of faults and fractures
8.3.1.4.2.2.4	Geologic mapping of the Exploratory Studies Facility
8.3.1.4.2.2.5	Seismic tomography/vertical seismic profiling
8.3.1.4.2.3.1	Development of a three-dimensional geologic model of the site area
8.3.1.4.3.1	Systematic acquisition of site-specific subsurface information
8.3.1.4.3.1.1	Systematic drilling program
8.3.1.5.1.1.1	Synoptic characterization of regional climate
8.3.1.5.1.2.1	Paleontologic analyses
8.3.1.5.1.2.2	Analysis of the stratigraphy-sedimentology of marsh lacustrine, and playa deposits
8.3.1.5.1.3.1	Analysis of pack rat middens
8.3.1.5.1.3.3	Determination of vegetation-climate relationships
8.3.1.5.1.4.1	Modeling of soil properties in the Yucca Mountain region
8.3.1.5.1.4.2	Surficial deposits mapping of the Yucca Mountain area
8.3.1.5.1.4.3	Eolian history of the Yucca Mountain region
8.3.1.5.1.5.1	Paleoclimate-paleoenvironmental synthesis
8.3.1.5.2.1.1	Regional paleoflood evaluation
8.3.1.5.2.1.2	Quaternary unsaturated zone hydrochemical analysis

<u>ACTIVITY NO.</u>	<u>ACTIVITY NAME</u>
8.3.1.5.2.1.3	Evaluation of past discharge areas
8.3.1.5.2.1.4	Analog recharge studies
8.3.1.5.2.1.5	Studies of calcite and opaline silica vein deposits
8.3.1.6.1.1.1	Development of a geomorphic map of Yucca Mountain
8.3.1.6.1.1.2	Analysis of the downcutting history of Fortymile Wash and its tributaries
8.3.1.6.1.1.3	An analysis of hillslope erosion at Yucca Mountain
8.3.1.6.2.1.1	Synthesis and data evaluation of impact of future climatic conditions on locations and rates of erosion
8.3.1.6.3.1.1	Synthesis and data evaluation of the impact of future uplift or subsidence and faulting on erosion at Yucca Mountain and vicinity
8.3.1.8.1.1.3	Presence of magma bodies in the vicinity of the site
8.3.1.8.1.2.1	Eruptive effects
8.3.1.8.3.2.2	Assessment of the effects of igneous intrusions on water-table elevations
8.3.1.8.3.2.5	Effects of faulting on water-table elevation
8.3.1.8.5.1.2	Geochronology studies
8.3.1.8.5.1.3	Field geologic studies
8.3.1.8.5.1.4	Geochemistry of scoria sequences
8.3.1.8.5.1.5	Geochemical cycles of basaltic volcanic fields
8.3.1.8.5.2.1	Evaluation of depth of curie temperature isotherm
8.3.1.8.5.2.3	Heat flow at Yucca Mountain and evaluation of regional ambient heat flow and local heat flow anomalies
8.3.1.9.2.1.1	Geochemical assessment of Yucca Mountain in relation to the potential for mineralization

<u>ACTIVITY NO.</u>	<u>ACTIVITY NAME</u>
8.3.1.9.2.1.4	Assessment of hydrocarbon resources at and near the site
8.3.1.9.2.2.1	Projected trends in local and regional ground-water development, and estimated withdrawal rates in southern Nevada, proximal to Yucca Mountain
8.3.1.12.2.1.1	Site meteorological monitoring program
8.3.1.14.2.1.1	Site reconnaissance
8.3.1.14.2.1.2	Preliminary and detailed exploration
8.3.1.14.2.1.3	Detailed exploration
8.3.1.14.2.2.1	Physical property and index laboratory tests
8.3.1.14.2.2.2	Mechanical and dynamic laboratory property tests
8.3.1.14.2.3	Field tests and characterization measurements
8.3.1.14.2.3.1	Physical property field tests and characterization measurements
8.3.1.14.2.3.2	Mechanical property field tests
8.3.1.14.2.3.3	Geophysical field measurements
8.3.1.15.1.1.1	Density and porosity characterization
8.3.1.15.1.1.3	Thermal conductivity characterization
8.3.1.15.1.2.1	Thermal expansion characterization
8.3.1.15.1.3	Laboratory determination of mechanical properties of intact rock
8.3.1.15.1.3.1	Compressive mechanical properties of intact rock at baseline experiment conditions
8.3.1.15.1.3.2	Effects of variable environmental conditions on mechanical properties
8.3.1.15.1.4	Laboratory determination of the mechanical properties of fractures
8.3.1.15.1.7.1	Plate loading tests

<u>ACTIVITY NO.</u>	<u>ACTIVITY NAME</u>
8.3.1.15.1.8.1	Evaluation of mining methods
8.3.1.15.2.1.2	Overcore stress experiments in the exploratory studies facility
8.3.1.15.2.2.1	Surface-based evaluation of ambient thermal conditions
8.3.1.16.1.1.1	Site flood and debris hazards studies
8.3.1.16.2.1.4	Identification and evaluation of potential effects of repository related withdrawals on the local flow system at Yucca Mountain, Nevada
8.3.1.17.2.1.2	Assess the potential for displacement on faults that intersect underground facilities
8.3.1.17.3.3.2	Select or develop empirical models for ground motion from underground nuclear explosions
8.3.1.17.3.5.1	Identify controlling seismic events
8.3.1.17.3.5.2	Characterize ground motion from the controlling seismic events
8.3.1.17.3.6.2	Evaluate ground motion probabilities
8.3.1.17.4.1.1	Compile historical earthquake record
8.3.1.17.4.1.2	Monitor current seismicity
8.3.1.17.4.1.3	Evaluate potential for induced seismicity at the site
8.3.1.17.4.2	Location and recency of faulting near prospective surface facilities
8.3.1.17.4.2.1	Identify appropriate trench locations in Midway Valley
8.3.1.17.4.3.1	Conduct and evaluate deep geophysical surveys in an east-west transect crossing the Furnace Creek fault zone, Yucca Mountain, and the Walker Lane
8.3.1.17.4.3.2	Evaluate Quaternary faults within 100 km of Yucca Mountain
8.3.1.17.4.3.4	Evaluate the Bare Mountain fault zone

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- 8.3.1.17.4.3.5 Evaluate structural domains and characterize the Yucca Mountain region with respect to regional patterns of faults and fractures
  - 8.3.1.17.4.4.1 Evaluate the Rock Valley fault system
  - 8.3.1.17.4.5.1 Evaluate the significance of the Miocene-Paleozoic contact in the Calico Hills area to detachment faulting within the site area
  - 8.3.1.17.4.5.2 Evaluate postulated detachment faults in the Beatty-Bare Mountain area
  - 8.3.1.17.4.6.1 Evaluate Quaternary geology and potential Quaternary faults at Yucca Mountain
  - 8.3.1.17.4.6.2 Evaluate age and recurrence of movement on suspected and known Quaternary faults
  - 8.3.1.17.4.7.1 Evaluate intermediate depth (2 to 3 km) reflection and refraction methods and plan potential application of these methods within the site area
  - 8.3.1.17.4.7.2 Detailed gravity survey of the site area
  - 8.3.1.17.4.7.3 Detailed aeromagnetic survey of the site area
  - 8.3.1.17.4.7.4 Detailed ground magnetic survey of specific features within the site area
  - 8.3.1.17.4.7.5 Evaluate surface geoelectric methods and plan potential application of these methods within the site area
  - 8.3.1.17.4.7.8 Evaluate shallow seismic reflection (mini-sosie) methods and, if appropriate, conduct surveys of selected structures at and proximal to the site area
  - 8.3.1.17.4.8.1 Evaluate present stress field within site area
  - 8.3.1.17.4.8.2 Evaluate and test shallow borehole hydrofrac and triaxial strain recovery methods for the determination of in situ stress and, if appropriate, plan potential application of these methods within and proximal to the site



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- 8.3.1.17.4.9.1 Evaluate age and extent of tectonically stable areas at and near Yucca Mountain
- 8.3.1.17.4.10.1 Relevel base-station network, Yucca Mountain and vicinity
- 8.3.1.17.4.10.2 Survey selected base stations, Yucca Mountain and vicinity, using global positioning satellite
- 8.3.1.17.4.10.3 Analyze existing releveling data, Yucca Mountain and vicinity
- 8.3.1.17.4.12.1 Evaluate tectonic processes and tectonic stability at the site
- 8.3.2.4.1.1 Design activity to verify access and drift usability
- 8.3.5.4.1.1 Refinement of site data parameters required for Issue 2.2
- 8.3.5.10.2.1 Characterization of the spent fuel waste form
- 8.3.5.10.2.2 Characterization of the glass waste form
- 8.3.5.10.3.2 Develop geochemical speciation and reaction model
- 8.3.5.10.5.1 Determine radionuclide transport parameters
- 8.3.5.10.5.2 Radionuclide transport modeling in the near-field waste package environment
- 8.3.5.12.1.1 Application of results
- 8.3.5.12.2.1 Model development
- 8.3.5.12.2.1.1 Development of a theoretical framework for calculational models
- 8.3.5.12.2.2 Verification and validation

## APPENDIX B

# GEOLOGIC AND ENGINEERING MATERIALS: BIBLIOGRAPHY OF CHEMICAL SPECIES (GEMBOCHS) DATA CATALOG

### Introduction

The GEMBOCHS database and software library together provide a suite of thermodynamic datafiles for use with geochemical modeling codes such as EQ3/6, which in turn are used to carry out aqueous speciation and fluid-rock mass transfer calculations that provide quantitative insight into the geochemical evolution of diverse geologic systems. In the context of Yucca Mountain Site Characterization Project (YMP) investigations, participant geochemists depend heavily on GEMBOCHS and EQ3/6 in their efforts to assess and predict the likely and potential geochemical consequences of the proposed subterranean repository.

This appendix lists the general types of data contained in the database and provides tabular summaries of the specific species, reference-state thermodynamic data, and literature references currently included in GEMBOCHS.

### GEMBOCHS Data Types

The following lists provide skeletal summaries of the compositional, reaction, and thermodynamic data included in GEMBOCHS for minerals, gases, and aqueous species. For a given species, some (or most) of these data may be lacking; conversely, for certain parameters, more than one referenced value is often available.

#### **Compositional Data for Minerals, Gases, and Aqueous Species**

- Elemental Composition
- Common Name

#### **Reaction Data for Aqueous Dissociation of Minerals, Gases, and Aqueous Species**

- Reaction Stoichiometry
- Equilibrium Constants
- Pressure, Temperature Conditions
- Standard Molal Gibbs Free Energies of Reaction
- Standard Molal Enthalpies of Reaction
- Standard Molal Entropies of Reaction

Standard Molal Volumes of Reaction  
Standard Molal Heat Capacities of Reaction  
Parameter Units -  
Literature References

**Thermodynamic Data for Minerals**

Standard Molal Gibbs Free Energy of Formation  
Standard Molal Enthalpy of Formation  
Standard Molal Entropy at Reference Pressure (*Pr*) and  
Temperature (*Tr*)  
Standard Molal Volume at *Pr*, *Tr*  
Standard Molal Heat Capacity at *Pr*, *Tr*  
Molecular Weight  
Heat Capacity Coefficients -  
Temperature Limits on Heat Capacity Coefficients  
Standard Molal Enthalpy of Transition  
Standard Molal Entropy of Transition  
Standard Molal Volume of Transition  
Clapeyron Slope  
Parameter Units  
Literature References

**Thermodynamic Data for Gases**

Standard Molal Gibbs Free Energy of Formation  
Standard Molal Enthalpy of Formation  
Standard Molal Entropy at *Pr*, *Tr*  
Standard Molal Volume at *Pr*, *Tr*  
Standard Molal Heat Capacity at *Pr*, *Tr*  
Molecular Weight  
Heat Capacity Coefficients  
Temperature Limits on Heat Capacity Coefficients  
Parameter Units  
Literature References

**Thermodynamic Data for Aqueous Species**

Standard Molal Gibbs Free Energy of Formation  
Standard Molal Enthalpy of Formation  
Standard Molal Entropy at *Pr*, *Tr*  
Standard Molal Volume at *Pr*, *Tr*  
Standard Molal Heat Capacity at *Pr*, *Tr*  
Molecular Weight  
Equation-of-State Coefficients  
Debye-Huckel Parameters  
Ionic Charge  
Electronic Entropy  
Parameter Units  
Literature References

## GEMBOCHS Species, Data, and References

Table B1 provides a comprehensive inventory of the chemical species for which at least some data are available in GEMBOCHS, a symbolic description of the data used to represent reference-state stability of individual species, and a matrix indicating the presence or absence of these species in each of the six standard thermodynamic datafiles currently provided for use with EQ3/6.

In the "species" section of the table, the common name for each distinct species is given in the "name" column, its chemical composition is provided in the "composition" column, and its "aqueous" or "mineral" nature in the "type" column. This last column requires some explanation. Although all aqueous species are grouped together in this table, within GEMBOCHS they are subdivided into "basis", "auxiliary basis", and "[other] aqueous" species, where the basis and auxiliary basis species are used in reactions that represent aqueous dissociation of minerals, gases, liquids, and other aqueous species. There is no physical differentiation associated with this subdivision, and from a thermodynamic standpoint such classification is completely arbitrary (albeit necessary from practical considerations).

Similarly, all minerals are grouped together here, although in the database itself they are subdivided into "[stoichiometric] solids", "solid solutions", "gases", and "liquids". However, in contrast to the case for aqueous species, these four subtypes are clearly distinct physically. In the following table, solid solutions are distinguished by the explicit parenthetical representation of cation mixing sites in their composition: e.g., Orthopyroxene:  $(\text{Fe},\text{Mg})\text{SiO}_3$ . Gases are denoted by their "(g)" suffix: e.g.,  $\text{CO}_2(\text{g})$ , and liquids by their "(1)" suffix: e.g.,  $\text{Br}_2(1)$ . All other species of type "mineral" are stoichiometric (pure) solids. Although these four species types are physically distinct, their thermodynamic behavior is represented with similar equations, hence, their grouping in this compilation.

Note that the composition column is blank whenever its specification would be redundant, and that the primary sort on the table is by species type; hence, all aqueous species are listed (alphabetically) in the first block, followed by the minerals (also alphabetized) in the second. Also note that the composition column, which is of 55-character length in the database, has been truncated to 28-character length below. This length restriction is rarely significant, although it can be in some instances (e.g., several Clinoptilolites).

In the "data" section, the "type" column refers to the type of data used to represent thermodynamic stability of the species at the reference T-P state of 25C, 1 bar. Type "1" denotes use of the standard molal Gibbs free energy of formation of the species from its elements in their standard state; type "2" refers to use of the standard molal enthalpy of formation and standard molal entropy to calculate the corresponding Gibbs free energy; type "3" signifies use of a reported equilibrium constant for aqueous dissociation of the species; type "4" indicates use of chemical potential data reported by Harvie et al. (1984); and finally, for species of the type "0", there is insufficient data to calculate the standard molal Gibbs free energy. Provided in the adjacent "lit. source" column is the literature source for the indicated data. These sources are given in standard squibb notation, which is simply a concatenation of the last two digits of the year of publication (20th century) and the first three letters of the author's last name; if there are two or more authors, the first three letters of the second author's last name are appended following a slash character. The literature references are provided in complete form in Table B2, which begins on page B-98.

Note that the summary of data used to calculate species stability in the reference state represents only a small fraction of the thermodynamic data contained in the GEMBOCHS database. Not tabulated or referenced here are the equation-of-state, heat-capacity, and phase-transition data used to calculate standard molal thermodynamic properties at elevated temperatures and pressures; Debye-Huckel parameters used to evaluate activity coefficients of aqueous species; site mixing parameters used to represent the thermodynamic behavior of solid solutions, etc.

The final "EQ3/6 Datafiles" section provides a matrix summary of the presence (indicated by an "X") or absence ("0") of a given species in each of the six thermodynamic datafiles provided for use with EQ3/6. The "com" file is a composite database that encompasses the broadest range of bulk chemical composition, at the expense of a somewhat reduced level of internal consistency; the "alt" file mirrors the "com" file with one exception: data for aqueous Np, Pu, and Am complexes are taken exclusively from Palmer et al. (1992), as described above. The "sup" file is based on equations and data taken from the SUPCRT92 software package (Johnson et al., 1992), which currently includes approximately 550 species and features a high level of internal consistency and a comprehensive equation-of-state for aqueous species. The "nea" file is based on the internally consistent, albeit bulk-composition restricted, CODATA (Cox et al., 1989) and NEA-Uranium (Grenthe et al., 1992) compilations. The "pit" (Pitzer, e.g., 1973, 1987) and "hmw" (Harvie et al., 1984) files

are primarily distinguished by their treatment of activity coefficients for aqueous species, which are based on Pitzer's equations. (In contrast, the "com", "alt", and "nea" files contain data which facilitate calculation of aqueous activity coefficients using an extended Debye-Huckel model, which is more appropriate for relatively dilute aqueous solutions.)

Each of these datafiles is particularly suited for use with certain geochemical modeling problems. For example, if the bulk chemistry of the system to be modeled is somewhat exotic (containing actinides, rare earths, etc.), then the "com" or "alt" files are likely the only choice; if the problem to be addressed involves common rock-forming minerals and relatively dilute aqueous solutions, then the "sup" file is recommended owing to its high level of internal consistency and aqueous-species equation of state. If the model environment is characterized by brines or other fluids of relatively high ionic strength, then the "pit" or "hmw" files are most appropriate. At present, the "nea" file is of limited practical use as its primarily restricted to Uranium species. However, this compilation will enjoy greatly enhanced applicability upon incorporation of the critical reviews of thermodynamic data currently in progress for Tc, Np, Pu, and Am species, which will be analogs to the Uranium volume of Grenthe et al. (1992).

Table B1: Summary of GEMBOCHS species, reference-state data, and EQ3/6 datafiles

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT.SOURCE	COM	ALT	SUP	PIT	NEA	HMW
(AmO2)2(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)2OH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)3(CO3)6(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)3(OH)4++		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)3(OH)5+		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)3(OH)7-		aqueous	3	92pal/sil	0	X	0	0	0	0
(AmO2)4(OH)7+		aqueous	3	92pal/sil	0	X	0	0	0	0
(NH4)2Sb2S4(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
(NpO2)2(OH)2++		aqueous	1	84lem	0	0	0	0	0	0
(NpO2)2(OH)2++		aqueous	3	84lem	X	0	0	0	0	0
(NpO2)2(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)2OH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)3(CO3)6(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)3(OH)4++		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)3(OH)5+		aqueous	1	84lem	0	0	0	0	0	0
(NpO2)3(OH)5+		aqueous	3	84lem	X	0	0	0	0	0
(NpO2)3(OH)5+		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)3(OH)7-		aqueous	3	92pal/sil	0	X	0	0	0	0
(NpO2)4(OH)7+		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)2(OH)2++		aqueous	1	80lem/tre	X	0	0	0	0	0
(PuO2)2(OH)2++		aqueous	3	80lem/tre	0	0	0	0	0	0
(PuO2)2(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)2OH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)3(CO3)6(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)3(OH)4++		aqueous	3	92pal/sil	X	X	0	0	0	0
(PuO2)3(OH)5+		aqueous	1	80lem/tre	X	0	0	0	0	0
(PuO2)3(OH)5+		aqueous	3	80lem/tre	0	0	0	0	0	0
(PuO2)3(OH)5+		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)3(OH)7-		aqueous	3	92pal/sil	0	X	0	0	0	0
(PuO2)4(OH)7+		aqueous	3	92pal/sil	0	X	0	0	0	0
(TcO(OH)2)2(aq)		aqueous	1	83rar	X	X	0	0	0	0
(UO2)11(CO3)6(OH)12--		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)2(CO3)(OH)3-		aqueous	3	84tri	0	0	0	0	0	0
(UO2)2(OH)2++		aqueous	0	chemval*	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW	
		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)2(OH)2++		aqueous	3	chemval*	0	0	0	0	0	0
(UO2)2(OH)2++		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)2CO3(OH)3-		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)2OH+++		aqueous	0	chemval*	0	0	0	0	0	0
(UO2)3(CO3)6(6-)		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3(CO3)6(6-)		aqueous	3	chemval*	0	0	0	0	0	0
(UO2)3(CO3)6(6-)		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3(OH)4++		aqueous	0	chemval*	0	0	0	0	0	0
(UO2)3(OH)5+		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3(OH)5+		aqueous	3	chemval*	0	0	0	0	0	0
(UO2)3(OH)5+		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3(OH)5CO2+		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3(OH)7-		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)3O(OH)2(HCO3)+		aqueous	1	92gre/fug	X	X	0	0	X	0
(UO2)4(OH)7+		aqueous	3	76bae/mes	X	X	0	0	0	0
(VO)2(OH)2++		aqueous	1	supcrt92**	X	X	X	0	0	0
1-Butanamine(aq)	C4H9NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Butanol(aq)	C4H9OH	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Butene(aq)	C4H8	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Butyne(aq)	C4H6	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Heptanamine(aq)	C7H15NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Heptanol(aq)	C7H15OH	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Heptene(aq)	C7H14	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Heptyne(aq)	C7H12	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Hexanamine(aq)	C6H13NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Hexanol(aq)	C6H13OH	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Hexene(aq)	C6H12	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Hexyne(aq)	C6H10	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Octanamine(aq)	C8H17NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Octanol(aq)	C8H17OH	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Octene(aq)	C8H16	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Octyne(aq)	C8H14	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Pentanamine(aq)	C5H11NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Pentanol(aq)	C5H11OH	aqueous	1	supcrt92**	X	X	X	0	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP'	PIT	NEA	HMW
1-Pentene(aq)	C5H10	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Pentyne(aq)	C5H8	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Propanamine(aq)	C3H7NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Propanol(aq)	C3H7OH	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Propene(aq)	C3H6	aqueous	1	supcrt92**	X	X	X	0	0	0
1-Propyne(aq)	C3H4	aqueous	1	supcrt92**	X	X	X	0	0	0
2-Butanone(aq)	C4H8O	aqueous	1	supcrt92**	X	X	X	0	0	0
2-Heptanone(aq)	C7H14O	aqueous	1	supcrt92**	X	X	X	0	0	0
2-Hexanone(aq)	C6H12O	aqueous	1	supcrt92**	X	X	X	0	0	0
2-Octanone(aq)	C8H16O	aqueous	1	supcrt92**	X	X	X	0	0	0
2-Pentanone(aq)	C5H10O	aqueous	1	supcrt92**	X	X	X	0	0	0
Acetaldehyde(aq)	CH3CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Acetamide(aq)	CH3CONH2	aqueous	1	93sho	X	X	X	0	0	0
Acetate	CH3COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Acetic acid(aq)	CH3COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Acetone(aq)	CH3COCH3	aqueous	1	supcrt92**	X	X	X	0	0	0
Ag(CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Ag(CO3)2---		aqueous	1	supcrt92**	X	X	X	0	0	0
Ag+		aqueous	1	supcrt92**	X	X	X	X	0	0
Ag++		aqueous	2	89cox/wag	0	0	0	0	0	0
AgCH3COO(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
AgCO3-		aqueous	1	93sho/kor	X	X	X	0	0	0
AgCl(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
AgCl2-		aqueous	1	supcrt92**	X	X	X	0	0	0
AgCl3--		aqueous	1	supcrt92**	X	X	X	0	0	0
AgCl4---		aqueous	1	supcrt92**	X	X	X	0	0	0
AgF(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
AgNO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Al(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Al(O-phth)+		aqueous	3	77mar/smi	0	0	0	0	0	0
Al(O-phth)2-		aqueous	3	89mar/smi	0	0	0	0	0	0
Al(OH)2+		aqueous	0	chemval*	0	0	0	0	0	0
Al(OH)2+		aqueous	3	93bou/kna	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Al(OH)2+		aqueous	3	chemval*	0	0	0	0	0	0
Al(OH)3(aq)		aqueous	3	93bou/kna	X	X	0	0	0	0
Al(OH)4-		aqueous	0	chemval*	0	0	0	0	0	0
Al(OH)4-		aqueous	3	93bou/kna	X	X	0	0	0	0
Al(OH)4-		aqueous	3	chemval*	0	0	0	0	0	0
Al(SO4)2-		aqueous	0	chemval*	0	0	0	0	0	0
Al(SO4)2-		aqueous	3	69iza/eat	X	X	0	0	0	0
Al(SO4)2-		aqueous	3	chemval*	0	0	0	0	0	0
Al+++		aqueous	1	supcrt92**	X	X	X	X	0	0
Al+++		aqueous	2	89cox/wag	0	0	0	0	0	0
Al13O4(OH)24(7+)		aqueous	3	76bae/mes	X	X	0	0	0	0
Al2(OH)2++++		aqueous	0	chemval*	0	0	0	0	0	0
Al2(OH)2++++		aqueous	3	76smi/mar	X	X	0	0	0	0
Al2(OH)2++++		aqueous	3	chemval*	0	0	0	0	0	0
Al3(OH)4(5+)		aqueous	0	chemval*	0	0	0	0	0	0
Al3(OH)4(5+)		aqueous	3	76smi/mar	X	X	0	0	0	0
Al3(OH)4(5+)		aqueous	3	chemval*	0	0	0	0	0	0
AlCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
AlCH3COO++		aqueous	3	77mar/smi	0	0	0	0	0	0
AlF++		aqueous	3	76smi/mar	X	X	0	0	0	0
AlF2+		aqueous	3	76smi/mar	X	X	0	0	0	0
AlF3(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
AlF4-		aqueous	3	76smi/mar	X	X	0	0	0	0
AlF5--		aqueous	0	76smi/mar	0	0	0	0	0	0
AlF6---		aqueous	0	76smi/mar	0	0	0	0	0	0
AlH2PO4++		aqueous	3	79lan	X	X	0	0	0	0
AlHPO4+		aqueous	3	79lan	X	X	0	0	0	0
AlO2-		aqueous	1	supcrt92**	0	0	0	0	0	0
AlOH++		aqueous	0	chemval*	0	0	0	0	0	0
AlOH++		aqueous	1	supcrt92**	X	X	X	0	0	0
AlOH++		aqueous	3	93bou/kna	0	0	0	0	0	0
AlOH++		aqueous	3	chemval*	0	0	0	0	0	0
AlSO4+		aqueous	0	chemval*	0	0	0	0	0	0
AlSO4+		aqueous	3	69iza/eat	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
ALSO4+		aqueous	3	chemval*	0	0	0	0	0	0
Alanine(aq)	C3H7NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
Alanylglycine(aq)	C5H10N2O3	aqueous	1	92sho	X	X	X	0	0	0
Am(CO3)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)2-		aqueous	1	84ker	0	0	0	0	0	0
Am(CO3)2-		aqueous	3	86ker/sil	X	0	0	0	0	0
Am(CO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)3--		aqueous	3	86ker/sil	X	0	0	0	0	0
Am(CO3)3---		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)3---		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(CO3)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)2+		aqueous	1	84ker	X	0	0	0	0	0
Am(H2PO4)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)3(aq)		aqueous	1	84ker	X	0	0	0	0	0
Am(H2PO4)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)4(aq)		aqueous	1	84ker	X	0	0	0	0	0
Am(H2PO4)4-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(H2PO4)4-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(HPO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(HPO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(HPO4)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(HPO4)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)2+		aqueous	1	84ker	X	0	0	0	0	0
Am(NO3)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(NO3)4(aq)		aqueous	1	84ker	0	0	0	0	0	0
Am(OH)2+		aqueous	3	86ker/sil	X	0	0	0	0	0
Am(OH)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(OH)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Am(OH)3(aq)		aqueous	1	84ker	0	0	0	0	0	0
Am(OH)3(aq)		aqueous	3	86ker/sil	X	0	0	0	0	0
Am(OH)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(OH)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(OH)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(OH)5-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(SO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(SO4)2-		aqueous	1	84ker	X	0	0	0	0	0
Am(SO4)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(SO4)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Am(SO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Am+++		aqueous	1	76fug/oet	X	X	0	0	0	0
Am++++		aqueous	1	76fug/oet	X	X	0	X	0	0
AmCO3+		aqueous	1	84ker	0	0	0	0	0	0
AmCO3+		aqueous	3	86ker/sil	X	0	0	0	0	0
AmCO3+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCl++		aqueous	1	84ker	X	0	0	0	0	0
AmCl++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCl+++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCl2+		aqueous	1	84ker	X	0	0	0	0	0
AmCl2+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCl2++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmCl3+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF++		aqueous	1	84ker	X	0	0	X	0	0
AmF++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF+++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF2+		aqueous	1	84ker	X	0	0	0	0	0
AmF2+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF2++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF3(aq)		aqueous	1	84ker	X	0	0	0	0	0
AmF3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF3+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmF5-		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
AmF6--		aqueous	3	92pal/sil	0	X	0	0	0	0
AmH2PO4++		aqueous	1	84ker	X	0	0	0	0	0
AmH2PO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmH2PO4+++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmHPO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmNO3++		aqueous	1	84ker	X	0	0	0	0	0
AmNO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmNO3+++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(CO3)2--		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(CO3)2---		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(CO3)3(5-)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(CO3)3----		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(H2PO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(NO3)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(NO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(OH)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(OH)3-		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(OH)4--		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2(SO4)2--		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2+		aqueous	1	76fug/oet	0	0	0	0	0	0
AmO2++		aqueous	1	76fug/oet	0	0	0	0	0	0
AmO2CO3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2CO3-		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2Cl(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2Cl+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2Cl2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2Cl2-		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2F(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2F+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2F2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2F3-		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2F4--		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2H2PO4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2H2PO4+		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
AmO2HCO3 (aq)		aqueous	1	84ker	0	0	0	0	0	0
AmO2HPO4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2HPO4 -		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2NO3 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2NO3+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2OH (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2OH+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2PO4 --		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2SO4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
AmO2SO4 -		aqueous	3	92pal/sil	0	X	0	0	0	0
AmOH++		aqueous	1	84ker	0	0	0	0	0	0
AmOH++		aqueous	3	86ker/sil	X	0	0	0	0	0
AmOH++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmOH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
AmSO4+		aqueous	1	84ker	X	0	0	0	0	0
AmSO4+		aqueous	3	92pal/sil	0	X	0	0	0	0
AmSO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
Ar (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
As (OH)3 (aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
As (OH)4 -		aqueous	3	76bae/mes	0	0	0	0	0	0
AsH3 (aq)		aqueous	1	69ser/kho	X	X	0	0	0	0
AsO2-		aqueous	2	92gre/fug	X	X	0	0	X	0
AsO2OH--		aqueous	1	69ser/kho	X	X	0	0	0	0
AsO3F--		aqueous	1	82wag/eva	X	X	0	0	0	0
AsO4 ---		aqueous	1	92gre/fug	0	0	0	0	X	0
AsO4 ---		aqueous	2	82wag/eva	X	X	0	X	0	0
Asparagine (aq)	C4H8N2O3	aqueous	1	supcrt92**	X	X	X	0	0	0
Aspartic acid (aq)	C4H7NO4	aqueous	1	supcrt92**	X	X	X	0	0	0
Au (CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Au+		aqueous	1	supcrt92**	X	X	X	0	0	0
Au+++		aqueous	1	supcrt92**	X	X	X	0	0	0
AuCH3COO (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
B (OH)3 (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
B (OH)3 (aq)		aqueous	2	89cox/wag	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
B(OH)4-		aqueous	3	72mes/bae	0	0	0	0	0	0
B(OH)4-		aqueous	3	80bas	0	0	0	0	0	0
B2O(OH)5-		aqueous	3	77bas	X	X	0	0	0	0
B3O3(OH)4-		aqueous	3	80bas	0	0	0	0	0	0
B4O5(OH)4--		aqueous	3	80bas	0	0	0	0	0	0
BF2(OH)2-		aqueous	1	80bas	X	X	0	0	0	0
BF3OH-		aqueous	1	80bas	X	X	0	0	0	0
BF4-		aqueous	1	supcrt92**	X	X	X	0	0	0
BH4-		aqueous	1	82wag/eva	X	X	0	0	0	0
BO2-		aqueous	1	supcrt92**	X	X	X	0	0	0
Ba(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ba(o-Phthalate)(aq)		aqueous	3	89mar/smi	X	X	0	0	0	0
Ba++		aqueous	1	supcrt92**	X	X	X	X	0	0
Ba++		aqueous	2	92gre/fug	0	0	0	0	X	0
BaB(OH)4+		aqueous	1	80bas	X	X	0	0	0	0
BaCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
BaCH3COO+		aqueous	3	89mar/smi	0	0	0	0	0	0
BaCO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
BaCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
BaF+		aqueous	1	supcrt92**	X	X	X	0	0	0
BaHCO3+		aqueous	1	supcrt92**	0	0	0	0	0	0
BaHCO3+		aqueous	1	supcrt92**	0	0	0	0	0	0
BaNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
BaOH+		aqueous	3	76bae/mes	X	X	0	0	0	0
BaSO4(aq)		aqueous	3	76smi/mar	0	0	0	0	0	0
Be(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Be++		aqueous	1	supcrt92**	X	X	X	X	0	0
BeCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
BeO2--		aqueous	1	supcrt92**	X	X	X	0	0	0
Benzene(aq)	C6H6	aqueous	1	supcrt92**	X	X	X	0	0	0
Bi(CH3COO)2+		aqueous	1	93sho/kor	0	0	0	0	0	0
Bi(CH3COO)3(aq)		aqueous	1	93sho/kor	0	0	0	0	0	0
BiCH3COO++		aqueous	1	93sho/kor	0	0	0	0	0	0
Br-		aqueous	1	supcrt92**	X	X	X	X	0	0
Br-		aqueous	2	89cox/wag	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Br3-		aqueous	1	supcrt92**	X	X	X	0	0	0
BrO-		aqueous	1	92gre/fug	0	0	0	0	X	0
BrO-		aqueous	1	supcrt92**	X	X	X	0	0	0
BrO3-		aqueous	1	supcrt92**	X	X	X	X	0	0
BrO3-		aqueous	2	92gre/fug	0	0	0	0	X	0
BrO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
Butanal(aq)	CH3(CH2)2CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Butanoate	C3H7COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Butanoic acid(aq)	C3H7COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
CN-		aqueous	1	supcrt92**	X	X	X	0	0	0
CO(aq)		aqueous	1	93sho/mck	X	X	X	0	0	0
CO2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CO2(aq)		aqueous	2	89cox/wag	0	0	0	0	0	0
CO2(aq)		aqueous	4	84har/mol	0	0	0	0	0	X
CO3--		aqueous	1	supcrt92**	X	X	X	0	0	0
CO3--		aqueous	2	89cox/wag	0	0	0	0	0	0
CO3--		aqueous	4	84har/mol	0	0	0	0	0	X
Ca(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ca(o-Phthalate)(aq)		aqueous	3	89mar/smi	X	X	0	0	0	0
Ca++		aqueous	1	supcrt92**	X	X	X	X	0	0
Ca++		aqueous	2	89cox/wag	0	0	0	0	0	0
Ca++		aqueous	4	84har/mol	0	0	0	0	0	X
CaB(OH)4+		aqueous	1	80bas	X	X	0	0	0	0
CaCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
CaCH3COO+		aqueous	3	89mar/smi	0	0	0	0	0	0
CaCO3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
CaCO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CaCO3(aq)		aqueous	3	82plu/bus	0	0	0	0	0	0
CaCO3(aq)		aqueous	3	chemval*	0	0	0	0	0	0
CaCO3(aq)		aqueous	3	data0R53	0	0	0	0	0	0
CaCO3(aq)		aqueous	4	84har/mol	0	0	0	0	0	X
CaCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
CaCl2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CaF+		aqueous	1	supcrt92**	X	X	X	0	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
CaH2PO4+		aqueous	3	76smi/mar	X	X	0	0	0	0
CaHCO3+		aqueous	0	chemval*	0	0	0	0	0	0
CaHCO3+		aqueous	1	87gar/par	0	0	0	0	0	0
CaHCO3+		aqueous	1	supcrt92**	X	X	X	0	0	0
CaHCO3+		aqueous	3	chemval*	0	0	0	0	0	0
CaHCO3+		aqueous	3	data0R53	0	0	0	0	0	0
CaHP2O7-		aqueous	3	76smi/mar	0	0	0	0	0	0
CaHPO4 (aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
CaNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
CaOH+		aqueous	3	76bae/mes	X	X	0	0	0	0
CaP2O7--		aqueous	3	76smi/mar	X	X	0	0	0	0
CaPO4-		aqueous	3	76smi/mar	X	X	0	0	0	10
CaSO4 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
CaSO4 (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CaSO4 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
Cd(CH3COO)2 (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Cd(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Cd++		aqueous	1	supcrt92**	X	X	X	X	0	0
Cd++		aqueous	2	89cox/wag	0	0	0	0	0	0
CdCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
CdSeO4 (aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Ce(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Ce(CH3COO)3 (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ce+++		aqueous	1	supcrt92**	X	X	X	X	0	0
CeCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Cl-		aqueous	1	supcrt92**	X	X	X	X	0	0
Cl-		aqueous	2	89cox/wag	0	0	0	0	0	0
Cl-		aqueous	4	84har/mol	0	0	0	0	0	X
ClO-		aqueous	1	92gre/fug	0	0	0	0	X	0
ClO-		aqueous	1	supcrt92**	X	X	X	0	0	0
ClO2-		aqueous	1	92gre/fug	0	0	0	0	X	0
ClO2-		aqueous	1	supcrt92**	X	X	X	0	0	0
ClO3-		aqueous	1	supcrt92**	X	X	X	X	0	0
ClO3-		aqueous	2	92gre/fug	0	0	0	0	X	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
ClO4-		aqueous	1	supcrt92**	X	X	X	X	0	0
ClO4-		aqueous	2	89cox/wag	0	0	0	0	0	0
Co(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Co(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Co(HS)2(aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
Co(OH)2(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
Co(OH)3-		aqueous	3	76smi/mar	0	0	0	0	0	0
Co(OH)4--		aqueous	3	76smi/mar	X	X	0	0	0	0
Co++		aqueous	1	supcrt92**	X	X	X	X	0	0
Co+++		aqueous	1	supcrt92**	X	X	X	0	0	0
Co2(OH)3+		aqueous	3	76bae/mes	X	X	0	0	0	0
Co4(OH)4++++		aqueous	3	76smi/mar	X	X	0	0	0	0
CoBr2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
CoCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
CoCl+		aqueous	1	74nau/ryz	X	X	0	0	0	0
CoCl+		aqueous	3	74nau/ryz	0	0	0	0	0	0
CoHS+		aqueous	1	74nau/ryz	X	X	0	0	0	0
CoI2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
CoNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
CoOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
CoS2O3(aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
CoSO4(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
CoSeO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Cr(OH)2+		aqueous	3	76bae/mes	X	X	0	0	0	0
Cr(OH)3(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
Cr(OH)4-		aqueous	3	76bae/mes	X	X	0	0	0	0
Cr++		aqueous	1	76del/hal	X	X	0	0	0	0
Cr+++		aqueous	2	76del/hal	X	X	0	X	0	0
Cr2(OH)2++++		aqueous	3	76bae/mes	X	X	0	0	0	0
Cr2O7--		aqueous	1	supcrt92**	X	X	X	0	0	0
Cr3(OH)4(5+)		aqueous	3	76bae/mes	X	X	0	0	0	0
CrBr++		aqueous	1	76del/hal	X	X	0	0	0	0
CrCl++		aqueous	1	76del/hal	X	X	0	0	0	0
CrCl2+		aqueous	1	76del/hal	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
CrO3Cl-		aqueous	1	76del/hal	X	X	0	0	0	0
CrO4--		aqueous	1	supcrt92**	X	X	X	X	0	0
CrO4---		aqueous	1	76del/hal	X	X	0	0	0	0
CrOH++		aqueous	3	76bae/mes	X	X	0	0	0	0
Cs(CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Cs+		aqueous	1	supcrt92**	X	X	X	X	0	0
Cs+		aqueous	2	89cox/wag	0	0	0	0	0	0
CsBr(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CsCH3COO(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
CsCl(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
CsI(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Cu(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Cu(CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Cu(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Cu(CO3)2--		aqueous	1	87woo/gar	X	X	0	0	0	0
Cu(NH3)2++		aqueous	1	82wag/eva	X	X	0	0	0	0
Cu(NH3)3++		aqueous	2	82wag/eva	X	X	0	0	0	0
Cu(NO2)2(aq)		aqueous	3	82hog	X	X	0	0	0	0
Cu+		aqueous	1	supcrt92**	X	X	X	X	0	0
Cu++		aqueous	1	supcrt92**	X	X	X	X	0	0
Cu++		aqueous	2	89cox/wag	0	0	0	0	0	0
CuCH3COO(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
CuCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
CuCO3(OH)2--		aqueous	1	87woo/gar	X	X	0	0	0	0
CuCO3(aq)		aqueous	1	87woo/gar	X	X	0	0	0	0
CuCl+		aqueous	1	82wag/eva	X	X	0	0	0	0
CuCl2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
CuCl2-		aqueous	1	82wag/eva	X	X	0	0	0	0
CuCl3--		aqueous	1	82wag/eva	X	X	0	0	0	0
CuCl4--		aqueous	1	87woo/gar	X	X	0	0	0	0
CuF+		aqueous	3	76smi/mar	X	X	0	0	0	0
CuH2PO4+		aqueous	3	79mat/spo	X	X	0	0	0	0
CuHPO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
CuNH3++		aqueous	3	76smi/mar	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
CuNO2+		aqueous	3	82hog	X	X	0	0	0	0
CuO2--		aqueous	1	82wag/eva	X	X	0	0	0	0
CuOH+		aqueous	1	87woo/gar	X	X	0	0	0	0
CuPO4-		aqueous	3	79mat/spo	X	X	0	0	0	0
Decanal(aq)	CH3(CH2)8CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Diglycine(aq)	C4H8N2O3	aqueous	1	92sho	X	X	X	0	0	0
Diketopiperazine(aq)	C4H6N2O2	aqueous	1	92sho	X	X	X	0	0	0
Dy(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Dy(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Dy+++		aqueous	1	supcrt92**	X	X	X	X	0	0
DyCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Er(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Er(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Er+++		aqueous	1	supcrt92**	X	X	X	X	0	0
ErCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Ethanamine(aq)	C2H5NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
Ethane(aq)	C2H6	aqueous	1	supcrt92**	X	X	X	0	0	0
Ethanol(aq)	C2H5OH	aqueous	1	supcrt92**	X	X	X	0	0	0
Ethylacetate(aq)	CH3COOCH2CH3	aqueous	1	93sho	X	X	X	0	0	0
Ethylbenzene(aq)	C6H5C2H5	aqueous	1	supcrt92**	X	X	X	0	0	0
Ethylene(aq)	C2H4	aqueous	1	supcrt92**	X	X	X	0	0	0
Ethyne(aq)	C2H2	aqueous	1	supcrt92**	X	X	X	0	0	0
Eu(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Eu(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Eu(CO3)2-		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(CO3)3---		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(HCO3)++		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(OH)2+		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(OH)2CO3-		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(OH)3(aq)		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(OH)4-		aqueous	1	87rar 2	X	X	0	0	0	0
Eu(SO4)2-		aqueous	1	85rar 2	X	X	0	0	0	0
Eu++		aqueous	1	supcrt92**	X	X	X	0	0	0
Eu+++		aqueous	1	supcrt92**	X	X	X	X	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Eu2(OH)2++++		aqueous	1	87rar 2	X	X	0	0	0	0
EuBr++		aqueous	1	85rar 2	X	X	0	0	0	0
EuBr2+		aqueous	1	85rar 2	X	X	0	0	0	0
EuBrO3++		aqueous	1	85rar 2	X	X	0	0	0	0
EuCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
EuCO3+		aqueous	1	87rar 2	X	X	0	0	0	0
EuCl++		aqueous	1	85rar 2	X	X	0	0	0	0
EuCl2+		aqueous	1	85rar 2	X	X	0	0	0	0
EuF++		aqueous	1	85rar 2	X	X	0	0	0	0
EuF2+		aqueous	1	85rar 2	X	X	0	0	0	0
EuIO3++		aqueous	1	85rar 2	X	X	0	0	0	0
EuNO3++		aqueous	1	85rar 2	X	X	0	0	0	0
EuOH(CO3)2--		aqueous	1	87rar 2	X	X	0	0	0	0
EuOH++		aqueous	1	87rar 2	X	X	0	0	0	0
EuOHCO3(aq)		aqueous	1	85rar 2	X	X	0	0	0	0
EuSO4+		aqueous	1	supcrt92**	X	X	X	X	0	0
F-		aqueous	2	89cox/wag	0	0	0	0	0	0
F-		aqueous	1	93sho/kor	X	X	X	0	0	0
Fe(CH3COO)2(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
Fe(CH3COO)2(aq)		aqueous	3	77mar/smi	0	0	0	0	0	0
Fe(CH3COO)2+		aqueous	3	77mar/smi	0	0	0	0	0	0
Fe(CH3COO)3(aq)		aqueous	3	77mar/smi	0	0	0	0	0	0
Fe(OH)2(aq)		aqueous	0	chemval*	0	0	0	0	0	0
Fe(OH)2(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
Fe(OH)2(aq)		aqueous	3	chemval*	0	0	0	0	0	0
Fe(OH)2+		aqueous	0	chemval*	0	0	0	0	0	0
Fe(OH)2+		aqueous	3	76bae/mes	X	X	0	0	0	0
Fe(OH)2+		aqueous	3	chemval*	0	0	0	0	0	0
Fe(OH)2+		aqueous	1	82wag/eva	X	X	0	0	0	0
Fe(OH)3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
Fe(OH)3-		aqueous	1	82wag/eva	X	X	0	0	0	0
Fe(OH)3-		aqueous	3	chemval*	0	0	0	0	0	0
Fe(OH)3-		aqueous	3	76bae/mes	X	X	0	0	0	0
Fe(OH)4-		aqueous	3	76bae/mes	X	X	0	0	0	0
Fe(SO4)2-		aqueous	1	82wag/eva	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Fe++		aqueous	1	supcrt92**	X	X	X	X	0	0
Fe+++		aqueous	0	chemval*	0	0	0	0	0	0
Fe+++		aqueous	1	supcrt92**	X	X	X	0	0	0
Fe+++		aqueous	3	chemval*	0	0	0	0	0	0
Fe+++		aqueous	0	chemval*	0	0	0	0	0	0
Fe2(OH)2++++		aqueous	1	82wag/eva	X	X	0	0	0	0
Fe2(OH)2++++		aqueous	3	chemval*	0	0	0	0	0	0
Fe2(OH)2++++		aqueous	3	76bae/mes	X	X	0	0	0	0
Fe3(OH)4(5+)		aqueous	1	93sho/kor	X	X	X	0	0	0
FeCH3COO+		aqueous	1	supcrt92**	0	0	0	0	0	0
FeCH3COO+		aqueous	3	77mar/smi	0	0	0	0	0	0
FeCH3COO++		aqueous	3	81tur/whi	X	X	0	0	0	0
FeCO3(aq)		aqueous	3	81tur/whi	X	X	0	0	0	0
FeCO3+		aqueous	1	supcrt92**	X	X	X	0	0	0
FeCl+		aqueous	0	chemval*	0	0	0	0	0	0
FeCl++		aqueous	1	82wag/eva	X	X	0	0	0	0
FeCl++		aqueous	3	chemval*	0	0	0	0	0	0
FeCl++		aqueous	1	supcrt92**	X	X	X	0	0	0
FeCl2(aq)		aqueous	3	90db 1	0	0	0	0	0	0
FeCl2(aq)		aqueous	3	69hel	X	X	0	0	0	0
FeCl2+		aqueous	0	chemval*	0	0	0	0	0	0
FeCl3(aq)		aqueous	1	82wag/eva	0	0	0	0	0	0
FeCl3(aq)		aqueous	3	chemval*	0	0	0	0	0	0
FeCl3(aq)		aqueous	3	69hel	X	X	0	0	0	0
FeCl4-		aqueous	3	90db 1	X	X	0	0	0	0
FeCl4--		aqueous	3	82hog	X	X	0	0	0	0
FeF+		aqueous	1	82wag/eva	X	X	0	0	0	0
FeF++		aqueous	1	82wag/eva	X	X	0	0	0	0
FeF2+		aqueous	3	82mar/smi	0	0	0	0	0	0
FeF3(aq)		aqueous	3	72nri 1	X	X	0	0	0	0
FeH2PO4+		aqueous	3	79lan	X	X	0	0	0	0
FeH2PO4++		aqueous	1	73ols/ome	0	0	0	0	0	0
FeH3SiO4++		aqueous	3	79mat/spo	X	X	0	0	0	0
FeHCO3+		aqueous	3	82hog	X	X	0	0	0	0
FeHPO4(aq)		aqueous	3							

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
FeHPO4+		aqueous	3	76smi/mar	X	X	0	0	0	0
FeHSO4++		aqueous	3	89mar/smi	0	0	0	0	0	0
FeHSeO3++		aqueous	3	76smi/mar	0	0	0	0	0	0
FeNO2++		aqueous	3	82mar/smi	X	X	0	0	0	0
FeNO3++		aqueous	3	76smi/mar	X	X	0	0	0	0
FeO(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
FeOH+		aqueous	0	chemval*	0	0	0	0	0	0
FeOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
FeOH+		aqueous	3	chemval*	0	0	0	0	0	0
FeOH++		aqueous	0	chemval*	0	0	0	0	0	0
FeOH++		aqueous	1	82wag/eva	X	X	0	0	0	0
FeOH++		aqueous	3	chemval*	0	0	0	0	0	0
FePO4-		aqueous	3	79mat/spo	X	X	0	0	0	0
FeSO4(aq)		aqueous	0	chemval*	0	0	0	0	0	0
FeSO4(aq)		aqueous	3	69iza/eat	X	X	0	0	0	0
FeSO4(aq)		aqueous	3	chemval*	0	0	0	0	0	0
FeSO4+		aqueous	0	chemval*	0	0	0	0	0	0
FeSO4+		aqueous	1	82wag/eva	X	X	0	0	0	0
FeSO4+		aqueous	3	chemval*	0	0	0	0	0	0
Formaldehyde(aq)	HCHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Formate	HCOO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Formic acid(aq)	HCOOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Ga+++		aqueous	1	supcrt92**	X	X	X	X	0	0
Gd(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Gd(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Gd+++		aqueous	1	supcrt92**	X	X	X	X	0	0
GdCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Glutamic acid(aq)	C5H9NO4	aqueous	1	supcrt92**	X	X	X	0	0	0
Glutamine(aq)	C5H10N2O3	aqueous	1	supcrt92**	X	X	X	0	0	0
Glycine(aq)	C2H5NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
H(o-Phthalate)-		aqueous	3	82mar/smi	X	X	0	0	0	0
H+		aqueous	1	supcrt92**	X	X	X	X	0	0
H+		aqueous	2	89cox/wag	0	0	0	0	0	0
H+		aqueous	4	84har/mol	0	0	0	0	0	X

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
H2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
H2AsO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
H2AsO3-		aqueous	2	92gre/fug	0	0	0	0	X	0
H2AsO4-		aqueous	1	supcrt92**	X	X	X	X	0	0
H2AsO4-		aqueous	2	92gre/fug	0	0	0	0	X	0
H2B4O7(aq)		aqueous	0	82wag/eva	0	0	0	0	0	0
H2CO3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
H2CO3(aq)		aqueous	3	chemval*	0	0	0	0	0	0
H2CrO4(aq)		aqueous	1	76del/hal	X	X	0	0	0	0
H2F2(aq)		aqueous	3	80bal/nor	X	X	0	0	0	0
H2O		aqueous	1	supcrt92**	X	X	X	X	0	0
H2O		aqueous	2	89cox/wag	0	0	0	0	0	0
H2O		aqueous	3	supcrt92**	0	0	X	X	0	0
H2O		aqueous	4	84har/mol	0	0	0	0	0	X
H2O		aqueous	0	92gre/fug	0	0	0	0	0	0
H2O2(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
H2P2O7--		aqueous	1	supcrt92**	X	X	X	0	0	0
H2P2O7--		aqueous	1	82wag/eva	X	X	0	0	0	0
H2PO3F(aq)		aqueous	1	supcrt92**	X	X	X	X	0	0
H2PO4-		aqueous	2	89cox/wag	0	0	0	0	0	0
H2PO4-		aqueous	1	85rar 1	0	0	0	0	0	0
H2RuO5(aq)		aqueous	0	chemval*	0	0	0	0	0	0
H2S(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
H2S(aq)		aqueous	2	89cox/wag	0	0	0	0	0	0
H2S(aq)		aqueous	3	chemval*	0	0	0	0	0	0
H2S(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
H2SO3(aq)		aqueous	3	82arn/sig	X	X	0	0	0	0
H2SO4(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
H2Se(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
H2SeO3(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
H2SeO3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
H2SiO4--		aqueous	1	74nau/ryz	X	X	0	0	0	0
H2SiO4--		aqueous	3	chemval*	0	0	0	0	0	0
H2SiO4--		aqueous	1	84rar	X	X	0	0	0	0
H2TcO4(aq)		aqueous	1	84rar	X	X	0	0	0	0



SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
H2VO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
H3AsO3(aq)		aqueous	2	92gre/fug	X	X	0	0	X	0
H3AsO4(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
H3AsO4(aq)		aqueous	2	92gre/fug	0	0	0	0	X	0
H3P2O7-		aqueous	1	92gre/fug	0	0	0	0	X	0
H3P2O7-		aqueous	1	supcrt92**	X	X	X	0	0	0
H3PO4(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
H3PO4(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
H3SiO4-		aqueous	1	76bae/mes	0	0	0	0	0	0
H3SiO4-		aqueous	3	76smi/mar	0	0	0	0	0	0
H3SiO4-		aqueous	3	chemval*	0	0	0	0	0	0
H4(H2SiO4)4----		aqueous	3	76smi/mar	X	X	0	0	0	0
H4P2O7(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
H4P2O7(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
H4P2O7(aq)		aqueous	3	76smi/mar	0	0	0	0	0	0
H6(H2SiO4)4--		aqueous	3	76smi/mar	X	X	0	0	0	0
HAsO2(aq)		aqueous	2	92gre/fug	X	X	0	0	X	0
HAsO3F-		aqueous	1	82wag/eva	X	X	0	0	0	0
HAsO4--		aqueous	1	supcrt92**	X	X	X	X	0	0
HAsO4--		aqueous	2	92gre/fug	0	0	0	0	X	0
HAsS2(aq)		aqueous	3	64sil/mar	X	X	0	0	0	0
HB4O7-		aqueous	0	82wag/eva	0	0	0	0	0	0
HBrO(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
HCN(aq)		aqueous	1	93sho/mck	X	X	X	0	0	0
HCO3-		aqueous	0	chemval*	0	0	0	0	0	0
HCO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
HCO3-		aqueous	2	89cox/wag	0	0	0	0	0	0
HCO3-		aqueous	3	chemval*	0	0	0	0	0	0
HCO3-		aqueous	4	84har/mol	0	0	0	0	0	X
HCl(aq)		aqueous	3	87rua/sew	X	X	0	0	0	0
HClO(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
HClO2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
HCoO2-		aqueous	1	82wag/eva	X	X	0	0	0	0
HCrO4-		aqueous	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
HF(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
HF(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
HF2-		aqueous	1	92gre/fug	0	0	0	0	X	0
HF2-		aqueous	1	supcrt92**	X	X	X	0	0	0
HFeO2-		aqueous	1	supcrt92**	0	0	0	0	0	0
HIO3(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
HN3(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
HNIO2-		aqueous	1	supcrt92**	0	0	X	0	0	0
HNO2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
HNO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
HO2-		aqueous	1	supcrt92**	X	X	X	0	0	0
HP2O7---		aqueous	1	82wag/eva	X	X	0	0	0	0
HP2O7---		aqueous	1	92gre/fug	0	0	0	0	X	0
HPO3F-		aqueous	1	82wag/eva	X	X	0	0	0	0
HPO4--		aqueous	1	supcrt92**	X	X	X	X	0	0
HPO4--		aqueous	2	89cox/wag	0	0	0	0	0	0
HPbO2-		aqueous	1	supcrt92**	0	0	0	0	0	0
HRuO5-		aqueous	1	85rar 1	X	X	0	0	0	0
HS-		aqueous	1	supcrt92**	X	X	X	0	0	0
HS-		aqueous	2	89cox/wag	0	0	0	0	0	0
HS2O3-		aqueous	1	92gre/fug	X	X	0	0	X	0
HSO3-		aqueous	1	92gre/fug	0	0	0	0	X	0
HSO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSO3-		aqueous	0	chemval*	0	0	0	0	0	0
HSO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSO4-		aqueous	2	89cox/wag	0	0	0	0	0	0
HSO4-		aqueous	3	chemval*	0	0	0	0	0	0
HSO4-		aqueous	4	84har/mol	0	0	0	0	0	X
HSO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSO5-		aqueous	3	89spy/ree	X	X	0	0	0	0
HSb2S4-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSe-		aqueous	1	92gre/fug	0	0	0	0	X	0
HSeO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSeO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
HSeO4-		aqueous	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
HSiO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
HTcO4-		aqueous	1	84rar	X	X	0	0	0	0
HVO4--		aqueous	1	supcrt92**	X	X	X	0	0	0
HZnO2-		aqueous	1	supcrt92**	0	0	0	0	0	0
He(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Heptanal(aq)	CH3(CH2)5CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Heptanoate	C6H13COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Heptanoic acid(aq)	C6H13COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Hexanal(aq)	CH3(CH2)4CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Hexanoate	C5H11COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Hexanoic acid(aq)	C5H11COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Hg(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Hg(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Hg++		aqueous	1	supcrt92**	X	X	X	0	0	0
Hg++		aqueous	2	89cox/wag	0	0	0	0	0	0
Hg2++		aqueous	1	supcrt92**	X	X	X	0	0	0
Hg2++		aqueous	2	89cox/wag	0	0	0	0	0	0
HgCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
Ho(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Ho(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ho+++		aqueous	1	supcrt92**	X	X	X	X	0	0
HoCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
I-		aqueous	1	supcrt92**	X	X	X	X	0	0
I-		aqueous	2	89cox/wag	0	0	0	0	0	0
I3-		aqueous	1	supcrt92**	X	X	X	0	0	0
IO-		aqueous	1	supcrt92**	X	X	X	0	0	0
IO3-		aqueous	1	supcrt92**	X	X	X	0	0	0
IO3-		aqueous	2	92gre/fug	0	0	0	0	X	0
IO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
In+++		aqueous	1	supcrt92**	X	X	X	X	0	0
Isoleucine(aq)	C6H13NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
K(CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
K+		aqueous	1	supcrt92**	X	X	X	X	0	0
K+		aqueous	2	89cox/wag	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
K+		aqueous	4	84har/mol	0	0	0	0	0	X
KBr(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
KCH3COO(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
KCl(aq)		aqueous	0	chemval*	0	0	0	0	0	0
KCl(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
KCl(aq)		aqueous	3	82arn/sig	0	0	0	0	0	0
KCl(aq)		aqueous	3	chemval*	0	0	0	0	0	0
KCl(aq)		aqueous	3	89mar/smi	X	X	0	0	0	0
KHPO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
KHSO4(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
KI(aq)		aqueous	0	chemval*	0	0	0	0	0	0
KOH(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
KOH(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
KOH(aq)		aqueous	3	chemval*	0	0	0	0	0	0
KOH(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
KP2O7---		aqueous	3	76smi/mar	0	0	0	0	0	0
KP2O7---		aqueous	0	chemval*	0	0	0	0	0	0
KSO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
KSO4-		aqueous	3	chemval*	0	0	0	0	0	0
KSO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
Kr(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
La(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
La(CH3COO)3(aq)		aqueous	1	supcrt92**	X	X	X	X	0	0
La+++		aqueous	1	93sho/kor	X	X	X	0	0	0
LaCH3COO++		aqueous	1	supcrt92**	X	X	X	0	0	0
Leucine(aq)	C6H13NO2	aqueous	1	92sho	X	X	X	0	0	0
Leucylglycine(aq)	C8H16N2O3	aqueous	1	93sho/kor	X	X	X	0	0	0
Li(CH3COO)2-		aqueous	1	supcrt92**	X	X	X	X	0	0
Li+		aqueous	2	89cox/wag	0	0	0	0	0	0
Li+		aqueous	1	93sho/kor	X	X	X	0	0	0
LiCH3COO(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
LiCl(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
LiOH(aq)		aqueous	3	82mar/smi	X	X	0	0	0	0
LiSO4-		aqueous	1	93sho/kor	X	X	X	0	0	0
Lu(CH3COO)2+		aqueous								

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Lu(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Lu+++		aqueous	1	supcrt92**	X	X	X	X	0	0
LuCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Methanamine(aq)	CH3NH2	aqueous	1	supcrt92**	X	X	X	0	0	0
Methane(aq)	CH4	aqueous	0	chemval*	0	0	0	0	0	0
Methane(aq)	CH4	aqueous	1	supcrt92**	X	X	X	0	0	0
Methane(aq)	CH4	aqueous	3	chemval*	0	0	0	0	0	0
Methanol(aq)	CH3OH	aqueous	1	supcrt92**	X	X	X	0	0	0
Methionine(aq)	C5H11NO2S	aqueous	1	supcrt92**	X	X	X	0	0	0
Mg(CH3COO)2(aq)		aqueous	1	supcrt92**	X	X	X	X	0	0
Mg++		aqueous	2	89cox/wag	0	0	0	0	0	0
Mg++		aqueous	4	84har/mol	0	0	0	0	0	X
Mg++		aqueous	4	84har/mol	0	0	0	0	0	X
Mg2CO3++		aqueous	0	82mar/smi	0	0	0	0	0	0
Mg2OH+++		aqueous	0	82mar/smi	0	0	0	0	0	0
Mg4(OH)4++++		aqueous	3	76bae/mes	X	X	0	0	0	0
MgB(OH)4+		aqueous	1	80bas	X	X	0	0	0	0
MgCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
MgCH3COO+		aqueous	3	89mar/smi	0	0	0	0	0	0
MgCO3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
MgCO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
MgCO3(aq)		aqueous	3	chemval*	0	0	0	0	0	0
MgCO3(aq)		aqueous	4	84har/mol	0	0	0	0	0	X
MgCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
MgF+		aqueous	1	supcrt92**	X	X	X	0	0	0
MgH2PO4+		aqueous	3	89mar/smi	X	X	0	0	0	0
MgHCO3+		aqueous	0	chemval*	0	0	0	0	0	0
MgHCO3+		aqueous	1	supcrt92**	X	X	X	0	0	0
MgHCO3+		aqueous	3	chemval*	0	0	0	0	0	0
MgHP2O7-		aqueous	3	76smi/mar	0	0	0	0	0	0
MgHPO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
MgOH+		aqueous	0	chemval*	0	0	0	0	0	0
MgOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
MgOH+		aqueous	3	chemval*	0	0	0	0	0	0

SPECIES			DATA	EQ3/6 DATAFILES						
*****			*****	*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
MgOH+		aqueous	4	84har/mol	0	0	0	0	0	X
MgP2O7--		aqueous	1	82wag/eva	X	X	0	0	0	0
MgP2O7--		aqueous	3	76smi/mar	0	0	0	0	0	0
MgPO4-		aqueous	3	74tru/jon	X	X	0	0	0	0
MgSO4 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
MgSO4 (aq)		aqueous	1	82mar/smi	X	X	0	0	0	0
MgSO4 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
Mn(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Mn(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Mn(NO3)2(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Mn(OH)2(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
Mn(OH)3-		aqueous	1	82wag/eva	X	X	0	0	0	0
Mn(OH)4--		aqueous	3	76bae/mes	X	X	0	0	0	0
Mn++		aqueous	1	supcrt92**	X	X	X	X	0	0
Mn+++		aqueous	1	76mac	X	X	0	0	0	0
Mn2(OH)3+		aqueous	3	76bae/mes	X	X	0	0	0	0
Mn2OH+++		aqueous	3	76bae/mes	X	X	0	0	0	0
MnCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
MnCO3(aq)		aqueous	3	79mat/spo	X	X	0	0	0	0
MnCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
MnCl2(aq)		aqueous	1	82wag/eva	0	0	0	0	0	0
MnCl3-		aqueous	1	82wag/eva	X	X	0	0	0	0
MnF+		aqueous	3	89mar/smi	X	X	0	0	0	0
MnH2PO4+		aqueous	3	79mat/spo	X	X	0	0	0	0
MnHCO3+		aqueous	1	82wag/eva	X	X	0	0	0	0
MnHCO3+		aqueous	3	79mat/spo	0	0	0	0	0	0
MnHCO3+		aqueous	3	79mat/spo	X	X	0	0	0	0
MnHPO4(aq)		aqueous	3	79mat/spo	X	X	0	0	0	0
MnNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
MnO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
MnO4--		aqueous	1	supcrt92**	X	X	X	0	0	0
MnOH+		aqueous	3	76bae/mes	X	X	0	0	0	0
MnPO4-		aqueous	3	79mat/spo	X	X	0	0	0	0
MnSO4(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
MnSeO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
MoO4 --		aqueous	1	supcrt92**	X	X	X	0	0	0
N2 (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
N3 -		aqueous	1	92gre/fug	X	X	0	0	X	0
NH3 (aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
NH3 (aq)		aqueous	1	supcrt92**	X	X	X	X	0	0
NH4 (CH3COO) 2-		aqueous	1	93sho/kor	X	X	X	0	0	0
NH4+		aqueous	1	supcrt92**	X	X	X	X	0	0
NH4+		aqueous	2	89cox/wag	0	0	0	0	0	0
NH4CH3COO (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
NH4SO4 -		aqueous	3	82mar/smi	X	X	0	0	0	0
NH4SbO2 (aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
NO2 -		aqueous	1	supcrt92**	X	X	X	X	0	0
NO3 -		aqueous	1	supcrt92**	X	X	X	X	0	0
NO3 -		aqueous	2	89cox/wag	0	0	0	0	0	0
Na (CH3COO) 2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Na (o-Phthalate) -		aqueous	3	89mar/smi	X	X	0	0	0	0
Na+		aqueous	1	supcrt92**	X	X	X	X	0	0
Na+		aqueous	2	89cox/wag	0	0	0	0	0	0
Na+		aqueous	4	84har/mol	0	0	0	0	0	X
Na2CO3 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
Na2CO3 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
Na2P2O7 --		aqueous	3	76smi/mar	X	X	0	0	0	0
Na2SO4 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
Na2SO4 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
NaB(OH)4 (aq)		aqueous	1	80bas	X	X	0	0	0	0
NaBr (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
NaCH3COO (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
NaCH3COO (aq)		aqueous	3	89mar/smi	0	0	0	0	0	0
NaCO3 -		aqueous	0	chemval*	0	0	0	0	0	0
NaCO3 -		aqueous	1	82wag/eva	X	X	0	0	0	0
NaCO3 -		aqueous	3	chemval*	0	0	0	0	0	0
NaCl (aq)		aqueous	0	chemval*	0	0	0	0	0	0
NaCl (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
NaCl (aq)		aqueous	3	chemval*	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
NaF(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
NaH3SiO4(aq)		aqueous	3	82arn/sig	0	0	0	0	0	0
NaHCO3(aq)		aqueous	0	chemval*	0	0	0	0	0	0
NaHCO3(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
NaHCO3(aq)		aqueous	3	chemval*	0	0	0	0	0	0
NaHP2O7--		aqueous	3	76smi/mar	X	X	0	0	0	0
NaHPO4-		aqueous	3	89mar/smi	X	X	0	0	0	0
NaHSiO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
NaI(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
NaOH(aq)		aqueous	0	chemval*	0	0	0	0	0	0
NaOH(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
NaOH(aq)		aqueous	3	chemval*	0	0	0	0	0	0
NaP2O7---		aqueous	1	82wag/eva	0	0	0	0	0	0
NaP2O7---		aqueous	3	76smi/mar	X	X	0	0	0	0
NaSO4-		aqueous	0	chemval*	0	0	0	0	0	0
NaSO4-		aqueous	3	82mar/smi	X	X	0	0	0	0
NaSO4-		aqueous	3	chemval*	0	0	0	0	0	0
Nd(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Nd(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Nd+++		aqueous	1	supcrt92**	X	X	X	X	0	0
NdCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Ne(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Ni(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ni(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Ni(NH3)2++		aqueous	1	82wag/eva	X	X	0	0	0	0
Ni(NH3)6++		aqueous	1	82wag/eva	X	X	0	0	0	0
Ni(NO3)2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
Ni(OH)2(aq)		aqueous	1	82wag/eva	0	0	0	0	0	0
Ni(OH)2(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Ni(OH)3-		aqueous	3	76smi/mar	X	X	0	0	0	0
Ni++		aqueous	1	supcrt92**	X	X	X	X	0	0
Ni2OH+++		aqueous	3	76bae/mes	X	X	0	0	0	0
Ni4(OH)4++++		aqueous	3	89mar/smi	X	X	0	0	0	0
NiBr+		aqueous	3	76smi/mar	X	X	0	0	0	0



SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
NiCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
NiCl+		aqueous	1	supcrt92**	X	X	X	0	0	10
NiHP2O7-		aqueous	1	82wag/eva	X	X	0	0	0	0
NiNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
NiO(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
NiOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
NiP2O7--		aqueous	1	82wag/eva	X	X	0	0	0	0
NiSO4(aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
NiSeO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Nonanal(aq)	CH3(CH2)7CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Np(CO3)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(CO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(CO3)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(CO3)3---		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(CO3)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(CO3)5(6-)		aqueous	1	84lem	0	0	0	0	0	0
Np(CO3)5(6-)		aqueous	3	84lem	X	0	0	0	0	0
Np(CO3)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(H2PO4)2+		aqueous	1	84lem	0	0	0	0	0	0
Np(H2PO4)2+		aqueous	3	84lem	X	0	0	0	0	0
Np(H2PO4)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(H2PO4)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(H2PO4)3(aq)		aqueous	1	84lem	0	0	0	0	0	0
Np(H2PO4)3(aq)		aqueous	3	84lem	X	0	0	0	0	0
Np(H2PO4)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(H2PO4)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(H2PO4)4-		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(HPO4)2(aq)		aqueous	1	84lem	0	0	0	0	0	0
Np(HPO4)2(aq)		aqueous	3	84lem	X	0	0	0	0	0
Np(HPO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(HPO4)3--		aqueous	1	84lem	0	0	0	0	0	0
Np(HPO4)3--		aqueous	3	84lem	X	0	0	0	0	0
Np(HPO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(HPO4)4----		aqueous	1	84lem	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Np(HPO4)4----		aqueous	3	84lem	X	0	0	0	0	0
Np(HPO4)4----		aqueous	3	92pal/sil	0	X	0	0	0	10
Np(HPO4)5(6-)		aqueous	1	84lem	0	0	0	0	0	0
Np(HPO4)5(6-)		aqueous	3	84lem	X	0	0	0	0	0
Np(HPO4)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(NO3)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(NO3)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(NO3)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(NO3)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(NO3)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)2++		aqueous	1	84lem	0	0	0	0	0	0
Np(OH)2++		aqueous	3	84lem	X	0	0	0	0	0
Np(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)3+		aqueous	1	84lem	0	0	0	0	0	0
Np(OH)3+		aqueous	3	84lem	X	0	0	0	0	0
Np(OH)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)4(aq)		aqueous	1	84lem	0	0	0	0	0	0
Np(OH)4(aq)		aqueous	3	84lem	X	0	0	0	0	0
Np(OH)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(OH)5-		aqueous	1	84lem	0	0	0	0	0	0
Np(OH)5-		aqueous	3	84lem	X	0	0	0	0	0
Np(OH)5-		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(SO4)2(aq)		aqueous	1	84lem	0	0	0	0	0	0
Np(SO4)2(aq)		aqueous	3	84lem	X	0	0	0	0	0
Np(SO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(SO4)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Np(SO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Np+++		aqueous	1	76fug/oet	0	0	0	0	0	0
Np+++		aqueous	1	84lem	X	X	0	0	0	0
Np++++		aqueous	1	76fug/oet	0	0	0	0	0	0
Np++++		aqueous	1	84lem	X	X	0	0	0	0
NpCO3+		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP'	PIT	NEA	HMW
NpCO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl+++		aqueous	1	84lem	0	0	0	0	0	0
NpCl+++		aqueous	3	84lem	X	0	0	0	0	0
NpCl+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl2+		aqueous	1	84lem	0	0	0	0	0	0
NpCl2++		aqueous	3	84lem	X	0	0	0	0	0
NpCl2++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl2++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpCl3+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF++		aqueous	1	84lem	0	0	0	0	0	0
NpF+++		aqueous	3	84lem	X	0	0	0	0	0
NpF+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF2+		aqueous	1	84lem	0	0	0	0	0	0
NpF2++		aqueous	3	84lem	X	0	0	0	0	0
NpF2++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF2++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF3+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF5-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpF6--		aqueous	1	84lem	0	0	0	0	0	0
NpH2PO4++		aqueous	3	84lem	X	0	0	0	0	0
NpH2PO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpH2PO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpH2PO4+++		aqueous	1	84lem	0	0	0	0	0	0
NpHPO4++		aqueous	3	84lem	X	0	0	0	0	0
NpHPO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpHPO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpHPO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpNO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpNO3+++		aqueous	1	84lem	0	0	0	0	0	0
NpO2(CO3)2--		aqueous	3	84lem	X	0	0	0	0	0
NpO2(CO3)2--										

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (CO3) 2--		aqueous	1	84lem	0	0	0	0	0	0
NpO2 (CO3) 2---		aqueous	3	84lem	X	0	0	0	0	0
NpO2 (CO3) 2----		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (CO3) 2----		aqueous	1	84lem	0	0	0	0	0	0
NpO2 (CO3) 3(5-)		aqueous	3	84lem	X	0	0	0	0	0
NpO2 (CO3) 3(5-)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (CO3) 3(5-)		aqueous	1	84lem	0	0	0	0	0	0
NpO2 (CO3) 3-----		aqueous	3	84lem	X	0	0	0	0	0
NpO2 (CO3) 3-----		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (CO3) 3-----		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (H2PO4) 2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (NO3) 2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (NO3) 2-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (OH) 2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (OH) 3-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (OH) 4--		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2 (SO4) 2--		aqueous	1	76fug/oet	0	0	0	0	0	0
NpO2+		aqueous	1	84lem	X	X	0	X	0	0
NpO2+		aqueous	1	76fug/oet	X	X	0	X	0	0
NpO2++		aqueous	1	84lem	X	X	0	0	0	0
NpO2++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2CO3 (aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2CO3-		aqueous	3	84lem	X	0	0	0	0	0
NpO2CO3-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2CO3-		aqueous	1	84lem	0	0	0	0	0	0
NpO2C1 (aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2C1 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2C1 (aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2C1+		aqueous	3	84lem	X	0	0	0	0	0
NpO2C1+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2C1+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2C12 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2C12-		aqueous	1	84lem	0	0	0	0	0	0
NpO2F (aq)										

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
NpO2F(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2F(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2F+		aqueous	1	84lem	0	0	0	0	0	0
NpO2F+		aqueous	3	84lem	X	0	0	0	0	0
NpO2F+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2F2(aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2F2(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2F2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2F3-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2F4--		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2H2PO4(aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2H2PO4(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2H2PO4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2H2PO4+		aqueous	1	84lem	0	0	0	0	0	0
NpO2H2PO4+		aqueous	3	84lem	X	0	0	0	0	0
NpO2H2PO4+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2HPO4(aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2HPO4(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2HPO4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2HPO4-		aqueous	1	84lem	0	0	0	0	0	0
NpO2HPO4-		aqueous	3	84lem	X	0	0	0	0	0
NpO2HPO4-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2NO3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2NO3+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2OH(aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2OH(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2OH(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2OH+		aqueous	1	84lem	0	0	0	0	0	0
NpO2OH+		aqueous	3	84lem	X	0	0	0	0	0
NpO2OH+		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2PO4--		aqueous	3	92pal/sil	0	X	0	0	0	0
NpO2SO4(aq)		aqueous	1	84lem	0	0	0	0	0	0
NpO2SO4(aq)		aqueous	3	84lem	X	0	0	0	0	0
NpO2SO4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
NpO2SO4-		aqueous	1	84lem	0	0	0	0	0	0
NpO2SO4-		aqueous	3	84lem	X	0	0	0	0	0
NpO2SO4-		aqueous	3	92pal/sil	0	X	0	0	0	0
NpOH++		aqueous	1	84lem	0	0	0	0	0	0
NpOH++		aqueous	3	84lem	X	0	0	0	0	0
NpOH++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpOH+++		aqueous	1	84lem	0	0	0	0	0	0
NpOH+++		aqueous	3	84lem	X	0	0	0	0	0
NpOH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpOH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpSO4+		aqueous	1	84lem	0	0	0	0	0	0
NpSO4++		aqueous	3	84lem	X	0	0	0	0	0
NpSO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
NpSO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
O2(aq)		aqueous	1	supcrt92**	X	X	X	X	0	0
O2(aq)		aqueous	2	89cox/wag	0	0	0	0	0	0
O2(g)		aqueous	2	89cox/wag	0	0	0	0	0	0
O2(g)		aqueous	4	84har/mol	0	0	0	0	0	X
OH-		aqueous	0	chemval*	0	0	0	0	0	0
OH-		aqueous	1	supcrt92**	X	X	X	X	0	0
OH-		aqueous	2	89cox/wag	0	0	0	0	0	0
OH-		aqueous	3	chemval*	0	0	0	0	0	0
OH-		aqueous	4	84har/mol	0	0	0	0	0	X
OH-		aqueous	1	93sch/sho	X	X	X	0	0	0
Octanal(aq)	CH3(CH2)6CHO	aqueous	1	supcrt92**	X	X	X	0	0	0
Octanoate	C7H15COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Octanoic acid(aq)	C7H15COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
P2O7----		aqueous	1	92gre/fug	0	0	0	0	X	0
P2O7----		aqueous	2	82wag/eva	X	X	0	X	0	0
PH4+		aqueous	1	82wag/eva	X	X	0	0	0	0
PO3F--		aqueous	1	82wag/eva	X	X	0	0	0	0
PO4---		aqueous	1	92gre/fug	0	0	0	0	X	0
PO4---		aqueous	1	supcrt92**	X	X	X	X	0	0
PO4---		aqueous	2	92gre/fug	0	0	0	0	X	0
PO4---		aqueous	1	93sho/kor	X	X	X	0	0	0
Pb(CH3COO)2(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
Pb(CH3COO)2(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Pb(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Pb++		aqueous	1	supcrt92**	X	X	X	X	0	0
Pb++		aqueous	2	89cox/wag	0	0	0	0	0	0
Pb++++		aqueous	1	74pou	X	X	0	0	0	0
PbCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
PbCH3COO+		aqueous	1	supcrt92**	0	0	0	0	0	0
PbCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
PbCl2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
PbCl3-		aqueous	1	supcrt92**	X	X	X	0	0	0
PbCl4--		aqueous	1	supcrt92**	X	X	X	0	0	0
PbF+		aqueous	1	82wag/eva	X	X	0	0	0	0
PbF2(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
PbF3-		aqueous	3	80bal/nor	0	0	0	0	0	0
PbF4--		aqueous	3	80bal/nor	0	0	0	0	0	0
PbH2PO4+		aqueous	3	76smi/mar	X	X	0	0	0	0
PbHPO4(aq)		aqueous	3	72nri 2	X	X	0	0	0	0
PbO(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
PbOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
Pd++		aqueous	1	supcrt92**	X	X	X	0	0	0
Pentanal(aq)	CH3(CH2)3CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Pentanoate	C4H9COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Pentanoic acid(aq)	C4H9COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Phenol(aq)	C6H5OH	aqueous	1	supcrt92**	X	X	X	0	0	0
Phenylalanine(aq)	C9H11NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
Pr(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Pr(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Pr+++		aqueous	1	supcrt92**	X	X	X	X	0	0
PrCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Propanal(aq)	CH3CH2CHO	aqueous	1	93sch/sho	X	X	X	0	0	0
Propane(aq)	C3H8	aqueous	1	supcrt92**	X	X	X	0	0	0
Propanoate	C2H5COO-	aqueous	1	supcrt92**	X	X	X	0	0	0
Propanoic acid(aq)	C2H5COOH	aqueous	1	supcrt92**	X	X	X	0	0	0
Pu(CO3)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(CO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Pu(CO3)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(CO3)3---		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(CO3)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(CO3)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(H2PO4)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(H2PO4)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(H2PO4)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(H2PO4)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(H2PO4)4-		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(HPO4)2(aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(HPO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(HPO4)2(aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(HPO4)3--		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(HPO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(HPO4)3---		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(HPO4)4----		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(HPO4)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(HPO4)4----		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(HPO4)5(6-)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(NO3)2+		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(NO3)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(NO3)3(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(NO3)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(NO3)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(OH)2+		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(OH)2++		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(OH)2++		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(OH)3(aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(OH)3+		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(OH)3+		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(OH)3+		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(OH)4(aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(OH)4(aq)		aqueous	3	80lem/tre	0	0	0	0	0	0



SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Pu(OH)4(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(OH)5-		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(OH)5-		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(OH)5-		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(SO4)2(aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
Pu(SO4)2(aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu(SO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(SO4)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu(SO4)2-		aqueous	3	chemval*	X	0	0	0	0	0
Pu(SO4)3--		aqueous	3	92pal/sil	0	X	0	0	0	0
Pu+++		aqueous	1	76fug/oet	0	0	0	0	0	0
Pu+++		aqueous	1	80lem/tre	X	X	0	0	0	0
Pu+++		aqueous	3	80lem/tre	0	0	0	0	0	0
Pu++++		aqueous	1	76fug/oet	0	0	0	0	0	0
Pu++++		aqueous	1	80lem/tre	X	X	0	0	0	0
PuCO3+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCO3++		aqueous	1	80lem/tre	0	0	0	0	0	0
PuCO3++		aqueous	3	85sil/nit	0	0	0	0	0	0
PuCO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCl++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCl+++		aqueous	1	80lem/tre	0	0	0	0	0	0
PuCl+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCl2+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCl2++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuCl3+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuCl3+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF+++		aqueous	1	80lem/tre	0	0	0	0	0	0
PuF+++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuF+++		aqueous	3	84nas/cle	X	0	0	0	0	0
PuF+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF2+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF2++		aqueous	3	84nas/cle	X	0	0	0	0	0
PuF2++		aqueous	3	92pal/sil	0	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
PuF3 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF3+		aqueous	3	84nas/cle	X	0	0	0	0	0
PuF3+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF4 (aq)		aqueous	3	84nas/cle	X	0	0	0	0	0
PuF4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF5-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuF6--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuH2PO4++		aqueous	1	80lem/tre	X	0	0	0	0	0
PuH2PO4++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuH2PO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuH2PO4+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuHPO4++		aqueous	1	80lem/tre	X	0	0	0	0	0
PuHPO4++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuHPO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuNO3++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuNO3+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(CO3)2--		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2(CO3)2--		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2(CO3)2--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(CO3)2---		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(CO3)3(5-)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(CO3)3----		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(H2PO4)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(NO3)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(NO3)2-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(OH)2(aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(OH)3-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(OH)4--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2(SO4)2--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2+		aqueous	1	76fug/oet	0	0	0	0	0	0
PuO2+		aqueous	1	80lem/tre	X	X	0	0	0	0
PuO2+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2++		aqueous	1	76fug/oet	0	0	0	0	0	0
PuO2++		aqueous	1	80lem/tre	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
PuO2++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2CO3 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2CO3-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2C1 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2C1+		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2C1+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2C1+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2C12 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2C12-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2F (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2F+		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2F+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2F+		aqueous	3	92pal/sil	0	X	0	0	0	10
PuO2F2 (aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2F2 (aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2F2 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2F3-		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2F3-		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2F3-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2F4--		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2F4--		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2F4--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2H2PO4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2H2PO4+		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2H2PO4+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2H2PO4+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2H2PO4+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2HPO4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2HPO4-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2NO3 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2NO3+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2OH (aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2OH (aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2OH (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2OH+		aqueous	1	80lem/tre	X	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
PuO2OH+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2OH+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2PO4--		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2SO4 (aq)		aqueous	1	80lem/tre	X	0	0	0	0	0
PuO2SO4 (aq)		aqueous	3	80lem/tre	0	0	0	0	0	0
PuO2SO4 (aq)		aqueous	3	92pal/sil	0	X	0	0	0	0
PuO2SO4-		aqueous	3	92pal/sil	0	X	0	0	0	0
PuOH++		aqueous	1	80lem/tre	X	0	0	0	0	0
PuOH++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuOH++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuOH+++		aqueous	1	80lem/tre	X	0	0	0	0	0
PuOH+++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuOH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuOH+++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuOH+++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuSO4+		aqueous	1	80lem/tre	X	0	0	0	0	0
PuSO4+		aqueous	3	80lem/tre	0	0	0	0	0	0
PuSO4+		aqueous	3	92pal/sil	0	X	0	0	0	0
PuSO4++		aqueous	1	80lem/tre	X	0	0	0	0	0
PuSO4++		aqueous	3	80lem/tre	0	0	0	0	0	0
PuSO4++		aqueous	3	92pal/sil	0	X	0	0	0	0
PuSO4++		aqueous	3	80lem/tre	0	0	0	0	0	0
Ra (CH3COO)2 (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Ra++		aqueous	1	supcrt92**	X	X	X	0	0	0
RaCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
Rb (CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Rb+		aqueous	1	supcrt92**	X	X	X	X	0	0
Rb+		aqueous	2	89cox/wag	0	0	0	0	0	0
RbBr (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
RbCH3COO (aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
RbCl (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
RbF (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
RbI (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
ReO4-		aqueous	1	supcrt92**	X	X	X	0	0	0
Rn (aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Ru (Cl)2+		aqueous	1	85rar 1	X	X	0	0	0	0
Ru (Cl)3 (aq)		aqueous	1	85rar 1	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Ru(OH) 2+		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2++		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2Cl+		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2Cl2(aq)		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2Cl3-		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2Cl4--		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 2SO4(aq)		aqueous	1	85rar 1	X	X	0	0	0	0
Ru(OH) 4(aq)		aqueous	1	87rar 1	X	X	0	0	0	0
Ru(SO4) 2-		aqueous	1	85rar 1	X	X	0	0	0	0
Ru++		aqueous	1	85rar 1	X	X	0	0	0	0
Ru+++		aqueous	1	85rar 1	X	X	0	0	0	0
Ru4(OH)12++++		aqueous	1	85rar 1	X	X	0	0	0	0
RuCl+		aqueous	1	85rar 1	X	X	0	0	0	0
RuCl++		aqueous	1	85rar 1	X	X	0	0	0	0
RuCl4-		aqueous	1	85rar 1	X	X	0	0	0	0
RuCl5--		aqueous	1	85rar 1	X	X	0	0	0	0
RuCl6---		aqueous	1	85rar 1	X	X	0	0	0	0
RuO4(aq)		aqueous	1	85rar 1	X	X	0	0	0	0
RuO4-		aqueous	1	85rar 1	X	X	0	0	0	0
RuO4--		aqueous	1	85rar 1	X	X	0	0	0	0
RuOH++		aqueous	1	85rar 1	X	X	0	0	0	0
RuSO4(aq)		aqueous	1	85rar 1	X	X	0	0	0	0
RuSO4+		aqueous	0	chemval*	0	0	0	0	0	0
S--		aqueous	1	82wag/eva	X	X	0	0	0	0
S--		aqueous	1	92gre/fug	0	0	0	0	X	0
S--		aqueous	3	chemval*	0	0	0	0	0	0
S2--		aqueous	0	chemval*	0	0	0	0	0	0
S2--		aqueous	1	supcrt92**	X	X	X	0	0	0
S2O3--		aqueous	1	92gre/fug	0	0	0	0	X	0
S2O3--		aqueous	1	supcrt92**	X	X	X	X	0	0
S2O4--		aqueous	1	supcrt92**	X	X	X	0	0	0
S2O5--		aqueous	1	supcrt92**	X	X	X	0	0	0
S2O6--		aqueous	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
S208--		aqueous	1	supcrt92**	X	X	X	0	0	0
S3--		aqueous	1	supcrt92**	X	X	X	0	0	0
S306--		aqueous	1	supcrt92**	X	X	X	0	0	0
S4--		aqueous	1	supcrt92**	X	X	X	0	0	0
S406--		aqueous	1	supcrt92**	X	X	X	0	0	0
S5--		aqueous	1	supcrt92**	X	X	X	0	0	0
S506--		aqueous	1	supcrt92**	X	X	X	0	0	0
SCN-		aqueous	1	92gre/fug	X	X	0	0	X	0
SO2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
SO3--		aqueous	1	92gre/fug	0	0	0	0	X	0
SO3--		aqueous	1	supcrt92**	X	X	X	0	0	0
SO4--		aqueous	0	chemval*	0	0	0	0	0	0
SO4--		aqueous	1	supcrt92**	X	X	X	X	0	0
SO4--		aqueous	2	89cox/wag	0	0	0	0	0	0
SO4--		aqueous	3	chemval*	0	0	0	0	0	0
SO4--		aqueous	4	84har/mol	0	0	0	0	0	X
Sb(OH)2+		aqueous	3	89spy/ree	X	X	0	0	0	0
Sb(OH)2F(aq)		aqueous	1	82wag/eva	0	0	0	0	0	0
Sb(OH)2F(aq)		aqueous	3	89spy/ree	X	X	0	0	0	0
Sb(OH)3(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
Sb(OH)4-		aqueous	3	89spy/ree	X	X	0	0	0	0
Sb2S4--		aqueous	3	89spy/ree	X	X	0	0	0	0
SbCl4-		aqueous	1	74nau/ryz	X	X	0	0	0	0
SbO+		aqueous	1	82wag/eva	0	0	0	0	0	0
SbO2-		aqueous	1	82wag/eva	0	0	0	0	0	0
SbOF(aq)		aqueous	1	82wag/eva	0	0	0	X	0	0
Sc(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Sc(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Sc+++		aqueous	1	supcrt92**	X	X	X	X	0	0
ScCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Se--		aqueous	1	74nau/ryz	X	X	0	0	0	0
SeO3--		aqueous	1	92gre/fug	0	0	0	0	X	0
SeO3--		aqueous	1	supcrt92**	X	X	X	0	0	0
SeO4--		aqueous	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Serine(aq)	C3H7NO3	aqueous	1	supcrt92**	X	X	X	0	0	0
Si(OH)4(aq)		aqueous	1	92gre/fug	0	0	0	0	X	0
Si2O2(OH)5-		aqueous	1	92gre/fug	0	0	0	0	X	0
Si2O3(OH)4--		aqueous	1	92gre/fug	0	0	0	0	X	0
Si3O5(OH)5---		aqueous	1	92gre/fug	0	0	0	0	X	0
Si3O6(OH)3---		aqueous	1	92gre/fug	0	0	0	0	X	0
Si4O7(OH)5---		aqueous	1	92gre/fug	X	X	0	0	X	0
Si4O8(OH)4----		aqueous	1	supcrt92**	X	X	X	0	0	0
SiF6--		aqueous	1	92gre/fug	0	0	0	0	X	0
SiO(OH)3-		aqueous	1	92gre/fug	0	0	0	0	X	0
SiO2(OH)2--		aqueous	1	supcrt92**	X	X	X	0	0	0
SiO2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Sm(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Sm(CH3COO)3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Sm++		aqueous	1	supcrt92**	X	X	X	X	0	0
Sm+++		aqueous	1	93sho/kor	X	X	X	0	0	0
SmCH3COO++		aqueous	1	84jac/hel	0	0	0	0	0	0
Sn(OH)2(aq)		aqueous	3	84jac/hel	X	X	0	0	0	0
Sn(OH)2(aq)		aqueous	1	84jac/hel	0	0	0	0	0	0
Sn(OH)2++		aqueous	3	84jac/hel	X	X	0	0	0	0
Sn(OH)2++		aqueous	1	84jac/hel	0	0	0	0	0	0
Sn(OH)3+		aqueous	3	84jac/hel	X	X	0	0	0	0
Sn(OH)3+		aqueous	1	84jac/hel	0	0	0	0	0	0
Sn(OH)3-		aqueous	3	84jac/hel	X	X	0	0	0	0
Sn(OH)3-		aqueous	1	84jac/hel	0	0	0	0	0	0
Sn(OH)4(aq)		aqueous	3	84jac/hel	X	X	0	0	0	0
Sn(OH)4(aq)		aqueous	1	82wag/eva	X	X	0	0	0	0
Sn(SO4)2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Sn++		aqueous	2	89cox/wag	0	0	0	0	0	0
Sn++		aqueous	1	84jac/hel	X	X	0	0	0	0
Sn++++		aqueous	3	84jac/hel	X	X	0	0	0	0
SnCl+		aqueous	3	84jac/hel	X	X	0	0	0	0
SnCl2(aq)		aqueous	3	84jac/hel	X	X	0	0	0	0
SnCl3-		aqueous	3	84jac/hel	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
SnF+		aqueous	3	84jac/hel	X	X	0	0	0	0
SnF+++		aqueous	0	84jac/hel	0	0	0	0	0	0
SnF2(aq)		aqueous	3	84jac/hel	X	X	0	0	0	0
SnF2++		aqueous	0	84jac/hel	0	0	0	0	0	0
SnF3+		aqueous	0	84jac/hel	0	0	0	0	0	0
SnF3-		aqueous	3	84jac/hel	X	X	0	0	0	0
SnF4(aq)		aqueous	0	84jac/hel	0	0	0	0	0	0
SnOH+		aqueous	1	84jac/hel	0	0	0	0	0	0
SnOH+		aqueous	3	84jac/hel	X	X	0	0	0	0
SnOH+++		aqueous	1	84jac/hel	0	0	0	0	0	0
SnOH+++		aqueous	3	84jac/hel	X	X	0	0	0	0
SnSO4++		aqueous	1	82wag/eva	X	X	0	0	0	0
Sr(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Sr++		aqueous	1	supcrt92**	X	X	X	X	0	0
Sr++		aqueous	2	92gre/fug	0	0	0	0	X	0
SrCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
SrCH3COO+		aqueous	3	89mar/smi	0	0	0	0	0	0
SrCO3(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
SrCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
SrCl2(aq)		aqueous	0	chemval*	0	0	0	0	0	0
SrCl2(aq)		aqueous	3	chemval*	0	0	0	0	0	0
SrF+		aqueous	1	supcrt92**	X	X	X	0	0	0
SrH2PO4+		aqueous	3	76smi/mar	X	X	0	0	0	0
SrHCO3+		aqueous	1	supcrt92**	0	0	0	0	0	0
SrHPO4(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
SrNO3+		aqueous	3	76smi/mar	X	X	0	0	0	0
SrOH+		aqueous	0	chemval*	0	0	0	0	0	0
SrOH+		aqueous	3	76bae/mes	X	X	0	0	0	0
SrOH+		aqueous	3	chemval*	0	0	0	0	0	0
SrP2O7--		aqueous	3	76smi/mar	X	X	0	0	0	0
SrSO4(aq)		aqueous	0	chemval*	0	0	0	0	0	0
SrSO4(aq)		aqueous	3	83rea	X	X	0	0	0	0
SrSO4(aq)		aqueous	3	chemval*	0	0	0	0	0	0
Tb(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0



SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Tb(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Tb+++		aqueous	1	supcrt92**	X	X	X	X	0	0
TbCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Tc++		aqueous	1	83rar	X	X	0	0	0	0
Tc+++		aqueous	1	83rar	X	X	0	0	0	0
TcO(OH)2(aq)		aqueous	1	83rar	X	X	0	0	0	0
TcO++		aqueous	1	83rar	X	X	0	0	0	0
TcO4-		aqueous	1	84rar	X	X	0	0	0	0
TcO4--		aqueous	1	84rar	X	X	0	0	0	0
TcO4---		aqueous	1	84rar	X	X	0	0	0	0
TcOOH+		aqueous	1	83rar	X	X	0	0	0	0
Th(H2PO4)2++		aqueous	1	80lan/her	X	X	0	0	0	0
Th(HPO4)2(aq)		aqueous	1	80lan/her	X	X	0	0	0	0
Th(HPO4)3--		aqueous	1	80lan/her	X	X	0	0	0	0
Th(OH)2++		aqueous	1	80lan/her	X	X	0	0	0	0
Th(OH)3+		aqueous	1	80lan/her	X	X	0	0	0	0
Th(OH)4(aq)		aqueous	1	80lan/her	X	X	0	0	0	0
Th(OH)4(aq)		aqueous	3	76bae/mes	0	0	0	0	0	0
Th(SO4)2(aq)		aqueous	1	80lan/her	X	X	0	0	0	0
Th(SO4)3--		aqueous	1	80lan/her	X	X	0	0	0	0
Th(SO4)4----		aqueous	1	80lan/her	X	X	0	0	0	0
Th++++		aqueous	2	76fug/oet	X	X	0	X	0	0
Th2(OH)2(6+)		aqueous	1	80lan/her	X	X	0	0	0	0
Th4(OH)8(8+)		aqueous	1	80lan/her	X	X	0	0	0	0
Th6(OH)15(9+)		aqueous	1	80lan/her	X	X	0	0	0	0
ThCl+++		aqueous	1	80lan/her	X	X	0	0	0	0
ThCl2++		aqueous	1	80lan/her	X	X	0	0	0	0
ThCl3+		aqueous	1	80lan/her	X	X	0	0	0	0
ThCl4(aq)		aqueous	1	80lan/her	X	X	0	0	0	0
ThF+++		aqueous	1	80lan/her	X	X	0	0	0	0
ThF2++		aqueous	1	80lan/her	X	X	0	0	0	0
ThF3+		aqueous	1	80lan/her	X	X	0	0	0	0
ThF4(aq)		aqueous	1	80lan/her	X	X	0	0	0	0
ThH2PO4+++		aqueous	1	80lan/her	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
ThH3PO4++++		aqueous	1	80lan/her	X	X	0	0	0	0
ThHPO4++		aqueous	1	80lan/her	X	X	0	0	0	0
ThOH+++		aqueous	1	82wag/eva	X	X	0	0	0	0
ThSO4++		aqueous	1	80lan/her	X	X	0	0	0	0
Threonine(aq)	C4H9NO3	aqueous	1	supcrt92**	X	X	X	0	0	0
Ti(OH)4(aq)		aqueous	1	81bar/lan	X	X	0	0	0	0
Tl(CH3COO)2-		aqueous	1	93sho/kor	X	X	X	0	0	0
Tl+		aqueous	1	supcrt92**	X	X	X	X	0	0
Tl+++		aqueous	1	supcrt92**	X	X	X	0	0	0
TlCH3COO(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Tm(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Tm(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Tm+++		aqueous	1	supcrt92**	X	X	X	X	0	0
TmCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Toluene(aq)	C6H5CH3	aqueous	1	supcrt92**	X	X	X	0	0	0
Tryptophan(aq)	C11H12N2O2	aqueous	1	supcrt92**	X	X	X	0	0	0
Tyrosine(aq)	C9H11NO3	aqueous	1	supcrt92**	X	X	X	0	0	0
U(CH3COO)2+		aqueous	1	93sho/kor	0	0	0	0	0	0
U(CH3COO)3(aq)		aqueous	1	93sho/kor	0	0	0	0	0	0
U(CO3)4----		aqueous	1	92gre/fug	X	X	0	0	X	0
U(CO3)5(6-)		aqueous	0	chemval*	0	0	0	0	0	0
U(CO3)5(6-)		aqueous	1	92gre/fug	X	X	0	0	X	0
U(CO3)5(6-)		aqueous	3	chemval*	0	0	0	0	0	0
U(HPO4)2(aq)		aqueous	1	78lan	0	0	0	0	0	0
U(HPO4)3--		aqueous	1	78lan	0	0	0	0	0	0
U(HPO4)4----		aqueous	1	78lan	0	0	0	0	0	0
U(NO3)2++		aqueous	1	92gre/fug	X	X	0	0	X	0
U(OH)2+		aqueous	3	80all/kip	0	0	0	0	0	0
U(OH)2++		aqueous	1	78lan	0	0	0	0	0	0
U(OH)3(aq)		aqueous	3	80all/kip	0	0	0	0	0	0
U(OH)3+		aqueous	1	78lan	0	0	0	0	0	0
U(OH)4(aq)		aqueous	0	chemval*	0	0	0	0	0	0
U(OH)4(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
U(OH)4(aq)		aqueous	3	chemval*	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
U(OH)4-		aqueous	3	80all/kip	0	0	0	0	0	0
U(OH)5-		aqueous	1	92gre/fug	0	0	0	0	0	0
U(SCN)2++		aqueous	1	92gre/fug	X	X	0	0	X	0
U(SO4)2(aq)		aqueous	0	chemval*	0	0	0	0	0	0
U(SO4)2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
U(SO4)2(aq)		aqueous	3	chemval*	0	0	0	0	0	0
U+++		aqueous	2	92gre/fug	X	X	0	0	X	0
U++++		aqueous	1	92gre/fug	X	X	0	0	X	0
U2(OH)2(6+)		aqueous	3	80all/kip	0	0	0	0	0	0
U2(OH)2++++		aqueous	3	80all/kip	0	0	0	0	0	0
U2(OH)3(5+)		aqueous	3	80all/kip	0	0	0	0	0	0
U2(OH)4++++		aqueous	3	80all/kip	0	0	0	0	0	0
U2(OH)5++++		aqueous	3	80all/kip	0	0	0	0	0	0
U6(OH)15(9+)		aqueous	1	78lan	0	0	0	0	0	0
UBr+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UCH3COO++		aqueous	1	93sho/kor	0	0	0	0	0	0
UCl+++		aqueous	0	chemval*	0	0	0	0	0	0
UCl+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UCl+++		aqueous	3	chemval*	0	0	0	0	0	0
UCl4(aq)		aqueous	1	82wag/eva	0	0	0	0	0	0
UF+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UF2++		aqueous	1	92gre/fug	X	X	0	0	X	0
UF3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UF4(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UF5-		aqueous	1	92gre/fug	X	X	0	0	X	0
UF6--		aqueous	1	92gre/fug	X	X	0	0	X	0
UHPO4++		aqueous	1	78lan	0	0	0	0	0	0
UI+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UNO3+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UNO3+++		aqueous	3	76smi/mar	0	0	0	0	0	0
UO2(CH3COO)2(aq)		aqueous	1	93sho/kor	0	0	0	0	0	0
UO2(CH3COO)2(aq)		aqueous	3	89mar/smi	0	0	0	0	0	0
UO2(CH3COO)3-		aqueous	1	93sho/kor	0	0	0	0	0	0
UO2(CH3COO)3-		aqueous	3	89mar/smi	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO2(CO3)2--		aqueous	0	chemval*	0	0	0	0	0	0
UO2(CO3)2--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(CO3)2--		aqueous	3	chemval*	0	0	0	0	0	0
UO2(CO3)3(5-)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(CO3)3----		aqueous	0	chemval*	0	0	0	0	0	0
UO2(CO3)3----		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(CO3)3----		aqueous	3	chemval*	0	0	0	0	0	0
UO2(H2PO4)(H3PO4)+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(H2PO4)(H3PO4)+		aqueous	3	84tri	0	0	0	0	0	0
UO2(H2PO4)2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(H2PO4)2(aq)		aqueous	3	84tri	0	0	0	0	0	0
UO2(H2PO4)3-		aqueous	1	78lan	0	0	0	0	0	0
UO2(HPO4)2--		aqueous	1	78lan	0	0	0	0	0	0
UO2(HPO4)2--		aqueous	3	82lan/don	0	0	0	0	0	0
UO2(IO3)2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(N3)2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(N3)3-		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(N3)4--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(NO3)2(aq)		aqueous	1	78cor/oha	0	0	0	0	0	0
UO2(OH)2(aq)		aqueous	1	92gre/fug	X	X	0	0	0	0
UO2(OH)2-		aqueous	3	80all/kip	0	0	0	0	0	0
UO2(OH)3-		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(OH)4--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(SCN)2(aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(SCN)3-		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(SO3)2--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(SO4)2--		aqueous	0	chemval*	0	0	0	0	0	0
UO2(SO4)2--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2(SO4)2--		aqueous	3	chemval*	0	0	0	0	0	0
UO2+		aqueous	0	chemval*	0	0	0	0	0	0
UO2+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2+		aqueous	3	chemval*	0	0	0	0	0	0
UO2++		aqueous	0	chemval*	0	0	0	0	0	0
UO2++		aqueous	2	89cox/wag	X	X	0	X	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
*****			*****		*****					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO2++		aqueous	3	chemval*	0	0	0	0	0	0
UO2Br+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2BrO3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2CH3COO+		aqueous	1	93sho/kor	0	0	0	0	0	0
UO2CH3COO+		aqueous	3	89mar/smi	0	0	0	0	0	0
UO2CO3 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
UO2CO3 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2CO3 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
UO2Cl+		aqueous	0	chemval*	0	0	0	0	0	0
UO2Cl+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2Cl+		aqueous	3	chemval*	0	0	0	0	0	0
UO2Cl2 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
UO2Cl2 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2Cl2 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
UO2ClO3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2F+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2F2 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2F3-		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2F4--		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2H2PO4+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2H2PO4+		aqueous	3	84tri	0	0	0	0	0	0
UO2H3PO4++		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2H3PO4++		aqueous	3	84tri	0	0	0	0	0	0
UO2HPO4 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2IO3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2N3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2NO3+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2OH (aq)		aqueous	3	80all/kip	0	0	0	0	0	0
UO2OH+		aqueous	0	chemval*	0	0	0	0	0	0
UO2OH+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2OH+		aqueous	3	chemval*	0	0	0	0	0	0
UO2OH+		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2PO4-		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2S2O3 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2SCN+		aqueous	1	92gre/fug	X	X	0	0	X	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO2SO3 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2SO4 (aq)		aqueous	0	chemval*	0	0	0	0	0	0
UO2SO4 (aq)		aqueous	1	92gre/fug	X	X	0	0	X	0
UO2SO4 (aq)		aqueous	3	chemval*	0	0	0	0	0	0
UO2SiO(OH)3+		aqueous	1	78lan	0	0	0	0	0	0
UOH++		aqueous	3	80all/kip	0	0	0	0	0	0
UOH+++		aqueous	0	chemval*	0	0	0	0	0	0
UOH+++		aqueous	1	92gre/fug	X	X	0	0	X	0
UOH+++		aqueous	3	chemval*	0	0	0	0	0	0
USCN+++		aqueous	1	92gre/fug	X	X	0	0	X	0
USO4++		aqueous	0	chemval*	0	0	0	0	0	0
USO4++		aqueous	1	92gre/fug	X	X	0	0	X	0
USO4++		aqueous	3	chemval*	0	0	0	0	0	0
Urea (aq)		aqueous	1	93sho/mck	X	X	X	0	0	0
V(OH)2+		aqueous	1	78lan	X	X	0	0	0	0
V+++		aqueous	1	76isr/mei	X	X	0	0	0	0
V2(OH)2++++		aqueous	3	76bae/mes	X	X	0	0	0	0
VO(OH)3(aq)		aqueous	3	76bae/mes	X	X	0	0	0	0
VO++		aqueous	1	supcrt92**	X	X	X	0	0	0
VO2(HPO4)2---		aqueous	3	82hog	X	X	0	0	0	0
VO2(OH)2-		aqueous	3	76bae/mes	X	X	0	0	0	0
VO2+		aqueous	1	supcrt92**	X	X	X	0	0	0
VO2F(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
VO2F2-		aqueous	3	76smi/mar	X	X	0	0	0	0
VO2F3--		aqueous	0	76smi/mar	0	0	0	0	0	0
VO2H2PO4(aq)		aqueous	3	82hog	X	X	0	0	0	0
VO2HPO4-		aqueous	3	82hog	X	X	0	0	0	0
VO2SO4-		aqueous	3	82hog	X	X	0	0	0	0
VO3OH--		aqueous	3	76bae/mes	X	X	0	0	0	0
VO4---		aqueous	1	82wag/eva	X	X	0	0	0	0
VOF+		aqueous	3	76smi/mar	X	X	0	0	0	0
VOF2(aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
VOF3-		aqueous	1	71ahr	0	0	0	0	0	0
VOF4--		aqueous	1	71ahr	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
VOH++		aqueous	3	76bae/mes	X	X	0	0	0	0
VOOH+		aqueous	3	76bae/mes	X	X	0	0	0	0
VOSO4 (aq)		aqueous	3	71bai	X	X	0	0	0	0
VSO4+		aqueous	3	82hog	X	X	0	0	0	0
Valine(aq)	C5H11NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
WO4--		aqueous	1	supcrt92**	X	X	X	0	0	0
Xe(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
Y(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Y(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Y+++		aqueous	1	supcrt92**	X	X	X	X	0	0
YCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Yb(CH3COO)2+		aqueous	1	93sho/kor	X	X	X	0	0	0
Yb(CH3COO)3(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Yb++		aqueous	1	supcrt92**	X	X	X	0	0	0
Yb+++		aqueous	1	supcrt92**	X	X	X	X	0	0
YbCH3COO++		aqueous	1	93sho/kor	X	X	X	0	0	0
Zn(CH3COO)2(aq)		aqueous	1	93sho/kor	X	X	X	0	0	0
Zn(CH3COO)2(aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
Zn(CH3COO)3-		aqueous	1	93sho/kor	X	X	X	0	0	0
Zn(CH3COO)3-		aqueous	1	supcrt92**	0	0	0	0	0	0
Zn++		aqueous	1	supcrt92**	X	X	X	X	0	0
Zn++		aqueous	2	89cox/wag	0	0	0	0	0	0
ZnCH3COO+		aqueous	1	93sho/kor	X	X	X	0	0	0
ZnCH3COO+		aqueous	1	supcrt92**	0	0	0	0	0	0
ZnCl+		aqueous	1	supcrt92**	X	X	X	0	0	0
ZnCl+		aqueous	3	87bou/bar	0	0	0	0	0	0
ZnCl2(aq)		aqueous	1	supcrt92**	X	X	X	0	0	0
ZnCl2(aq)		aqueous	3	87bou/bar	0	0	0	0	0	0
ZnCl3-		aqueous	1	supcrt92**	X	X	X	0	0	0
ZnCl3-		aqueous	3	87bou/bar	0	0	0	0	0	0
ZnCl4--		aqueous	1	supcrt92**	X	X	X	0	0	0
ZnCl4--		aqueous	3	87bou/bar	0	0	0	0	0	0
ZnF+		aqueous	3	76smi/mar	X	X	0	0	0	0
ZnH2PO4+		aqueous	3	76smi/mar	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
ZnHCO3+		aqueous	3	87bou/bar	X	X	0	0	0	0
ZnHPO4 (aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
ZnO (aq)		aqueous	1	supcrt92**	0	0	0	0	0	0
ZnO2--		aqueous	1	supcrt92**	0	0	0	0	0	0
ZnOH+		aqueous	1	supcrt92**	0	0	0	0	0	0
ZnOH+		aqueous	3	87bou/bar	X	X	0	0	0	0
ZnPO4-		aqueous	3	79mat/spo	X	X	0	0	0	0
ZnSeO4 (aq)		aqueous	3	76smi/mar	X	X	0	0	0	0
Zr(OH)2++		aqueous	1	74nau/ryz	X	X	0	0	0	0
Zr(OH)3+		aqueous	1	74nau/ryz	X	X	0	0	0	0
Zr(OH)4 (aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
Zr(SO4)2(aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
Zr(SO4)3--		aqueous	1	74nau/ryz	X	X	0	0	0	0
Zr++++		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF+++		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF2++		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF3+		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF4 (aq)		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF5-		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrF6--		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrOH+++		aqueous	1	74nau/ryz	X	X	0	0	0	0
ZrSO4++		aqueous	1	74nau/ryz	X	X	0	0	0	0
a-Aminobutyric acid(aq)	C4H9NO2	aqueous	1	supcrt92**	X	X	X	0	0	0
m-Xylene(aq)	C6H4(CH3)2	aqueous	1	supcrt92**	0	0	0	0	0	0
n-Butane(aq)	C4H10	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Butylbenzene(aq)	C6H5C4H9	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Heptane(aq)	C7H16	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Heptylbenzene(aq)	C6H5C7H15	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Hexane(aq)	C6H14	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Hexylbenzene(aq)	C6H5C6H13	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Octane(aq)	C8H18	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Octylbenzene(aq)	C6H5C8H17	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Pentane(aq)	C5H12	aqueous	1	supcrt92**	X	X	X	0	0	0
n-Pentylbenzene(aq)	C6H5C5H11	aqueous	1	supcrt92**	X	X	X	0	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
n-Propylbenzene(aq)	C6H5C3H7	aqueous	1	supcrt92**	X	X	X	0	0	0
o-Phthalate	C8O4H4	aqueous	1	85wol	X	X	0	0	0	0
o-Phthalic acid(aq)		aqueous	3	89mar/smi	X	X	0	0	0	0
o-Xylene(aq)	C6H4(CH3)2	aqueous	1	supcrt92**	0	0	0	0	0	0
p-Xylene(aq)	C6H4(CH3)2	aqueous	1	supcrt92**	0	0	0	0	0	0
(As2O5)3·5H2O		mineral	0	92gre/fug	0	0	0	0	0	0
(Pb(OH)2)3·PbCl2		mineral	1	82wag/eva	X	X	0	X	0	0
(UO2)2As2O7		mineral	2	92gre/fug	X	X	0	X	X	0
(UO2)2Cl3		mineral	2	92gre/fug	X	X	0	0	X	0
(UO2)2P2O7		mineral	2	92gre/fug	X	X	0	X	X	0
(UO2)3(AsO4)2		mineral	2	92gre/fug	X	X	0	X	X	0
(UO2)3(PO4)2		mineral	2	92gre/fug	X	X	0	X	X	0
(UO2)3(PO4)2		mineral	3	84tri	0	0	0	0	0	0
(UO2)3(PO4)2·4H2O		mineral	1	92gre/fug	X	X	0	X	X	0
(VO)3(PO4)2		mineral	1	82wag/eva	X	X	0	0	0	0
Acanthite	Ag2S	mineral	1	supcrt92**	X	X	X	0	0	0
Acmite	NaFeSi2O6	mineral	1	supcrt92**	0	0	0	0	0	0
Afwillite	Ca3Si2O4(OH)6	mineral	1	82sar/bar	X	X	0	0	0	0
Ag		mineral	1	supcrt92**	X	X	X	X	0	0
Ag		mineral	2	89cox/wag	0	0	0	0	0	0
Ag(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Ag3PO4		mineral	0	73don	0	0	0	0	0	0
Ag3PO4		mineral	3	76smi/mar	X	X	0	X	0	0
Ahlfeldite	NiSeO3·2H2O	mineral	1	74nau/ryz	X	X	0	0	0	0
Akermanite	Ca2MgSi2O7	mineral	1	supcrt92**	X	X	X	0	0	0
Al		mineral	2	89cox/wag	X	X	0	X	0	0
Al(OH)3(am)		mineral	3	74tru/jon	0	0	0	0	0	0
Al(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Al2(SO4)3		mineral	1	79rob/hem	X	X	0	X	0	0
Al2(SO4)3·6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
AlF3		mineral	2	89cox/wag	X	X	0	X	0	0
Alabandite	MnS	mineral	1	supcrt92**	X	X	X	0	0	0
Alamosite	PbSiO3	mineral	1	82wag/eva	X	X	0	0	0	0
Albite	NaAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Albite high	NaAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0
Albite low	NaAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0
Almandine	Al2Fe3(SiO4)3	mineral	1	supcrt92**	0	0	0	0	0	0
Alstonite	BaCa(CO3)2	mineral	1	82wag/eva	X	X	0	0	0	0
Alum-K	KAl(SO4)2·12H2O	mineral	2	73bar/kna	X	X	0	X	0	0
Alunite	KAl3(OH)6(SO4)2	mineral	1	supcrt92**	X	X	X	X	0	0
Am		mineral	1	76oet/ran	X	X	0	0	0	0
Am(OH)3		mineral	3	86ker/sil	X	X	0	X	0	0
Am(OH)3(am)		mineral	3	86ker/sil	X	X	0	X	0	0
AmOHCO3		mineral	3	86ker/sil	X	X	0	X	0	0
Amesite-14A	Mg4Al4Si2O10(OH)8	mineral	1	78wol	X	X	0	0	0	0
Amesite-14A	Mg4Al4Si2O10(OH)8	mineral	1	supcrt92**	0	0	0	0	0	0
Amesite-7a	Mg2Al2SiO5(OH)4	mineral	1	78wol	0	0	0	0	0	0
Amesite-7a	Mg2Al2SiO5(OH)4	mineral	1	supcrt92**	0	0	0	0	0	0
Analcime	Na.96Al.96Si2.04O6:H2O	mineral	1	82joh/flo	X	X	0	0	0	0
Analcime	Na.96Al.96Si2.04O6:H2O	mineral	1	supcrt92**	0	0	X	0	0	0
Analcime-dehy	Na.96Al.96Si2.04O6	mineral	1	82joh/flo	X	X	0	0	0	0
Analcime-dehy	Na.96Al.96Si2.04O6	mineral	1	supcrt92**	0	0	X	0	0	0
Andalusite	Al2SiO5	mineral	1	supcrt92**	X	X	X	0	0	0
Andradite	Ca3Fe2(SiO4)3	mineral	1	supcrt92**	X	X	X	0	0	0
Anglesite	PbSO4	mineral	1	supcrt92**	X	X	X	X	0	0
Anglesite	PbSO4	mineral	2	89cox/wag	0	0	0	0	0	0
Anhydrite	CaSO4	mineral	1	supcrt92**	X	X	X	X	0	0
Anhydrite	CaSO4	mineral	4	84har/mol	0	0	0	0	0	X
Annite	KFe3AlSi3O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Anorthite	CaAl2(SiO4)2	mineral	1	supcrt92**	X	X	X	0	0	0
Antarcticite	CaCl2·6H2O	mineral	1	84har/mol	X	X	0	X	0	X
Antarcticite	CaCl2·6H2O	mineral	4	84har/mol	0	0	0	X	0	X
Anthophyllite	Mg7Si8O22(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Antigorite	Mg48Si24O85(OH)62	mineral	1	supcrt92**	X	X	X	0	0	0
Antlerite	Cu3(SO4)(OH)4	mineral	1	82wag/eva	X	X	0	X	0	0
Aphthitalite	NaK3(SO4)2	mineral	1	84har/mol	X	X	0	X	0	X
Aphthitalite	NaK3(SO4)2	mineral	4	84har/mol	0	0	0	X	0	X
Ar(g)		mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Ar(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Aragonite	CaCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Aragonite	CaCO3	mineral	4	84har/mol	0	0	0	0	0	X
Arcanite	K2SO4	mineral	1	79rob/hem	X	X	0	X	0	0
Arcanite	K2SO4	mineral	4	84har/mol	0	0	0	0	0	X
Arsenolite	As2O3	mineral	1	79rob/hem	X	X	0	0	0	0
Arsenopyrite	FeAsS	mineral	1	82wag/eva	X	X	0	0	0	0
Artinite	Mg2CO3(OH)2·3H2O	mineral	1	supcrt92**	X	X	X	0	0	0
As		mineral	1	79rob/hem	X	X	0	0	0	0
As		mineral	1	92gre/fug	0	0	0	0	X	0
As2O5		mineral	2	82wag/eva	X	X	0	X	0	0
As2O5		mineral	2	92gre/fug	0	0	0	0	X	0
As4O6 (mono)		mineral	2	92gre/fug	X	X	0	X	X	0
As4O6 (octa)		mineral	2	92gre/fug	X	X	0	X	X	0
Atacamite	Cu4Cl2(OH)6	mineral	1	87woo/gar	X	X	0	X	0	0
Au		mineral	1	supcrt92**	X	X	X	0	0	0
Autunite-H	H2(UO2)2(PO4)2	mineral	1	78lan	0	0	0	0	0	0
Autunite-K	K2(UO2)2(PO4)2	mineral	1	78lan	0	0	0	0	0	0
Autunite-Na	Na2(UO2)2(PO4)2	mineral	1	78lan	0	0	0	0	0	0
Autunite-Sr	Sr(UO2)2(PO4)2	mineral	1	78lan	0	0	0	0	0	0
Azurite	Cu3(CO3)2(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
B		mineral	2	89cox/wag	X	X	0	0	0	0
B(g)		mineral	2	89cox/wag	X	X	0	0	0	0
B2O3		mineral	2	89cox/wag	X	X	0	0	0	0
BF3(g)		mineral	2	89cox/wag	X	X	0	0	0	0
Ba		mineral	1	79rob/hem	X	X	0	X	0	0
Ba		mineral	1	92gre/fug	0	0	0	0	X	0
Ba(OH)2·8H2O		mineral	1	82wag/eva	X	X	0	X	0	0
Ba2CaUO6		mineral	0	92gre/fug	0	0	0	0	0	0
Ba2MgUO6		mineral	0	92gre/fug	0	0	0	0	0	0
Ba2Si3O8		mineral	1	82wag/eva	X	X	0	0	0	0
Ba2SiO4		mineral	1	82wag/eva	X	X	0	0	0	0
Ba2SrUO6		mineral	0	92gre/fug	0	0	0	0	0	0
Ba2U2O7		mineral	2	92gre/fug	X	X	0	X	X	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Ba3(AsO4)2		mineral	0	82wag/eva	0	0	0	0	0	0
Ba3UO6		mineral	2	92gre/fug	X	X	0	X	X	0
BaBr2		mineral	1	82wag/eva	X	X	0	X	0	0
BaBr2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
BaCl2		mineral	1	82wag/eva	X	X	0	X	0	0
BaCl2		mineral	2	92gre/fug	0	0	0	0	X	0
BaCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
BaCl2:H2O		mineral	1	82wag/eva	X	X	0	X	0	0
BaCrO4		mineral	1	76del/hal	X	X	0	X	0	0
BaHPO4		mineral	0	90crc	0	0	0	0	0	0
BaHPO4		mineral	3	76smi/mar	X	X	0	X	0	0
BaI2		mineral	1	85cha/dav	X	X	0	X	0	0
BaMnO4		mineral	1	82wag/eva	X	X	0	0	0	0
BaO		mineral	1	82wag/eva	X	X	0	X	0	0
BaO		mineral	2	92gre/fug	0	0	0	0	X	0
BaS		mineral	1	82wag/eva	X	X	0	0	0	0
BaSeO3		mineral	1	82wag/eva	X	X	0	0	0	0
BaSeO4		mineral	1	82wag/eva	X	X	0	0	0	0
BaSiF6		mineral	1	82wag/eva	X	X	0	0	0	0
BaSiO3		mineral	2	82wag/eva	0	0	0	0	0	0
BaU2O7		mineral	2	92gre/fug	X	X	0	X	X	0
BaUO3		mineral	0	92gre/fug	0	0	0	0	0	0
BaUO4		mineral	2	92gre/fug	X	X	0	X	X	0
BaZrO3		mineral	1	74nau/ryz	X	X	0	0	0	0
Baddeleyite	ZrO2	mineral	1	79rob/hem	X	X	0	0	0	0
Barite	BaSO4	mineral	1	supcrt92**	X	X	X	X	0	0
Barytocalcite	BaCa(CO3)2	mineral	1	82wag/eva	X	X	0	0	0	0
Bassanite	CaSO4:1/2H2O	mineral	1	82wag/eva	X	X	0	X	0	0
Bassetite	Fe(UO2)2(PO4)2	mineral	1	78lan	X	X	0	X	0	0
Be		mineral	1	89cox/wag	X	X	0	X	0	0
Be(g)		mineral	2	89cox/wag	0	0	0	X	0	0
Be13U		mineral	2	92gre/fug	X	X	0	0	0	0
Beidellite-Ca	Ca.165Al2.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Beidellite-Cs	Cs.33Si3.67Al2.33O10(OH)2	mineral	1	88db 4	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Beidellite-H	H. 33Al2.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Beidellite-K	K. 33Al2.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Beidellite-Mg	Mg. 165Al2.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Beidellite-Na	Na. 33Al2.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Berlinite	AlPO4	mineral	1	82wag/eva	X	X	0	X	0	0
Berndtite	SnS2	mineral	1	supcrt92**	X	X	X	0	0	0
Bi		mineral	1	79rob/hem	0	0	0	0	0	0
Bieberite	CoSO4:7H2O	mineral	1	82wag/eva	X	X	0	X	0	0
Biotite	K(Mg, Fe)3AlSi3O10(OH)2	mineral	1	ss***	X	X	0	0	0	0
Birnessite	Mn8O14:5H2O	mineral	1	83ker	X	X	0	X	0	0
Bischofite	MgCl2:6H2O	mineral	1	84har/mol	X	X	0	X	0	X
Bischofite	MgCl2:6H2O	mineral	4	84har/mol	0	0	0	X	0	X
Bixbyite	Mn2O3	mineral	1	79rob/hem	X	X	0	X	0	0
Bloedite	Na2Mg(SO4)2:4H2O	mineral	1	84har/mol	X	X	0	X	0	X
Bloedite	Na2Mg(SO4)2:4H2O	mineral	4	84har/mol	0	0	0	X	0	X
Boehmite	AlO2H	mineral	1	supcrt92**	X	X	X	X	0	0
Boltwoodite	KH3OUO2SiO4	mineral	1	82hem	X	X	0	0	0	0
Boltwoodite-Na	Na. 7K. 3H3O1UO2SiO4:H2O	mineral	1	82hem	X	X	0	0	0	0
Borax	Na2[B4O5(OH)4]:8H2O	mineral	1	82wag/eva	X	X	0	0	0	0
Boric acid	B(OH)3	mineral	2	89cox/wag	X	X	0	0	0	0
Bornite	Cu5FeS4	mineral	1	supcrt92**	X	X	X	0	0	0
Br(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Br2(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Br2(l)		mineral	2	89cox/wag	X	X	0	X	0	0
Brezinaite	Cr3S4	mineral	2	78vau/cra	X	X	0	0	0	0
Brochantite	Cu4(SO4)(OH)6	mineral	1	87woo/gar	X	X	0	X	0	0
Bromellite	BeO	mineral	1	supcrt92**	0	0	0	0	0	0
Bromellite	BeO	mineral	2	89cox/wag	X	X	0	X	0	0
Brucite	Mg(OH)2	mineral	1	supcrt92**	X	X	X	X	0	0
Brucite	Mg(OH)2	mineral	4	84har/mol	0	0	0	0	0	X
Brushite	CaHPO4:2H2O	mineral	0	90crc	0	0	0	0	0	0
Brushite	CaHPO4:2H2O	mineral	3	76ben/ada	X	X	0	X	0	0
Bunsenite	NiO	mineral	1	supcrt92**	X	X	X	X	0	0
Burkeite	Na6CO3(SO4)2	mineral	1	84har/mol	X	X	0	0	0	X
Burkeite	Na6CO3(SO4)2	mineral	4	84har/mol	0	0	0	0	0	X

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
C		mineral	1	supcrt92**	X	X	X	0	0	0
C		mineral	2	89cox/wag	0	0	0	0	0	0
C(g)		mineral	2	89cox/wag	X	X	0	0	0	0
C2H4(g)		mineral	1	93sho	X	X	X	0	0	0
CH4(g)		mineral	1	supcrt92**	X	X	X	0	0	0
CO(g)		mineral	1	93sho	X	X	X	0	0	0
CO(g)		mineral	2	89cox/wag	X	X	0	0	0	0
CO2(g)		mineral	1	supcrt92**	X	X	X	0	0	0
CO2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
CO2(g)		mineral	4	84har/mol	0	0	0	0	0	X
Ca		mineral	2	89cox/wag	X	X	0	X	0	0
Ca(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Ca-Al Pyroxene	CaAl2SiO6	mineral	1	supcrt92**	X	X	X	0	0	0
Ca2Al2O5·8H2O		mineral	1	82sar/bar	X	X	0	X	0	0
Ca2Cl2(OH)2·H2O		mineral	1	84har/mol	X	X	0	X	0	X
Ca2Cl2(OH)2·H2O		mineral	4	84har/mol	0	0	0	X	0	X
Ca2V2O7		mineral	1	82wag/eva	X	X	0	0	0	0
Ca3(AsO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
Ca3Al2O6		mineral	1	82sar/bar	X	X	0	X	0	0
Ca3UO6		mineral	0	92gre/fug	0	0	0	0	0	0
Ca3V2O8		mineral	1	82wag/eva	X	X	0	0	0	0
Ca4Al2Fe2O10		mineral	1	82sar/bar	X	X	0	0	0	0
Ca4Al2O7·13H2O		mineral	1	82sar/bar	X	X	0	X	0	0
Ca4Al2O7·19H2O		mineral	1	82sar/bar	X	X	0	X	0	0
Ca4C12(OH)6·13H2O		mineral	1	84har/mol	X	X	0	X	0	X
Ca4C12(OH)6·13H2O		mineral	4	84har/mol	0	0	0	X	0	X
Ca6Al4Fe2O15		mineral	0	82sar/bar	0	0	0	0	0	0
CaAl2O4		mineral	1	82sar/bar	X	X	0	X	0	0
CaAl2O4·10H2O		mineral	1	82sar/bar	X	X	0	X	0	0
CaAl4O7		mineral	1	82sar/bar	X	X	0	X	0	0
CaC12·4H2O		mineral	4	84har/mol	0	0	0	0	0	X
CaC12·H2O		mineral	2	82wag/eva	0	0	0	0	0	0
CaSO4·0.5H2O(beta)		mineral	1	82wag/eva	X	X	0	X	0	0
CaSeO3·2H2O		mineral	1	74nau/ryz	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
CaSeO4		mineral	0	90crc	0	0	0	0	0	0
CaSeO4		mineral	3	76smi/mar	X	X	0	0	0	0
CaUO4		mineral	0	chemval*	0	0	0	0	0	0
CaUO4		mineral	2	92gre/fug	X	X	0	X	X	0
CaUO4		mineral	3	chemval*	0	0	0	0	0	0
CaV2O6		mineral	1	82wag/eva	X	X	0	0	0	0
CaZrO3		mineral	1	74nau/ryz	X	X	0	0	0	0
Cadmoseelite	CdSe	mineral	2	74mil	X	X	0	0	0	0
Calcite	CaCO3	mineral	0	chemval*	0	0	0	0	0	0
Calcite	CaCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Calcite	CaCO3	mineral	3	chemval*	0	0	0	0	0	0
Calcite	CaCO3	mineral	4	84har/mol	0	0	0	0	0	X
Calomel	Hg2Cl2	mineral	2	89cox/wag	X	X	0	0	0	0
Carbonate-Calcite	(Ca, Mn, Zn, Mg, Fe, Sr)CO3	mineral	1	ss***	X	X	0	0	0	0
Carnallite	KMgCl3:6H2O	mineral	1	84har/mol	X	X	0	X	0	X
Carnallite	KMgCl3:6H2O	mineral	4	84har/mol	0	0	0	X	0	X
Carnotite	K2(UO2)2(VO4)2	mineral	1	78lan	X	X	0	0	0	0
Cassiterite	SnO2	mineral	1	supcrt92**	X	X	X	0	0	0
Cassiterite	SnO2	mineral	2	89cox/wag	0	0	0	0	0	0
Cattierite	CoS2	mineral	1	78vau/cra	X	X	0	X	0	0
Cd		mineral	2	89cox/wag	X	X	0	X	0	0
Cd(g)		mineral	2	89cox/wag	X	X	0	X	0	0
CdCr2O4		mineral	1	76del/hal	X	X	0	X	0	0
CdSO4:2.667H2O		mineral	2	92gre/fug	X	X	0	X	X	0
CdSeO3		mineral	1	82wag/eva	X	X	0	0	0	0
CdSeO4		mineral	1	82wag/eva	X	X	0	0	0	0
Ce		mineral	1	79rob/hem	X	X	0	X	0	0
Celadonite	KMgAlSi4O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Celadonite	KMgAlSi4O10(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Celestite	SrSO4	mineral	0	chemval*	0	0	0	0	0	0
Celestite	SrSO4	mineral	1	supcrt92**	X	X	X	X	0	0
Celestite	SrSO4	mineral	3	chemval*	0	0	0	0	0	0
Cerussite	PbCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Chalcanthite	CuSO4:5H2O	mineral	1	82wag/eva	X	X	0	X	0	0
Chalcedony	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Chalcocite	Cu2S	mineral	1	supcrt92**	X	X	X	0	0	0
Chalcocyanite	CuSO4	mineral	2	89cox/wag	X	X	0	X	0	0
Chalcopyrite	CuFeS2	mineral	1	supcrt92**	X	X	X	0	0	0
Chamosite-7A	Fe2Al2SiO5(OH)4	mineral	1	78wol	X	X	0	0	0	0
Chamosite-7A	Fe2Al2SiO5(OH)4	mineral	1	supcrt92**	0	0	0	0	0	0
Chlorargyrite	AgCl	mineral	1	supcrt92**	X	X	X	X	0	0
Chlorargyrite	AgCl	mineral	2	89cox/wag	0	0	0	0	0	0
Chlorite-ss	(Fe,Mg)5Al2Si3O10(OH)8	mineral	1	ss***	X	X	0	0	0	0
Chloritoid	FeAl2SiO5(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Chlorocalcite	KCaCl3	mineral	0		0	0	0	0	0	0
Chloromagnesite	MgCl2	mineral	1	79rob/hem	X	X	0	X	0	0
Chromite	FeCr2O4	mineral	1	82wag/eva	X	X	0	X	0	0
Chrysocolla	CuSiH4O5	mineral	1	87woo/gar	X	X	0	0	0	0
Chrysotile	Mg3Si2O5(OH)4	mineral	1	supcrt92**	X	X	X	0	0	0
Cinnabar	HgS	mineral	1	supcrt92**	X	X	X	0	0	0
Cl(g)		mineral	1	89cox/wag	0	0	0	0	0	0
Cl2(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Claudetite	As2O3	mineral	1	79rob/hem	X	X	0	0	0	0
Clausthalite	PbSe	mineral	2	82wag/eva	X	X	0	0	0	0
Clinochalcomenite	CuSeO3·2H2O	mineral	1	74nau/ryz	X	X	0	0	0	0
Clinochlore-14A	Mg5Al2Si3O10(OH)8	mineral	1	supcrt92**	X	X	X	0	0	0
Clinochlore-7A	Mg5Al2Si3O10(OH)8	mineral	1	supcrt92**	X	X	X	0	0	0
Clinoptilolite	Na.954K.543Ca.761Mg.124Sr.03	mineral	1	89db 6	X	X	0	0	0	0
Clinoptilolite-Ba	Ba1.7335Al3.45Fe.017Si14.533	mineral	1	89db2	0	0	0	0	0	0
Clinoptilolite-Ca	Ca1.7335Al3.45Fe.017Si14.533	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-Cs	Cs3.467Al3.45Fe.017Si14.5330	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-K	K3.467Al3.45Fe.017Si14.53303	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-Mg	Mg1.7335Al3.45Fe.017Si14.533	mineral	1	89db2	0	0	0	0	0	0
Clinoptilolite-Mn	Mn1.7335Al3.45Fe.017Si14.533	mineral	1	89db2	0	0	0	0	0	0
Clinoptilolite-NH4	(NH4)3.467Al3.45Fe.017Si14.5	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-Na	Na3.467Al3.45Fe.017Si14.5330	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-Sr	Sr1.7335Al3.45Fe.017Si14.533	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-dehy	Sr.036Mg.124Ca.761Mn.002Ba.0	mineral	1	89db 6	X	X	0	0	0	0
Clinoptilolite-dehy-Ca	Ca1.7335Al3.45Fe.017Si14.533	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-dehy-Cs	Cs3.467Al3.45Fe.017Si14.5330	mineral	1	89db 7	X	X	0	0	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Clinoptilolite-dehy-K	K3.467Al3.45Fe.017Si14.53303	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-dehy-NH4	(NH4)3.467Al3.45Fe.017Si14.5	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-dehy-Na	Na3.467Al3.45Fe.017Si14.5330	mineral	1	89db 7	X	X	0	0	0	0
Clinoptilolite-dehy-Sr	Sr1.7335Al3.45Fe.017Si14.533	mineral	1	89db.7	X	X	0	0	0	0
Clinoptilolite-hy-Ca	Ca1.7335Al3.45Fe.017Si14.533	mineral	1	viani	X	X	0	0	0	0
Clinoptilolite-hy-Cs	Cs3.467Al3.45Fe.017Si14.5330	mineral	1	viani	X	X	0	0	0	0
Clinoptilolite-hy-K	K3.467Al3.45Fe.017Si14.53303	mineral	1	viani	X	X	0	0	0	0
Clinoptilolite-hy-Na	Na3.467Al3.45Fe.017Si14.5330	mineral	1	viani	X	X	0	0	0	0
Clinoptilolite-hy-Sr	Sr1.7335Al3.45Fe.017Si14.533	mineral	1	viani	X	X	0	0	0	0
Clinoptilolite-hy-ss	(Na,K,Cs,NH4,Ca.5,Sr.5)3.467	mineral	1	ss***	X	X	0	0	0	0
Clinoptilolite-ss	(Na,K,Cs,NH4,Ca.5,Sr.5)3.467	mineral	1	ss***	X	X	0	0	0	0
Clinozoisite	Ca2Al3Si3O12(OH)	mineral	1	supcrt92**	X	X	X	0	0	0
Co		mineral	1	79rob/hem	X	X	0	X	0	0
Co(NO3)2		mineral	1	65gar/chr	X	X	0	X	0	0
Co(OH)2		mineral	0	73don	0	0	0	0	0	0
Co(OH)2		mineral	3	76bae/mes	X	X	0	X	0	0
Co2SiO4		mineral	2	82wag/eva	X	X	0	0	0	0
Co3(AsO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
Co3(PO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
CoBr2		mineral	0	82wag/eva	0	0	0	0	0	0
CoCl2		mineral	1	82wag/eva	X	X	0	X	0	0
CoCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
CoCl2:6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
CoF2		mineral	1	82wag/eva	X	X	0	X	0	0
CoF3		mineral	2	79kub/alc	X	X	0	0	0	0
CoFe2O4		mineral	1	74nau/ryz	X	X	0	0	0	0
CoHPO4		mineral	1	82wag/eva	X	X	0	X	0	0
CoO		mineral	1	82wag/eva	X	X	0	X	0	0
CoS		mineral	1	74nau/ryz	X	X	0	0	0	0
CoSO4		mineral	1	82wag/eva	X	X	0	X	0	0
CoSO4.3Co(OH)2		mineral	1	82wag/eva	X	X	0	X	0	0
CoSO4:6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
CoSO4:H2O		mineral	1	74nau/ryz	X	X	0	X	0	0
CoSeO3		mineral	3	76smi/mar	X	X	0	0	0	0
CoWO4		mineral	1	74nau/ryz	X	X	0	0	0	0
Coesite	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Coffinite	USiO4	mineral	0	chemval*	0	0	0	0	0	0
Coffinite	USiO4	mineral	1	82hem	0	0	0	0	0	0
Coffinite	USiO4	mineral	1	92gre/fug	X	X	0	0	X	0
Coffinite	USiO4	mineral	3	chemval*	0	0	0	0	0	0
Colemanite	Ca2B6O11:5H2O	mineral	1	77bas	X	X	0	0	0	0
Cordierite anhyd	Mg2Al4Si5O18	mineral	1	supcrt92**	X	X	X	0	0	0
Cordierite hydr	Mg2Al4Si5O18:H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Corkite	PbFe3(PO4)(SO4)(OH)6	mineral	1	78ric/nri	X	X	0	0	0	0
Corundum	Al2O3	mineral	1	supcrt92**	X	X	X	X	0	0
Corundum	Al2O3	mineral	2	89cox/wag	0	0	0	0	0	0
Cotunnite	PbCl2	mineral	1	82wag/eva	X	X	0	X	0	0
Covellite	CuS	mineral	1	supcrt92**	X	X	X	0	0	0
Cr		mineral	1	79rob/hem	X	X	0	X	0	0
CrCl3		mineral	2	82wag/eva	X	X	0	X	0	0
CrF3		mineral	2	76del/hal	X	X	0	X	0	0
CrF4		mineral	2	76del/hal	X	X	0	X	0	0
CrI3		mineral	2	76del/hal	X	X	0	X	0	0
CrO2		mineral	2	76del/hal	X	X	0	X	0	0
CrO3		mineral	2	76del/hal	X	X	0	X	0	0
CrS		mineral	1	76del/hal	X	X	0	0	0	0
Cristobalite	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0
Cristobalite-a	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0
Cristobalite-b	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0
Crocoite	PbCrO4	mineral	1	76del/hal	X	X	0	X	0	0
Cronstedtite-7A	Fe2Fe2SiO5(OH)4	mineral	1	78wol	X	X	0	0	0	0
Cronstedtite-7A	Fe2Fe2SiO5(OH)4	mineral	1	supcrt92**	0	0	0	0	0	0
Cs		mineral	2	89cox/wag	X	X	0	X	0	0
Cs(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Cs2U2O7		mineral	2	92gre/fug	X	X	0	X	X	0
Cs2U4O12		mineral	2	92gre/fug	X	X	0	X	X	0
Cs2UO4		mineral	1	82hem	0	0	0	0	0	0
Cs2UO4		mineral	2	92gre/fug	X	X	0	X	X	0
Cs2UO4		mineral	1	supcrt92**	X	X	X	X	0	0
Cu		mineral	1	supcrt92**	X	X	X	X	0	0
Cu		mineral	2	89cox/wag	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Cu(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Cu <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>		mineral	1	82wag/eva	X	X	0	X	0	0
Cu <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> :3H <sub>2</sub> O		mineral	3	80bal/nor	X	X	0	X	0	0
CuCl <sub>2</sub>		mineral	1	82wag/eva	X	X	0	X	0	0
CuCr <sub>2</sub> O <sub>4</sub>		mineral	1	76del/hal	X	X	0	X	0	0
CuF		mineral	0	73don	0	0	0	0	0	0
CuF		mineral	3	80bal/nor	X	X	0	X	0	0
CuF <sub>2</sub>		mineral	0	90crc	0	0	0	0	0	0
CuF <sub>2</sub>		mineral	3	80bal/nor	X	X	0	X	0	0
CuF <sub>2</sub> :2H <sub>2</sub> O		mineral	0	90crc	0	0	0	0	0	0
CuF <sub>2</sub> :2H <sub>2</sub> O		mineral	3	80bal/nor	X	X	0	X	0	0
CuSeO <sub>3</sub>		mineral	1	82wag/eva	X	X	0	0	0	0
Cumingtonite	Mg <sub>7</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	mineral	1	supcrt92**	0	0	0	0	0	0
Cuprite	Cu <sub>2</sub> O	mineral	1	supcrt92**	X	X	X	X	0	0
Daphnite-14A	Fe <sub>5</sub> AlAlSi <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>	mineral	1	78wol	X	X	0	0	0	0
Daphnite-14A	Fe <sub>5</sub> AlAlSi <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>	mineral	1	supcrt92**	0	0	0	0	0	0
Daphnite-7A	Fe <sub>5</sub> AlAlSi <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>	mineral	1	78wol	X	X	0	0	0	0
Daphnite-7A	Fe <sub>5</sub> AlAlSi <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>	mineral	1	supcrt92**	0	0	0	0	0	0
Dawsonite	NaAlCO <sub>3</sub> (OH) <sub>2</sub>	mineral	1	79rob/hem	X	X	0	0	0	0
Delafossite	CuFeO <sub>2</sub>	mineral	1	74nau/ryz	X	X	0	X	0	0
Diaspore	AlHO <sub>2</sub>	mineral	1	supcrt92**	X	X	X	X	0	0
Dicalcium silicate	Ca <sub>2</sub> SiO <sub>4</sub>	mineral	2	82wag/eva	X	X	0	0	0	0
Dickite	Al <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub>	mineral	1	supcrt92**	0	0	0	0	0	0
Diopside	CaMgSi <sub>2</sub> O <sub>6</sub>	mineral	1	supcrt92**	X	X	X	0	0	0
Dioptase	CuSiO <sub>2</sub> (OH) <sub>2</sub>	mineral	1	87woo/gar	X	X	0	0	0	0
Dolomite	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	0	chemval*	0	0	0	0	0	0
Dolomite	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	1	supcrt92**	X	X	X	0	0	0
Dolomite	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	3	chemval*	0	0	0	0	0	0
Dolomite	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	4	84har/mol	0	0	0	0	0	X
Dolomite-dis	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	1	supcrt92**	X	X	X	0	0	0
Dolomite-ord	CaMg(CO <sub>3</sub> ) <sub>2</sub>	mineral	1	supcrt92**	X	X	X	0	0	0
Downeyite	SeO <sub>2</sub>	mineral	0	92gre/fug	0	0	0	0	0	0
Downeyite	SeO <sub>2</sub>	mineral	2	74mil	X	X	0	0	0	0
Dy		mineral	1	79rob/hem	X	X	0	X	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Edenite	NaCa2Mg5Si7AlO22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Enstatite	MgSiO3	mineral	1	supcrt92**	X	X	X	0	0	0
Epidote	Ca2FeAl2Si3O12OH	mineral	1	supcrt92**	X	X	X	0	0	0
Epidote-ord	FeCa2Al2(OH)(SiO4)3	mineral	1	supcrt92**	X	X	X	0	0	10
Epidote-ss	Ca2(Fe,Al)Al2Si3O12(OH)	mineral	1	ss***	X	X	0	0	0	0
Epsomite	MgSO4:7H2O	mineral	1	84har/mol	X	X	0	X	0	X
Epsomite	MgSO4:7H2O	mineral	4	84har/mol	0	0	0	X	0	X
Er		mineral	1	79rob/hem	X	X	0	X	0	0
Erythrite	Co3(AsO4)2:8H2O	mineral	1	74nau/ryz	X	X	0	X	0	0
Eskolaite	Cr2O3	mineral	1	82wag/eva	X	X	0	X	0	0
Ettringite	Ca6Al2(SO4)3(OH)12:26H2O	mineral	2	82sar/bar	X	X	0	X	0	0
Eu		mineral	1	85rar 2	X	X	0	X	0	0
Eu(IO3)3:2H2O		mineral	1	85rar 2	X	X	0	X	0	0
Eu(NO3)3:6H2O		mineral	1	85rar 2	X	X	0	X	0	0
Eu(OH)2.5Cl.5		mineral	1	85rar 2	X	X	0	X	0	0
Eu(OH)2Cl		mineral	1	85rar 2	X	X	0	X	0	0
Eu(OH)3		mineral	1	87rar 2	X	X	0	X	0	0
Eu2(CO3)3:3H2O		mineral	1	87rar 2	X	X	0	0	0	0
Eu2(SO4)3:8H2O		mineral	1	85rar 2	X	X	0	X	0	0
Eu2O3(cubic)		mineral	1	85rar 2	X	X	0	X	0	0
Eu2O3(monoclinic)		mineral	1	85rar 2	X	X	0	X	0	0
Eu3O4		mineral	1	85rar 2	X	X	0	X	0	0
EuBr3		mineral	1	85rar 2	X	X	0	X	0	0
EuCl2		mineral	2	87rar 2	X	X	0	X	0	0
EuCl3		mineral	1	85rar 2	X	X	0	X	0	0
EuCl3:6H2O		mineral	1	85rar 2	X	X	0	X	0	0
EuF3:0.5H2O		mineral	1	85rar 2	X	X	0	X	0	0
EuO		mineral	1	87rar 2	X	X	0	X	0	0
EuOC1		mineral	1	85rar 2	X	X	0	0	0	0
EuS		mineral	1	85rar 2	X	X	0	X	0	0
EuSO4		mineral	1	85rar 2	X	X	0	X	0	0
Eucryptite	LiAlSiO4	mineral	1	82wag/eva	X	X	0	0	0	0
F(g)		mineral	2	89cox/wag	0	0	0	0	0	0
F2(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Fayalite	Fe2SiO4	mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Fe		mineral	1	supcrt92**	X	X	X	X	0	0
Fe(OH)2		mineral	1	82wag/eva	X	X	0	X	0	0
Fe(OH)3		mineral	0	chemval*	0	0	0	0	0	0
Fe(OH)3		mineral	1	82wag/eva	X	X	0	0	0	0
Fe(OH)3		mineral	3	chemval*	0	0	0	0	0	0
Fe2(SO4)3		mineral	1	79rob/hem	X	X	0	0	0	0
FeAsO4		mineral	3	64sil/mar	X	X	0	0	0	0
FeF2		mineral	1	82wag/eva	X	X	0	X	0	0
FeF3		mineral	2	79kub/alc	X	X	0	0	0	0
FeO		mineral	1	supcrt92**	X	X	X	X	0	0
FeSO4		mineral	1	82wag/eva	X	X	0	X	0	0
FeSe		mineral	2	78vau/cra	0	0	0	0	0	0
FeV2O4		mineral	2	79kub/alc	X	X	0	0	0	0
Ferrite-Ca	CaFe2O4	mineral	1	82sar/bar	X	X	0	0	0	0
Ferrite-Cu	CuFe2O4	mineral	1	82wag/eva	X	X	0	0	0	0
Ferrite-Dicalcium	Ca2Fe2O5	mineral	1	79rob/hem	X	X	0	0	0	0
Ferrite-Mg	MgFe2O4	mineral	1	79rob/hem	X	X	0	0	0	0
Ferrite-Zn	ZnFe2O4	mineral	1	82wag/eva	X	X	0	0	0	0
Ferroedenite	NaCa2Fe5Si7AlO22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Ferrogedrite	Fe5Al4Si6O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Ferropargasite	NaCa2Fe4Al3Si6O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Ferroselite	FeSe2	mineral	2	74mil	X	X	0	0	0	0
Ferrosilite	FeSiO3	mineral	1	supcrt92**	X	X	X	0	0	0
Ferrotremolite	Ca2Fe5Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Fluorapatite	Ca5(PO4)3F	mineral	1	79rob/hem	X	X	0	X	0	0
Fluoredenite	NaCa2Mg5Si7AlO22F2	mineral	1	supcrt92**	0	0	0	0	0	0
Fluorite	CaF2	mineral	1	supcrt92**	X	X	X	X	0	0
Fluorophlogopite	KAlMg3Si3O10F2	mineral	1	supcrt92**	0	0	0	0	0	0
Fluortremolite	Ca2Mg5Si8O22F2	mineral	1	supcrt92**	0	0	0	0	0	0
Forsterite	Mg2SiO4	mineral	1	supcrt92**	X	X	X	0	0	0
Foshagite	Ca4Si3O9(OH)2:0.5H2O	mineral	1	82sar/bar	X	X	0	0	0	0
Fr		mineral	1	82wag/eva	0	0	0	0	0	0
Frankdicksonite	BaF2	mineral	1	82wag/eva	0	0	0	0	0	0
Frankdicksonite	BaF2	mineral	3	76smi/mar	X	X	0	X	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Freboldite	CoSe	mineral	1	78vau/cra	X	X	0	0	0	0
Ga		mineral	1	79rob/hem	X	X	0	X	0	0
Galena	PbS	mineral	1	supcrt92**	X	X	X	0	0	0
Garnet-ss	Ca3(Al, Fe)2Si3O12	mineral	1	ss***	X	X	0	0	0	0
Gaylussite	CaNa2(CO3)2·5H2O	mineral	1	84har/mol	X	X	0	0	0	X
Gaylussite	CaNa2(CO3)2·5H2O	mineral	4	84har/mol	0	0	0	0	0	X
Gd		mineral	1	79rob/hem	X	X	0	X	0	0
Ge		mineral	1	89cox/wag	0	0	0	0	0	0
Ge(g)		mineral	2	89cox/wag	0	0	0	0	0	0
GeF4(g)		mineral	2	89cox/wag	0	0	0	0	0	0
GeO2		mineral	2	89cox/wag	0	0	0	0	0	0
Gehlenite	Ca2Al2SiO7	mineral	1	supcrt92**	X	X	X	0	0	0
Gibbsite	Al(OH)3	mineral	1	supcrt92**	X	X	X	X	0	0
Gismondine	Ca2Al4Si4O16·9H2O	mineral	1	89db 3	X	X	0	0	0	0
Glauberite	Na2Ca(SO4)2	mineral	1	84har/mol	X	X	0	X	0	X
Glauberite	Na2Ca(SO4)2	mineral	4	84har/mol	0	0	0	X	0	X
Glaucophane	Na2Al2Mg3Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Goethite	FeOOH	mineral	1	79rob/hem	X	X	0	0	0	0
Greenalite	Fe3Si2O5(OH)4	mineral	1	78wol	X	X	0	0	0	0
Greenalite	Fe3Si2O5(OH)4	mineral	1	supcrt92**	0	0	0	0	0	0
Grossular	Ca3Al2(SiO4)3	mineral	1	supcrt92**	X	X	X	0	0	0
Grunerite	Fe7Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Gypsum	CaSO4·2H2O	mineral	0	chemval*	0	0	0	0	0	0
Gypsum	CaSO4·2H2O	mineral	1	79rob/hem	X	X	0	X	0	0
Gypsum	CaSO4·2H2O	mineral	3	chemval*	0	0	0	0	0	0
Gypsum	CaSO4·2H2O	mineral	4	84har/mol	0	0	0	0	0	X
Gyrolite	Ca2Si3O7(OH)2·1.5H2O	mineral	1	82sar/bar	X	X	0	0	0	0
H(g)		mineral	2	89cox/wag	0	0	0	0	0	0
H-Autunite	H2(UO2)2(PO4)2	mineral	1	92gre/fug	X	X	0	X	X	0
H2(g)		mineral	1	supcrt92**	X	X	X	X	0	0
H2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
H2(g)		mineral	4	84har/mol	0	0	0	0	0	X
H2O(g)		mineral	1	supcrt92**	X	X	X	X	0	0
H2O(g)		mineral	2	89cox/wag	0	0	0	0	0	0
H2S(g)		mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
H2S(g)		mineral	2	89cox/wag	0	0	0	0	0	0
H3OUF6		mineral	0	92gre/fug	0	0	0	0	0	0
HBr(g)		mineral	2	89cox/wag	X	X	0	X	0	0
HCl(g)		mineral	2	89cox/wag	X	X	0	X	0	0
HF		mineral	1	79rob/hem	0	0	0	0	0	0
HF(g)		mineral	2	89cox/wag	X	X	0	X	0	0
HI(g)		mineral	2	89cox/wag	X	X	0	X	0	0
HTcO4		mineral	1	83rar	X	X	0	0	0	0
Haiweeite	Ca(UO2)2(Si2O5)3·5H2O	mineral	1	82hem	X	X	0	0	0	0
Halite	NaCl	mineral	1	supcrt92**	X	X	X	X	0	0
Halite	NaCl	mineral	4	84har/mol	0	0	0	0	0	X
Halloysite	Al2Si2O5(OH)4	mineral	1	supcrt92**	0	0	0	0	0	0
Hastingsite	NaAl2Ca2Fe5Si6O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Hatrurite	Ca3SiO5	mineral	1	82sar/bar	X	X	0	0	0	0
Hausmannite	Mn3O4	mineral	1	79rob/hem	X	X	0	X	0	0
He(g)		mineral	1	supcrt92**	X	X	X	0	0	0
He(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Heazlewoodite	Ni3S2	mineral	1	82wag/eva	X	X	0	0	0	0
Hedenbergite	CaFe(SiO3)2	mineral	1	supcrt92**	X	X	X	0	0	0
Hematite	Fe2O3	mineral	1	supcrt92**	X	X	X	0	0	0
Hercynite	FeAl2O4	mineral	1	79rob/hem	X	X	0	X	0	0
Herzenbergite	SnS	mineral	1	supcrt92**	X	X	X	0	0	0
Heulandite	Ba.065Sr.175Ca.585K.132Na.38	mineral	1	85joh/flo	X	X	0	0	0	0
Heulandite	Ba.065Sr.175Ca.585K.132Na.38	mineral	1	supcrt92**	0	0	0	0	0	0
Hexahydrite	MgSO4·6H2O	mineral	1	84har/mol	X	X	0	X	0	X
Hexahydrite	MgSO4·6H2O	mineral	4	84har/mol	0	0	0	X	0	X
Hg(g)		mineral	2	89cox/wag	X	X	0	0	0	0
Hg(l)		mineral	1	supcrt92**	X	X	X	0	0	0
Hg(l)		mineral	2	89cox/wag	0	0	0	0	0	0
Hg2SO4		mineral	2	89cox/wag	X	X	0	0	0	0
Hg2SeO3		mineral	1	82wag/eva	X	X	0	0	0	0
HgSeO3		mineral	1	82wag/eva	X	X	0	0	0	0
Hillebrandite	Ca2SiO3(OH)2·0.17H2O	mineral	1	82sar/bar	X	X	0	0	0	0
Hinsdalite	Al3PPbSO8(OH)6	mineral	0	86jen	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Hinsdalite	Al3PPbSO8(OH)6	mineral	3	80bal/nor	X	X	0	X	0	0
Ho		mineral	1	82wag/eva	X	X	0	X	0	0
Hopeite	Zn3(PO4)2:4H2O	mineral	0	90crc	0	0	0	0	0	0
Hopeite	Zn3(PO4)2:4H2O	mineral	3	76smi/mar	X	X	0	X	0	0
Huntite	CaMg3(CO3)4	mineral	1	supcrt92**	X	X	X	0	0	0
Hydroboracite	MgCaB6O11:6H2O	mineral	1	77bas	X	X	0	0	0	0
Hydrocerussite	Pb3(CO3)2(OH)2	mineral	1	78ric/nri	X	X	0	0	0	0
Hydromagnesite	Mg5(CO3)4(OH)2:4H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Hydrophilite	CaCl2	mineral	1	79rob/hem	X	X	0	X	0	0
Hydroxylapatite	Ca5(OH)(PO4)3	mineral	1	79rob/hem	X	X	0	X	0	0
I(g)		mineral	2	89cox/wag	0	0	0	0	0	0
I2		mineral	2	89cox/wag	X	X	0	X	0	0
I2(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Ice	H2O	mineral	2	87kee/rup	X	X	0	X	0	0
Illite	K0.6Mg0.25Al1.8Al0.5Si3.5O10	mineral	1	78wol	X	X	0	0	0	0
Ilmenite	FeTiO3	mineral	1	79rob/hem	X	X	0	0	0	0
In		mineral	1	79rob/hem	X	X	0	X	0	0
Ir		mineral	1	79rob/hem	0	0	0	0	0	0
Jadeite	NaAl(SiO3)2	mineral	1	supcrt92**	X	X	X	0	0	0
Jarosite	KFe3(SO4)2(OH)6	mineral	1	75kas/bor	X	X	0	0	0	0
Jarosite-Na	Fe3(SO4)2(OH)6	mineral	1	75kas/bor	X	X	0	0	0	0
K		mineral	2	89cox/wag	X	X	0	X	0	0
K(g)		mineral	2	89cox/wag	X	X	0	X	0	0
K-Feldspar	KAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0
K2CO3:3/2H2O		mineral	1	84har/mol	X	X	0	0	0	X
K2CO3:3/2H2O		mineral	4	84har/mol	0	0	0	0	0	X
K2CaCl4		mineral	0		0	0	0	0	0	0
K2O		mineral	1	supcrt92**	X	X	X	X	0	0
K2Se		mineral	2	74mil	X	X	0	0	0	0
K2SiO3		mineral	2	77pau	0	0	0	0	0	0
K2TeCl6		mineral	0	83rar	0	0	0	0	0	0
K2U2O7		mineral	0	92gre/fug	0	0	0	0	0	0
K2UO4		mineral	2	92gre/fug	X	X	0	X	X	0
K3H(SO4)2		mineral	1	84har/mol	X	X	0	X	0	X



SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
K3H(SO4)2		mineral	4	84har/mol	0	0	0	X	0	X
K8H4(CO3)6:3H2O		mineral	1	84har/mol	X	X	0	0	0	X
K8H4(CO3)6:3H2O		mineral	4	84har/mol	0	0	0	0	0	X
KAl(SO4)2		mineral	1	79rob/hem	X	X	0	X	0	0
KBr		mineral	2	82wag/eva	X	X	0	X	0	0
KMgCl3		mineral	2	82wag/eva	X	X	0	X	0	0
KMgCl3:2H2O		mineral	2	82wag/eva	X	X	0	X	0	0
KNaCO3:6H2O		mineral	1	84har/mol	X	X	0	0	0	X
KNaCO3:6H2O		mineral	4	84har/mol	0	0	0	0	0	X
KTcO4		mineral	1	83rar	X	X	0	0	0	0
KUO2AsO4		mineral	1	82wag/eva	X	X	0	X	0	0
KUO3		mineral	0	92gre/fug	0	0	0	0	0	0
Kainite	KMgClSO4:3H2O	mineral	1	84har/mol	X	X	0	X	0	X
Kainite	KMgClSO4:3H2O	mineral	4	84har/mol	0	0	0	X	0	X
Kalicinite	KHCO3	mineral	1	84har/mol	X	X	0	0	0	X
Kalicinite	KHCO3	mineral	4	84har/mol	0	0	0	0	0	X
Kalsilite	KAlSiO4	mineral	1	supcrt92**	X	X	X	0	0	0
Kaolinite	Al2Si2O5(OH)4	mineral	1	supcrt92**	X	X	X	0	0	0
Karelianite	V2O3	mineral	1	82wag/eva	X	X	0	0	0	0
Kasolite	Pb(UO2)SiO4:H2O	mineral	1	82hem	X	X	0	0	0	0
Katoite	Ca3Al2H12O12	mineral	1	82sar/bar	X	X	0	X	0	0
Kieserite	MgSO4:H2O	mineral	1	84har/mol	X	X	0	X	0	X
Kieserite	MgSO4:H2O	mineral	4	84har/mol	0	0	0	X	0	X
Klockmannite	CuSe	mineral	2	74mil	X	X	0	0	0	0
Kr(g)		mineral	1	supcrt92**	X	X	X	0	0	0
Kr(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Krutaitite	CuSe2	mineral	2	78vau/cra	X	X	0	0	0	0
Kyanite	Al2SiO5	mineral	1	supcrt92**	X	X	X	0	0	0
La		mineral	1	79rob/hem	X	X	0	X	0	0
Lammerite	Cu3(AsO4)2	mineral	1	82wag/eva	X	X	0	X	0	0
Lanarkite	Pb2(SO4)O	mineral	1	82wag/eva	X	X	0	X	0	0
Lansfordite	MgCO3:5H2O	mineral	1	82wag/eva	X	X	0	0	0	0
Larnite	Ca2SiO4	mineral	1	supcrt92**	0	0	0	0	0	0
Larnite	Ca2SiO4	mineral	2	82sar/bar	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Laumontite	CaAl2Si4O12:4H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Laurite	RuS2	mineral	1	85rar 1	X	X	0	0	0	0
Lawrencite	FeCl2	mineral	1	79rob/hem	X	X	0	X	0	0
Lawsonite	CaAl2Si2O7(OH)2:H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Leonhardite	Ca2Al4Si8O24:7H2O	mineral	1	supcrt92**	0	0	0	0	0	0
Leonite	K2Mg(SO4)2:4H2O	mineral	1	84har/mol	X	X	0	X	0	X
Leonite	K2Mg(SO4)2:4H2O	mineral	4	84har/mol	0	0	0	X	0	X
Li		mineral	2	89cox/wag	X	X	0	X	0	0
Li(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Li2Se		mineral	2	74mil	X	X	0	0	0	0
Li2SiO3		mineral	3	81wag	0	0	0	0	0	0
Li2U2O7		mineral	0	92gre/fug	0	0	0	0	0	0
Li2U3O10		mineral	0	92gre/fug	0	0	0	0	0	0
Li2UO4		mineral	2	92gre/fug	X	X	0	X	X	0
Li4UO5		mineral	0	92gre/fug	0	0	0	0	0	0
LiUO2AsO4		mineral	1	82wag/eva	X	X	0	X	0	0
LiUO3		mineral	0	92gre/fug	0	0	0	0	0	0
Lime	CaO	mineral	1	supcrt92**	X	X	X	X	0	0
Lime	CaO	mineral	2	89cox/wag	0	0	0	0	0	0
Linnæite	Co3S4	mineral	1	78vau/cra	X	X	0	X	0	0
Litharge	PbO	mineral	1	82wag/eva	X	X	0	X	0	0
Lopezite	K2Cr2O7	mineral	1	76del/hal	X	X	0	X	0	0
Lu		mineral	1	79rob/hem	X	X	0	X	0	0
Magadiite	NaSi7O13(OH)3:3H2O	mineral	3	74tru/jon	0	0	0	0	0	0
Magnesiochromite	MgCr2O4	mineral	2	82wag/eva	X	X	0	X	0	0
Magnesiohastingsite	NaAl2Ca2FeMg4Si6O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Magnesioriebeckite	Na2Fe2Mg3Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Magnesite	MgCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Magnesite	MgCO3	mineral	4	84har/mol	0	0	0	0	0	X
Magnetite	Fe3O4	mineral	1	supcrt92**	X	X	X	0	0	0
Malachite	Cu2CO3(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Manganite	MnHO2	mineral	1	65bri	X	X	0	X	0	0
Manganosite	MnO	mineral	1	supcrt92**	X	X	X	X	0	0
Margarite	CaAl4Si2O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Massicot	PbO	mineral	1	82wag/eva	X	X	0	X	0	0
Matlockite	PbFC1	mineral	0	67rob/bet	0	0	0	0	0	0
Matlockite	PbFC1	mineral	3	80bal/nor	X	X	0	X	0	0
Maximum Microcline	KAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0
Mayenite	Ca12Al14O33	mineral	1	82sar/bar	X	X	0	X	0	0
Melanterite	FeSO4:7H2O	mineral	1	79rob/hem	X	X	0	X	0	0
Mercallite	KHSO4	mineral	1	84har/mol	X	X	0	X	0	X
Mercallite	KHSO4	mineral	4	84har/mol	0	0	0	X	0	X
Merwinite	MgCa3(SiO4)2	mineral	1	supcrt92**	X	X	X	0	0	0
Mesolite	Na.676Ca.657Al1.99Si3.01O10:	mineral	1	89db 6	X	X	0	0	0	0
Mesolite	Na.676Ca.657Al1.99Si3.01O10:	mineral	2	83joh/flo	0	0	0	0	0	0
Metacinnabar	HgS	mineral	1	supcrt92**	X	X	X	0	0	0
Metasilicate-Na	Na2SiO3:9H2O	mineral	0	82wag/eva	0	0	0	0	0	0
Mg		mineral	2	89cox/wag	X	X	0	X	0	0
Mg(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Mg1.25SO4(OH)0.5:0.5H2O		mineral	1	82jan	X	X	0	0	0	0
Mg1.5SO4(OH)		mineral	1	82jan	X	X	0	0	0	0
Mg2V2O7		mineral	1	82wag/eva	X	X	0	0	0	0
Mg3(AsO4)2		mineral	3	64sil/mar	X	X	0	X	0	0
MgBr2		mineral	2	73bar/kna	X	X	0	X	0	0
MgBr2:6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MgCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MgCl2:4H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MgCl2:H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MgOHC1		mineral	2	73bar/kna	X	X	0	X	0	0
MgSO4		mineral	1	82wag/eva	X	X	0	X	0	0
MgSeO3		mineral	2	77bar/kna	X	X	0	0	0	0
MgSeO3:6H2O		mineral	1	74nau/ryz	X	X	0	0	0	0
MgU3O10		mineral	0	92gre/fug	0	0	0	0	0	0
MgUO4		mineral	0	chemval*	0	0	0	0	0	0
MgUO4		mineral	2	92gre/fug	X	X	0	X	X	0
MgUO4		mineral	3	chemval*	0	0	0	0	0	0
MgV2O6		mineral	1	82wag/eva	X	X	0	0	0	0
Millerite	NiS	mineral	1	82wag/eva	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUR	PIT	NEA	HMW
Minium	Pb3O4	mineral	1	82wag/eva	X	X	0	0	0	0
Minnesotaite	Fe3Si4O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Minnesotaite	Fe3Si4O10(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Mirabilite	Na2SO4:10H2O	mineral	1	79rob/hem	X	X	0	X	0	0
Mirabilite	Na2SO4:10H2O	mineral	4	84har/mol	0	0	0	0	0	X
Misenite	K8H6(SO4)7	mineral	1	84har/mol	X	X	0	X	0	X
Misenite	K8H6(SO4)7	mineral	4	84har/mol	0	0	0	X	0	X
Mn		mineral	1	79rob/hem	X	X	0	X	0	0
Mn(OH)2(am)		mineral	1	82wag/eva	X	X	0	X	0	0
Mn(OH)3		mineral	3	76plu/jon	X	X	0	0	0	0
Mn3(AsO4)2		mineral	0	73don	0	0	0	0	0	0
Mn3(AsO4)2		mineral	3	64sil/mar	X	X	0	X	0	0
Mn3(PO4)2		mineral	0	86jen	0	0	0	0	0	0
Mn3(PO4)2		mineral	3	76plu/jon	X	X	0	X	0	0
MnCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MnCl2:4H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MnCl2:H2O		mineral	1	82wag/eva	X	X	0	X	0	0
MnHPO4		mineral	3	76plu/jon	X	X	0	X	0	0
MnO2(gamma)		mineral	1	65bri	X	X	0	X	0	0
MnSO4		mineral	1	79rob/hem	X	X	0	X	0	0
MnSe		mineral	2	74mil	X	X	0	0	0	0
MnSeO3		mineral	3	76smi/mar	X	X	0	0	0	0
MnSeO3:2H2O		mineral	1	74nau/ryz	X	X	0	0	0	0
MnV2O6		mineral	1	76isr/mei	X	X	0	0	0	0
Mo		mineral	1	79rob/hem	X	X	0	0	0	0
MoSe2		mineral	2	74mil	X	X	0	0	0	0
Modderite	CoAs	mineral	1	74nau/ryz	X	X	0	0	0	0
Molybdomenite	PbSeO3	mineral	0	82wag/eva	0	0	0	0	0	0
Molysite	FeCl3	mineral	1	79rob/hem	X	X	0	0	0	0
Monohydrocalcite	CaCO3:H2O	mineral	1	79rob/hem	X	X	0	0	0	0
Monteponite	CdO	mineral	2	89cox/wag	X	X	0	X	0	0
Monticellite	CaMgSiO4	mineral	1	supcrt92**	X	X	X	0	0	0
Montmor-Ca	Ca.165Mg.33Al1.67Si4O10(OH)2	mineral	1	88db 3	X	X	0	0	0	0
Montmor-Cs	Cs.33Mg.33Al1.67Si4O10(OH)2	mineral	1	88db 4	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Montmor-K	K.33Mg.33Al1.67Si4O10(OH)2	mineral	1	88db 3	X	X	0	0	0	0
Montmor-Mg	Mg.495Al1.67Si4O10(OH)2	mineral	1	88db 3	X	X	0	0	0	0
Montmor-Na	Na.33Mg.33Al1.67Si4O10(OH)2	mineral	1	88db 3	X	X	0	0	0	0
Montroydite	HgO	mineral	2	89cox/wag	X	X	0	0	0	0
Mordenite	Ca.2895Na.361Al.94Si5.06O12:	mineral	1	91joh/tas	X	X	0	0	0	0
Mordenite-dehy	Ca.2895Na.361Al.94Si5.06O12	mineral	1	91joh/tas	X	X	0	0	0	0
Morenosite	NiSO4:7H2O	mineral	1	82wag/eva	X	X	0	X	0	0
Muscovite	KAl3Si3O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
N(g)		mineral	2	89cox/wag	0	0	0	0	0	0
N2(g)		mineral	1	supcrt92**	X	X	X	X	0	0
N2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
NH3(g)		mineral	1	supcrt92**	X	X	X	X	0	10
NH3(g)		mineral	2	89cox/wag	0	0	0	0	0	0
NH4HSe		mineral	1	82wag/eva	X	X	0	0	0	0
Na		mineral	2	89cox/wag	X	X	0	X	0	0
Na(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Na2CO3		mineral	2	82wag/eva	X	X	0	0	0	0
Na2CO3:7H2O		mineral	1	82wag/eva	X	X	0	0	0	0
Na2CO3:7H2O		mineral	4	84har/mol	0	0	0	0	0	X
Na2Cr2O7		mineral	2	76del/hal	X	X	0	X	0	0
Na2CrO4		mineral	2	76del/hal	X	X	0	X	0	0
Na2Mg(SO4)2		mineral	0		0	0	0	0	0	0
Na2O		mineral	1	supcrt92**	X	X	X	X	0	0
Na2Se		mineral	2	74mil	X	X	0	0	0	0
Na2Se2		mineral	2	74mil	X	X	0	0	0	0
Na2SiO3		mineral	2	73bar/kna	X	X	0	0	0	0
Na2U2O7		mineral	2	92gre/fug	X	X	0	X	X	0
Na2UO4(alpha)		mineral	0	chemval*	0	0	0	0	0	0
Na2UO4(alpha)		mineral	2	92gre/fug	X	X	0	X	X	0
Na2UO4(alpha)		mineral	3	chemval*	0	0	0	0	0	0
Na2UO4(beta)		mineral	0	92gre/fug	0	0	0	0	0	0
Na3H(SO4)2		mineral	1	84har/mol	X	X	0	X	0	X
Na3H(SO4)2		mineral	4	84har/mol	0	0	0	X	0	X
Na3UO4		mineral	0	chemval*	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Na3UO4		mineral	2	92gre/fug	X	X	0	0	X	0
Na3UO4		mineral	3	chemval*	0	0	0	0	0	0
Na4Ca(SO4)3·2H2O		mineral	1	84har/mol	X	X	0	X	0	X
Na4Ca(SO4)3·2H2O		mineral	4	84har/mol	0	0	0	X	0	X
Na4SiO4		mineral	2	73bar/kna	X	X	0	0	0	0
Na4UO2(CO3)3		mineral	1	92gre/fug	X	X	0	0	X	0
Na4UO5		mineral	0	92gre/fug	0	0	0	0	0	0
Na6Si2O7		mineral	2	73bar/kna	X	X	0	0	0	0
Na6U7O24		mineral	0	92gre/fug	0	0	0	0	0	0
NaBr		mineral	2	82wag/eva	X	X	0	X	0	0
NaBr·2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
NaFeO2		mineral	1	82wag/eva	X	X	0	0	0	0
NaNpO2CO3·3.5H2O		mineral	1	84lem	X	X	0	0	0	0
NaTcO4		mineral	1	83rar	X	X	0	0	0	0
NaUO3		mineral	0	chemval*	0	0	0	0	0	0
NaUO3		mineral	2	92gre/fug	X	X	0	X	X	0
NaUO3		mineral	3	chemval*	0	0	0	0	0	0
Nahcolite	NaHCO3	mineral	2	73bar/kna	X	X	0	0	0	0
Nahcolite	NaHCO3	mineral	4	84har/mol	0	0	0	0	0	X
Nantokite	CuCl	mineral	1	82wag/eva	X	X	0	X	0	0
Natrolite	Na2Al2Si3O10·2H2O	mineral	1	83joh/flo	X	X	0	0	0	0
Natrolite	Na2Al2Si3O10·2H2O	mineral	1	supcrt92**	0	0	0	0	0	0
Natron	Na2CO3·10H2O	mineral	1	82wag/eva	X	X	0	0	0	0
Natron	Na2CO3·10H2O	mineral	4	84har/mol	0	0	0	0	0	X
Natrosilite	Na2Si2O5	mineral	2	77bar/kna	X	X	0	0	0	0
Naumannite	Ag2Se	mineral	1	82wag/eva	X	X	0	0	0	0
Nb		mineral	1	79rob/hem	0	0	0	0	0	0
Nd		mineral	1	79rob/hem	X	X	0	X	0	0
Ne(g)		mineral	1	supcrt92**	X	X	X	0	0	0
Ne(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Nepheline	NaAlSiO4	mineral	1	supcrt92**	X	X	X	0	0	0
Nesquehonite	MgCO3·3H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Nesquehonite	MgCO3·3H2O	mineral	4	84har/mol	0	0	0	0	0	X
Ni		mineral	1	supcrt92**	X	X	X	X	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Ni(OH)2		mineral	1	82wag/eva	X	X	0	X	0	0
Ni2P2O7		mineral	1	82wag/eva	X	X	0	X	0	0
Ni2SiO4		mineral	1	74nau/ryz	X	X	0	0	0	0
Ni3(PO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
NiCO3		mineral	1	82wag/eva	X	X	0	0	0	0
NiCl2		mineral	1	82wag/eva	X	X	0	X	0	0
NiCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
NiCl2:4H2O		mineral	1	82wag/eva	X	X	0	X	0	0
NiCr2O4		mineral	0	76del/hal	0	0	0	0	0	0
NiF2		mineral	1	82wag/eva	X	X	0	X	0	0
NiF2:4H2O		mineral	1	82wag/eva	X	X	0	X	0	0
NiSO4		mineral	1	82wag/eva	X	X	0	X	0	0
NiSO4:6H2O(alpha)		mineral	1	82wag/eva	X	X	0	X	0	0
Nickelbischofite	NiCl2:6H2O	mineral	1	82wag/eva	X	X	0	X	0	0
Ningyoite	CaUP2O8:2H2O	mineral	1	78lan	X	X	0	0	0	0
Niter	KNO3	mineral	2	79rob/hem	X	X	0	X	0	0
Nitrobarite	Ba(NO3)2	mineral	1	82wag/eva	X	X	0	X	0	0
Nontronite-Ca	Ca.165Fe2Al.33Si3.67H2O12	mineral	1	78wol	X	X	0	0	0	0
Nontronite-Cs	Cs.33Si4Fe1.67Mg.33H2O12	mineral	1	88db 4	X	X	0	0	0	0
Nontronite-H	H.33Fe2Al.33Si3.67H2O12	mineral	1	78wol	X	X	0	0	0	0
Nontronite-K	K.33Fe2Al.33Si3.67H2O12	mineral	1	78wol	X	X	0	0	0	0
Nontronite-Mg	Mg.165Fe2Al.33Si3.67H2O12	mineral	1	78wol	X	X	0	0	0	0
Nontronite-Na	Na.33Fe2Al.33Si3.67H2O12	mineral	1	78wol	X	X	0	0	0	0
Np		mineral	1	84lem	X	X	0	0	0	0
Np(HPO4)2		mineral	1	84lem	X	X	0	0	0	0
Np(HPO4)2		mineral	3	84lem	0	0	0	0	0	0
Np(OH)4		mineral	1	84lem	X	X	0	0	0	0
Np(OH)4		mineral	3	84lem	0	0	0	0	0	0
Np2O5		mineral	1	84lem	0	0	0	0	0	0
Np2O5		mineral	3	84lem	X	X	0	0	0	0
NpO2		mineral	1	84lem	X	X	0	0	0	0
NpO2		mineral	3	84lem	0	0	0	0	0	0
NpO2(OH)2		mineral	1	84lem	X	X	0	0	0	0
NpO2(OH)2		mineral	3	84lem	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
NpO2OH (am)		mineral	1	84lem	X	X	0	0	0	0
NpO2OH (am)		mineral	3	84lem	0	0	0	0	0	0
O(g)		mineral	2	89cox/wag	0	0	0	0	0	0
O2		mineral	1	supcrt92**	X	X	X	X	0	0
O2		mineral	2	89cox/wag	0	0	0	0	0	0
O2		mineral	4	84har/mol	0	0	0	0	0	X
Okenite	CaSi2O4(OH)2:H2O	mineral	1	82sar/bar	X	X	0	0	0	0
Olivine	(Fe,Mg)2SiO4	mineral	1	ss***	0	0	0	0	0	0
Orpiment	As2S3	mineral	1	82wag/eva	X	X	0	0	0	0
Orthopyroxene	(Fe,Mg)SiO3	mineral	1	ss***	X	X	0	0	0	0
Os		mineral	1	79rob/hem	0	0	0	0	0	0
Otavite	CdCO3	mineral	1	84sve	X	X	0	0	0	0
Ottemannite	Sn2S3	mineral	2	79kub/alc	X	X	0	0	0	0
Oxychloride-Mg	Mg2Cl(OH)3:4H2O	mineral	1	84har/mol	X	X	0	X	0	X
Oxychloride-Mg	Mg2Cl(OH)3:4H2O	mineral	4	84har/mol	0	0	0	X	0	X
P		mineral	2	89cox/wag	X	X	0	X	0	0
P(am)		mineral	0	92gre/fug	0	0	0	0	0	0
P(g)		mineral	2	89cox/wag	0	0	0	0	0	0
P2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
P4(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Paragonite	NaAl3Si3O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Paralaurionite	PbClOH	mineral	1	78ric/nri	X	X	0	X	0	0
Pargasite	NaCa2Al3Mg4Si6O22(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Parsonsite	Pb2UO2(PO4)2:2H2O	mineral	1	78ric/nri	X	X	0	X	0	0
Pb		mineral	2	89cox/wag	X	X	0	X	0	0
Pb(H2PO4)2		mineral	3	73nri	X	X	0	X	0	0
Pb(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Pb2SiO4		mineral	1	82wag/eva	X	X	0	0	0	0
Pb3(PO4)2		mineral	1	72nri 2	X	X	0	X	0	0
Pb3SO6		mineral	1	78ric/nri	X	X	0	X	0	0
Pb4O(PO4)2		mineral	1	72nri 2	X	X	0	X	0	0
Pb4SO7		mineral	1	78ric/nri	X	X	0	X	0	0
PbCO3 . PbO		mineral	1	82wag/eva	X	X	0	0	0	0
PbF2		mineral	1	82wag/eva	0	0	0	0	0	0
PbF2		mineral	3	76smi/mar	X	X	0	X	0	0
PbHPO4		mineral	1	74nri	X	X	0	X	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
PbSO4.2NH3		mineral	1	82wag/eva	X	X	0	X	0	0
PbSeO4		mineral	1	82wag/eva	X	X	0	0	0	0
Pd		mineral	1	79rob/hem	X	X	0	0	0	0
Pd-Oxyannite	KFe3AlSi3O10(OH)O-	mineral	1	78wol	0	0	0	0	0	0
Pd-Oxyannite	KFe3AlSi3O10(OH)O-	mineral	1	supcrt92**	0	0	0	0	0	0
Penroseite	NiSe2	mineral	2	74mil	X	X	0	0	0	0
Pentahydrite	MgSO4:5H2O	mineral	1	80har/wea	X	X	0	X	0	0
Periclase	MgO	mineral	1	supcrt92**	X	X	X	X	0	0
Periclase	MgO	mineral	2	89cox/wag	0	0	0	0	0	0
Petalite	LiAlSi4O10	mineral	1	82wag/eva	X	X	0	0	0	0
Phlogopite	KAlMg3Si3O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Phosgenite	Pb2(CO3)Cl2	mineral	1	78ric/nri	X	X	0	0	0	0
Picromerite	K2Mg(SO4)2:6H2O	mineral	1	84har/mol	X	X	0	X	0	X
Picromerite	K2Mg(SO4)2:6H2O	mineral	4	84har/mol	0	0	0	X	0	X
Pirssonite	Na2Ca(CO3)2:2H2O	mineral	1	84har/mol	X	X	0	0	0	X
Pirssonite	Na2Ca(CO3)2:2H2O	mineral	4	84har/mol	0	0	0	0	0	X
Plagioclase	CaAl2Si2O8-NaAlSi3O8	mineral	1	ss***	X	X	0	0	0	0
Plattnerite	PbO2	mineral	1	82wag/eva	X	X	0	0	0	0
Plumbogummite	PbAl3(PO4)2(OH)5:H2O	mineral	0	86jen	0	0	0	0	0	0
Plumbogummite	PbAl3(PO4)2(OH)5:H2O	mineral	3	80bal/nor	X	X	0	X	0	0
Polydymite	Ni3S4	mineral	1	78vau/cra	X	X	0	0	0	0
Polyhalite	K2MgCa2(SO4)4:2H2O	mineral	1	84har/mol	X	X	0	X	0	X
Polyhalite	K2MgCa2(SO4)4:2H2O	mineral	4	84har/mol	0	0	0	X	0	X
Portlandite	Ca(OH)2	mineral	1	79rob/hem	X	X	0	X	0	0
Portlandite	Ca(OH)2	mineral	4	84har/mol	0	0	0	0	0	X
Pr		mineral	1	79rob/hem	X	X	0	X	0	0
Prehnite	Ca2Al2Si3O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Przhevalskite	Pb(UO2)2(PO4)2	mineral	1	78lan	X	X	0	X	0	0
Pseudowollastonite	CaSiO3	mineral	2	77bar/kna	X	X	0	0	0	0
Pt		mineral	1	79rob/hem	0	0	0	0	0	0
Pu		mineral	1	86mor	X	X	0	0	0	0
Pu(HPO4)2		mineral	1	80lem/tre	X	X	0	0	0	0
Pu(HPO4)2		mineral	3	80lem/tre	0	0	0	0	0	0
Pu(OH)3		mineral	1	80lem/tre	X	X	0	0	0	0
Pu(OH)3		mineral	3	80lem/tre	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
*****		*****		*****						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Pu(OH)4		mineral	1	80lem/tre	X	X	0	0	0	0
Pu(OH)4		mineral	3	80lem/tre	0	0	0	0	0	0
Pu2O3		mineral	1	80lem/tre	X	X	0	0	0	0
Pu2O3		mineral	3	80lem/tre	0	0	0	0	0	0
Pu2O3(alpha)		mineral	1	66oet	0	0	0	0	0	0
PuF3		mineral	1	80lem/tre	X	X	0	0	0	0
PuF3		mineral	3	80lem/tre	0	0	0	0	0	0
PuF4		mineral	1	80lem/tre	X	X	0	0	0	0
PuF4		mineral	3	80lem/tre	0	0	0	0	0	0
PuO2		mineral	1	80lem/tre	X	X	0	0	0	0
PuO2		mineral	3	80lem/tre	0	0	0	0	0	0
PuO2(OH)2		mineral	1	80lem/tre	X	X	0	0	0	0
PuO2(OH)2		mineral	3	80lem/tre	0	0	0	0	0	0
PuO2HPO4		mineral	1	80lem/tre	X	X	0	0	0	0
PuO2HPO4		mineral	3	80lem/tre	0	0	0	0	0	0
PuO2OH(am)		mineral	1	80lem/tre	X	X	0	0	0	0
PuO2OH(am)		mineral	3	80lem/tre	0	0	0	0	0	0
Pyrite	FeS2	mineral	0	chemval*	0	0	0	0	0	0
Pyrite	FeS2	mineral	1	supcrt92**	X	X	X	0	0	0
Pyrite	FeS2	mineral	3	chemval*	0	0	0	0	0	0
Pyrolusite	MnO2	mineral	1	79rob/hem	X	X	0	X	0	0
Pyromorphite	Pb5(PO4)3Cl	mineral	1	73nri	X	X	0	X	0	0
Pyromorphite-OH	Pb5(OH)(PO4)3	mineral	1	72nri 2	X	X	0	X	0	0
Pyrope	Mg3Al2(SiO4)3	mineral	1	supcrt92**	0	0	0	0	0	0
Pyrophyllite	Al2Si4O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Pyrrhotite	FeS	mineral	1	supcrt92**	X	X	X	0	0	0
Quartz	SiO2	mineral	1	supcrt92**	X	X	X	0	0	0
Quartz	SiO2	mineral	2	89cox/wag	0	0	0	0	0	0
Ra		mineral	1	82wag/eva	X	X	0	0	0	0
Ra(NO3)2		mineral	1	82wag/eva	X	X	0	0	0	0
RaCl2:2H2O		mineral	1	82wag/eva	X	X	0	0	0	0
RaSO4		mineral	1	82wag/eva	X	X	0	0	0	0
Rankinite	Ca3Si2O7	mineral	2	77bar/kna	X	X	0	0	0	0
Rb		mineral	2	89cox/wag	X	X	0	X	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Rb(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Rb2U2O7		mineral	0	92gre/fug	0	0	0	0	0	0
Rb2UO4		mineral	2	92gre/fug	X	X	0	X	X	0
RbUO3		mineral	0	92gre/fug	0	0	0	0	0	0
Re		mineral	1	79rob/hem	X	X	0	0	0	0
Realgar	AsS	mineral	1	79rob/hem	X	X	0	0	0	0
Rh		mineral	1	79rob/hem	0	0	0	0	0	0
Rhodochrosite	MnCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Rhodonite	MnSiO3	mineral	1	79rob/hem	X	X	0	0	0	0
Richterite	Na2CaMg5Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Riebeckite	Na2Fe5Si8O22(OH)2	mineral	1	supcrt92**	0	0	0	0	0	0
Ripidolite-14A	Mg3Fe2Al2Si3O10(OH)8	mineral	1	78wol	X	X	0	0	0	0
Ripidolite-7A	Mg3Fe2Al2Si3O10(OH)8	mineral	1	78wol	X	X	0	0	0	0
Rn(g)		mineral	1	supcrt92**	X	X	X	0	0	0
Romarchite	SnO	mineral	1	supcrt92**	X	X	X	0	0	0
Romarchite	SnO	mineral	2	89cox/wag	0	0	0	0	0	0
Ru		mineral	1	85rar 1	X	X	0	0	0	0
Ru(OH)3·H2O(am)		mineral	1	85rar 1	X	X	0	0	0	0
Ru(g)		mineral	1	85rar 1	0	0	0	0	0	0
RuBr3		mineral	1	85rar 1	X	X	0	0	0	0
RuCl3		mineral	1	85rar 1	X	X	0	0	0	0
RuCl3(g)		mineral	0	85rar 1	0	0	0	0	0	0
RuI3		mineral	1	85rar 1	X	X	0	0	0	0
RuO2		mineral	1	85rar 1	X	X	0	0	0	0
RuO2·2H2O(am)		mineral	1	85rar 1	X	X	0	0	0	0
RuO3(g)		mineral	0	85rar 1	0	0	0	0	0	0
RuO4		mineral	1	85rar 1	X	X	0	0	0	0
RuO4(g)		mineral	0	85rar 1	0	0	0	0	0	0
RuO4(l)		mineral	0	85rar 1	0	0	0	0	0	0
RuSe2		mineral	0	85rar 1	0	0	0	0	0	0
RuTe2		mineral	0	85rar 1	0	0	0	0	0	0
Rutherfordine	UO2CO3	mineral	1	92gre/fug	X	X	0	0	X	0
Rutile	TiO2	mineral	1	supcrt92**	X	X	0	0	0	0
Rutile	TiO2	mineral	2	89cox/wag	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
S		mineral	2	89cox/wag	X	X	0	0	0	0
S(g)		mineral	2	89cox/wag	0	0	0	0	0	0
S2(g)		mineral	1	supcrt92**	X	X	X	0	0	0
S2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
SO2(g)		mineral	1	supcrt92**	X	X	X	X	0	0
SO2(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Safflorite	CoAs2	mineral	1	74nau/ryz	X	X	0	0	0	0
Saleeite	Mg(UO2)2(PO4)2	mineral	1	78lan	X	X	0	X	0	0
Sanbornite	BaSi2O5	mineral	1	82wag/eva	X	X	0	0	0	0
Sanidine high	KAlSi3O8	mineral	1	supcrt92**	X	X	X	0	0	0
Sanidine-ss	(K,Na)AlSi3O8	mineral	1	ss***	X	X	0	0	0	0
Saponite-Ca	Ca.165Mg3Al.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Saponite-Cs	Cs.33Si3.67Al.33Mg3O10(OH)2	mineral	1	88db 4	X	X	0	0	0	0
Saponite-H	H.33Mg3Al.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Saponite-K	K.33Mg3Al.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	10
Saponite-Mg	Mg3.165Al.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Saponite-Na	Na.33Mg3Al.33Si3.67O10(OH)2	mineral	1	78wol	X	X	0	0	0	0
Saponite-tri	(Ca.5,H,K,Mg.5,Na).33Mg3Al.3	mineral	1	ss***	X	X	0	0	0	0
Sb		mineral	1	82wag/eva	X	X	0	0	0	0
Sb		mineral	1	92gre/fug	0	0	0	0	0	0
Sb(OH)3		mineral	1	82wag/eva	X	X	0	X	0	0
Sb2O3		mineral	3	89spy/ree	X	X	0	0	0	0
Sb2O4		mineral	1	82wag/eva	X	X	0	0	0	0
Sb2O5		mineral	1	82wag/eva	X	X	0	0	0	0
Sb2S3		mineral	1	82wag/eva	0	0	0	0	0	0
Sb4O6(cubic)		mineral	1	82wag/eva	X	X	0	X	0	0
Sb4O6(orthorhombic)		mineral	1	82wag/eva	X	X	0	X	0	0
SbBr3		mineral	1	82wag/eva	X	X	0	X	0	0
SbCl3		mineral	1	79rob/hem	X	X	0	X	0	0
Sc		mineral	1	82wag/eva	X	X	0	X	0	0
Scacchite	MnCl2	mineral	1	82wag/eva	X	X	0	X	0	0
Schoepite	UO3:2H2O	mineral	1	88oha/lew	0	0	0	0	0	0
Schoepite	UO3:2H2O	mineral	2	92gre/fug	X	X	0	X	X	0
Schoepite-dehy(.393)	UO3:.393H2O	mineral	0	92gre/fug	0	0	0	0	0	0
Schoepite-dehy(.393)	UO3:.393H2O	mineral	2	88oha/lew	X	X	0	X	0	0
Schoepite-dehy(.648)	UO3:.648H2O	mineral	0	92gre/fug	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Schoepite-dehy(.648)	UO3:.648H2O	mineral	2	88oha/lew	X	X	0	X	0	0
Schoepite-dehy(.85)	UO3:.85H2O	mineral	2	88oha/lew	X	X	0	X	0	0
Schoepite-dehy(.9)	UO3:.9H2O	mineral	2	92gre/fug	X	X	0	X	X	0
Schoepite-dehy(1.0)	UO3:H2O	mineral	2	88oha/lew	X	X	0	X	0	0
Scolecite	CaAl2Si3O10:3H2O	mineral	1	83joh/flo	X	X	0	0	0	0
Se		mineral	1	79rob/hem	X	X	0	0	0	0
Se		mineral	1	92gre/fug	0	0	0	0	X	0
Se2O5		mineral	2	74mil	X	X	0	0	0	0
SeCl4		mineral	2	74mil	X	X	0	0	0	0
SeO3		mineral	2	74mil	X	X	0	0	0	0
Sellaite	MgF2	mineral	2	89cox/wag	X	X	0	X	0	0
Sepiolite	Mg4Si6O15(OH)2:6H2O	mineral	1	supcrt92**	X	X	X	0	0	0
Shcherbinaite	V2O5	mineral	1	82wag/eva	X	X	0	0	0	0
Si		mineral	2	89cox/wag	X	X	0	0	0	0
Si(g)		mineral	2	89cox/wag	X	X	0	0	0	0
SiF4(g)		mineral	2	89cox/wag	X	X	0	0	0	0
SiO2(am)		mineral	0	chemval*	0	0	0	0	0	0
SiO2(am)		mineral	1	supcrt92**	X	X	X	0	0	0
SiO2(am)		mineral	3	chemval*	0	0	0	0	0	0
Siderite	FeCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Sillimanite	Al2SiO5	mineral	1	supcrt92**	X	X	X	0	0	0
Sinjarite	CaCl2:2H2O	mineral	2	82wag/eva	0	0	0	0	0	0
Sklodowskite	Mg(H3O)2(UO2)2(SiO4)2:4H2O	mineral	1	82hem	X	X	0	0	0	0
Sm		mineral	1	79rob/hem	X	X	0	0	0	0
Smd-Celad(Fe,Al)-Ca	CaAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-Cs	CsAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-K	KAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-Li	LiAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-Mg	MgAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-Na	NaAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Fe,Al)-Sr	SrAlFeSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-Ca	CaAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-Cs	CsAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-K	KAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Smd-Celad(Mg,Al)-Li	LiAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-Mg	MgAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-Na	NaAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Celad(Mg,Al)-Sr	SrAlMgSi4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Ferripyrophyllite	Fe2Si4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Ca	CaAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Cs	CsAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-H	HA13Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-K	KA13Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Li	LiAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Mg	MgAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Na	NaAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Al)-Sr	SrAl3Si3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Ca	CaFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Cs	CsFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-H	HFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-K	KFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Li	LiFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Mg	MgFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Na	NaFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Muscovite(Fe)-Sr	SrFe2AlSi3O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smd-Pyrophyllite	Al2Si4O10(OH)2	mineral	3	viani	0	0	0	0	0	0
Smectite-Reykjanes	Mn.01K.03Na.33Ca.66Fe++.33Fe	mineral	0	78wol	0	0	0	0	0	0
Smectite-di	(Na,K,Ca.5,Mg.5).33(Al,Mg,Fe	mineral	1	ss***	X	X	0	0	0	0
Smectite-high-Fe-Mg	Ca.025Na.1K.2Fe++.5Fe+++ .2Mg	mineral	1	78wol	X	X	0	0	0	0
Smectite-low-Fe-Mg	Ca.02Na.15K.2Fe++.29Fe+++ .16	mineral	1	78wol	X	X	0	0	0	0
Smithsonite	ZnCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Sn		mineral	1	supcrt92**	X	X	X	0	0	0
Sn		mineral	2	89cox/wag	0	0	0	0	0	0
Sn(OH)2		mineral	1	82wag/eva	X	X	0	0	0	0
Sn(SO4)2		mineral	2	79kub/alc	X	X	0	0	0	0
Sn(g)		mineral	2	89cox/wag	X	X	0	0	0	0
Sn3S4		mineral	2	79kub/alc	X	X	0	0	0	0
SnBr2		mineral	2	79kub/alc	X	X	0	0	0	0
SnBr4		mineral	1	82wag/eva	X	X	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
SnCl2		mineral	2	79kub/alc	X	X	0	0	0	0
SnSO4		mineral	2	79kub/alc	X	X	0	0	0	0
SnSe		mineral	2	79kub/alc	X	X	0	0	0	0
SnSe2		mineral	2	79kub/alc	X	X	0	0	0	0
Soddyite	(UO2)2(SiO4):2H2O	mineral	1	82hem	X	X	0	0	0	0
Spessartine	Al2Mn3(SiO4)3	mineral	1	supcrt92**	0	0	0	0	0	0
Sphaerocobaltite	CoCO3	mineral	1	84sve	X	X	0	0	0	0
Sphalerite	ZnS	mineral	1	supcrt92**	X	X	X	0	0	0
Spinel	Al2MgO4	mineral	1	supcrt92**	X	X	X	X	0	0
Spinel-Co	Co3O4	mineral	2	82wag/eva	X	X	0	X	0	0
Spodumene	LiAlSi2O6	mineral	1	82wag/eva	X	X	0	0	0	0
Sr		mineral	1	79rob/hem	X	X	0	X	0	0
Sr		mineral	1	92gre/fug	0	0	0	0	X	0
Sr(NO3)2		mineral	1	79rob/hem	X	X	0	X	0	0
Sr(NO3)2		mineral	2	92gre/fug	0	0	0	0	X	0
Sr(NO3)2:4H2O		mineral	1	82wag/eva	X	X	0	X	0	0
Sr(OH)2		mineral	1	85cha/dav	X	X	0	X	0	0
Sr2SiO4		mineral	1	82wag/eva	X	X	0	0	0	0
Sr2U3O11		mineral	0	92gre/fug	0	0	0	0	0	0
Sr2UO5		mineral	0	92gre/fug	0	0	0	0	0	0
Sr3(AsO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
Sr3UO6		mineral	0	92gre/fug	0	0	0	0	0	0
SrBr2		mineral	1	82wag/eva	X	X	0	X	0	0
SrBr2:6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
SrBr2:H2O		mineral	1	82wag/eva	X	X	0	X	0	0
SrCl2		mineral	1	82wag/eva	X	X	0	X	0	0
SrCl2		mineral	2	92gre/fug	0	0	0	0	X	0
SrCl2:2H2O		mineral	1	82wag/eva	X	X	0	X	0	0
SrCl2:6H2O		mineral	1	82wag/eva	X	X	0	X	0	0
SrCl2:H2O		mineral	1	82wag/eva	X	X	0	X	0	0
SrCrO4		mineral	1	76del/hal	X	X	0	X	0	0
SrF2		mineral	1	82wag/eva	0	0	0	0	0	0
SrF2		mineral	3	76smi/mar	X	X	0	X	0	0
SrHPO4		mineral	1	82wag/eva	X	X	0	X	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
SrI2		mineral	1	85cha/dav	X	X	0	X	0	0
SrO		mineral	1	82wag/eva	X	X	0	X	0	0
SrO		mineral	2	92gre/fug	0	0	0	0	X	0
SrS		mineral	1	82wag/eva	X	X	0	0	0	0
SrSe		mineral	0	74mil	0	0	0	0	0	0
SrSeO3		mineral	3	76smi/mar	0	0	0	0	0	0
SrSeO4		mineral	0	90crc	0	0	0	0	0	0
SrSeO4		mineral	3	76smi/mar	X	X	0	0	0	0
SrSiO3		mineral	1	82wag/eva	X	X	0	0	0	0
SrU4O13		mineral	0	92gre/fug	0	0	0	0	0	0
SrUO4 (alpha)		mineral	2	92gre/fug	X	X	0	X	X	0
SrUO4 (beta)		mineral	0	92gre/fug	0	0	0	0	0	0
SrZrO3		mineral	1	74nau/ryz	X	X	0	0	0	0
Starkeyite	MgSO4:4H2O	mineral	1	80har/wea	X	X	0	X	0	0
Staurolite	Fe2Al9Si4O24H	mineral	1	supcrt92**	0	0	0	0	0	0
Stibnite	Sb2S3	mineral	3	89spy/ree	X	X	0	0	0	0
Stilbite	Ca1.019Na.136K.006Al2.18Si6.	mineral	1	90how/joh	X	X	0	0	0	0
Stilbite	Ca1.019Na.136K.006Al2.18Si6.	mineral	1	supcrt92**	0	0	0	0	0	0
Stilleite	ZnSe	mineral	1	78vau/cra	X	X	0	0	0	0
Strengite	FePO4:2H2O	mineral	1	79rob/hem	X	X	0	0	0	0
Strontianite	SrCO3	mineral	0	chemval*	0	0	0	0	0	0
Strontianite	SrCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Strontianite	SrCO3	mineral	3	chemval*	0	0	0	0	0	0
Sylvite	KCl	mineral	1	supcrt92**	X	X	X	X	0	0
Sylvite	KCl	mineral	4	84har/mol	0	0	0	0	0	X
Syngenite	K2Ca(SO4)2:H2O	mineral	1	84har/mol	X	X	0	X	0	X
Syngenite	K2Ca(SO4)2:H2O	mineral	4	84har/mol	0	0	0	X	0	X
Ta		mineral	1	79rob/hem	0	0	0	0	0	0
Tachyhydrite	Mg2CaCl6:12H2O	mineral	1	84har/mol	X	X	0	X	0	X
Tachyhydrite	Mg2CaCl6:12H2O	mineral	4	84har/mol	0	0	0	X	0	X
Talc	Mg3Si4O10(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Tarapacaite	K2CrO4	mineral	2	76del/hal	X	X	0	X	0	0
Tb		mineral	1	79rob/hem	X	X	0	X	0	0
Tc		mineral	1	83rar	X	X	0	X	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Tc(OH)2		mineral	1	83rar	X	X	0	0	0	0
Tc(OH)3		mineral	1	83rar	X	X	0	0	0	0
Tc2O7		mineral	1	83rar	X	X	0	0	0	0
Tc2O7(g)		mineral	1	83rar	X	X	0	0	0	0
Tc2S7		mineral	2	83rar	X	X	0	0	0	0
Tc3O4		mineral	1	83rar	X	X	0	0	0	0
Tc4O7		mineral	1	83rar	X	X	0	0	0	0
TcF6		mineral	0	83rar	0	0	0	0	0	0
TcF6(g)		mineral	0	83rar	0	0	0	0	0	0
TcO2:2H2O(am)		mineral	1	83rar	X	X	0	0	0	0
TcO3		mineral	2	83rar	X	X	0	0	0	0
TcO3Cl(g)		mineral	0	83rar	0	0	0	0	0	0
TcOH		mineral	1	83rar	X	X	0	0	0	0
TcS2		mineral	2	83rar	X	X	0	0	0	0
TcS3		mineral	2	83rar	X	X	0	0	0	0
Te		mineral	1	79rob/hem	0	0	0	0	0	0
Te		mineral	1	92gre/fug	0	0	0	0	0	0
Tenorite	CuO	mineral	1	supcrt92**	X	X	X	X	0	0
Tephroite	Mn2SiO4	mineral	1	82wag/eva	X	X	0	0	0	0
Th		mineral	2	89cox/wag	X	X	0	X	0	0
Th(NO3)4:5H2O		mineral	1	82wag/eva	X	X	0	X	0	0
Th(OH)4		mineral	1	74nau/ryz	X	X	0	X	0	0
Th(SO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
Th(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Th2S3		mineral	1	82wag/eva	X	X	0	0	0	0
Th2Se3		mineral	2	74mil	X	X	0	0	0	0
Th7S12		mineral	1	82wag/eva	X	X	0	0	0	0
ThBr4		mineral	1	82wag/eva	X	X	0	X	0	0
ThCl4		mineral	1	80lan/her	X	X	0	X	0	0
ThF4		mineral	1	80lan/her	X	X	0	X	0	0
ThF4:2.5H2O		mineral	1	82wag/eva	X	X	0	X	0	0
ThI4		mineral	1	82wag/eva	X	X	0	X	0	0
ThS		mineral	1	82wag/eva	X	X	0	0	0	0
ThS2		mineral	1	82wag/eva	X	X	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Thenardite	Na2SO4	mineral	1	79rob/hem	X	X	0	X	0	0
Thenardite	Na2SO4	mineral	4	84har/mol	0	0	0	0	0	X
Thermonatrite	Na2CO3:H2O	mineral	1	82wag/eva	X	X	0	0	0	0
Thermonatrite	Na2CO3:H2O	mineral	4	84har/mol	0	0	0	0	0	X
Thorianite	ThO2	mineral	2	89cox/wag	X	X	0	X	0	0
Ti		mineral	2	89cox/wag	X	X	0	0	0	0
Ti(g)		mineral	2	89cox/wag	X	X	0	0	0	0
TiCl4(g)		mineral	2	89cox/wag	X	X	0	0	0	0
Tiemannite	HgSe	mineral	2	78vau/cra	X	X	0	0	0	0
Titanite	CaTiSiO5	mineral	1	supcrt92**	X	X	0	0	0	0
Tl		mineral	1	79rob/hem	X	X	0	X	0	0
Tl2CrO4		mineral	0	76del/hal	0	0	0	0	0	0
Tm		mineral	1	79rob/hem	X	X	0	X	0	0
Tobermorite-11A	Ca5Si6H11O22.5	mineral	1	82sar/bar	X	X	0	0	0	0
Tobermorite-14A	Ca5Si6H21O27.5	mineral	1	82sar/bar	X	X	0	0	0	0
Tobermorite-9A	Ca5Si6H6O20	mineral	1	82sar/bar	X	X	0	0	0	0
Todorokite	Mn7O12:3H2O	mineral	1	83ker	X	X	0	X	0	0
Torbernite	Cu(UO2)2(PO4)2	mineral	1	78lan	X	X	0	X	0	0
Tremolite	Ca2Mg5Si8O22(OH)2	mineral	1	supcrt92**	X	X	X	0	0	0
Trevorite	NiFe2O4	mineral	1	79rob/hem	X	X	0	0	0	0
Tridymite	SiO2	mineral	1	82wag/eva	X	X	0	0	0	0
Troilite	FeS	mineral	1	79rob/hem	X	X	0	0	0	0
Trona	Na3H(CO3)2:2H2O	mineral	0	84har/mol	0	0	0	0	0	X
Trona	Na3H(CO3)2:2H2O	mineral	4	84har/mol	0	0	0	0	0	X
Trona-K	K2NaH(CO3)2:2H2O	mineral	1	84har/mol	X	X	0	0	0	X
Trona-K	K2NaH(CO3)2:2H2O	mineral	4	84har/mol	0	0	0	0	0	X
Tsumebite	Pb2Cu(PO4)(OH)3:3H2O	mineral	3	80bal/nor	X	X	0	X	0	0
Tyuyamunite	Ca(UO2)2(VO4)2	mineral	1	78lan	X	X	0	0	0	0
U		mineral	2	89cox/wag	X	X	0	X	0	0
U(CO3)2		mineral	1	92gre/fug	X	X	0	0	X	0
U(HPO4)2:4H2O		mineral	1	92gre/fug	X	X	0	0	X	0
U(OH)2SO4		mineral	1	92gre/fug	X	X	0	0	X	0
U(OH)3		mineral	3	80all/kip	0	0	0	0	0	0
U(OH)4		mineral	3	80all/kip	0	0	0	0	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
U(SO3)2		mineral	2	92gre/fug	X	X	0	0	X	0
U(SO4)2		mineral	2	92gre/fug	X	X	0	0	X	0
U(SO4)2:4H2O		mineral	2	92gre/fug	X	X	0	0	0	0
U(SO4)2:8H2O		mineral	2	92gre/fug	X	X	0	0	X	0
U(g)		mineral	2	89cox/wag	X	X	0	0	0	0
U2C3		mineral	2	92gre/fug	X	X	0	0	X	0
U2Cl10(g)		mineral	1	92gre/fug	X	X	0	0	X	0
U2Cl8(g)		mineral	2	92gre/fug	X	X	0	0	X	0
U2F10(g)		mineral	2	92gre/fug	X	X	0	0	X	0
U2F9		mineral	1	92gre/fug	X	X	0	0	X	0
U2O2C15		mineral	2	92gre/fug	X	X	0	0	X	0
U2O3F6		mineral	2	92gre/fug	X	X	0	X	X	0
U2S3		mineral	2	92gre/fug	X	X	0	0	X	0
U2S5		mineral	0	92gre/fug	0	0	0	0	0	0
U2Se3		mineral	2	92gre/fug	X	X	0	0	X	0
U3As4		mineral	2	92gre/fug	X	X	0	0	X	0
U3O5F8		mineral	2	92gre/fug	X	X	0	X	X	0
U3O7(alpha)		mineral	0	92gre/fug	0	0	0	0	0	0
U3O8		mineral	2	89cox/wag	0	0	0	0	0	0
U3O8(alpha)		mineral	0	chemval*	0	0	0	0	0	0
U3O8(alpha)		mineral	3	chemval*	0	0	0	0	0	0
U3P4		mineral	2	92gre/fug	X	X	0	0	X	0
U3S5		mineral	2	92gre/fug	X	X	0	0	X	0
U3Sb4		mineral	2	92gre/fug	X	X	0	0	0	0
U3Se4		mineral	2	92gre/fug	X	X	0	0	X	0
U3Se5		mineral	2	92gre/fug	X	X	0	0	X	0
U4F17		mineral	1	92gre/fug	X	X	0	0	X	0
U4O9		mineral	0	chemval*	0	0	0	0	0	0
U4O9		mineral	3	chemval*	0	0	0	0	0	0
U4Sb3		mineral	0	92gre/fug	0	0	0	0	0	0
U5O12Cl		mineral	2	92gre/fug	X	X	0	0	X	0
UAs		mineral	2	92gre/fug	X	X	0	0	X	0
UAs2		mineral	2	92gre/fug	X	X	0	X	X	0
UAsO5		mineral	0	92gre/fug	0	0	0	0	0	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UAsS		mineral	0	92gre/fug	0	0	0	0	0	0
UAsSe		mineral	0	92gre/fug	0	0	0	0	0	0
UAsTe		mineral	0	92gre/fug	0	0	0	0	0	0
UBr(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UBr2(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UBr2Cl		mineral	2	92gre/fug	X	X	0	0	X	0
UBr2Cl2		mineral	2	92gre/fug	X	X	0	0	X	0
UBr2I2		mineral	0	92gre/fug	0	0	0	0	0	0
UBr3		mineral	2	92gre/fug	X	X	0	0	0	0
UBr3(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UBr3Cl		mineral	2	92gre/fug	X	X	0	0	X	0
UBr3I		mineral	0	92gre/fug	0	0	0	0	0	0
UBr4		mineral	2	92gre/fug	X	X	0	0	X	0
UBr4(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UBr5		mineral	2	92gre/fug	X	X	0	0	X	0
UBr5(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UBrCl2		mineral	2	92gre/fug	X	X	0	0	X	0
UBrCl3		mineral	2	92gre/fug	X	X	0	0	X	0
UBrI3		mineral	0	92gre/fug	0	0	0	0	0	0
UC		mineral	1	92gre/fug	X	X	0	0	X	0
UC1.94(alpha)		mineral	1	92gre/fug	X	X	0	0	X	0
UC1(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UC12(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UC12F2		mineral	2	92gre/fug	X	X	0	0	X	0
UC12I2		mineral	2	92gre/fug	X	X	0	0	X	0
UC13		mineral	2	92gre/fug	X	X	0	0	X	0
UC13(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UC13F		mineral	2	92gre/fug	X	X	0	0	X	0
UC13I		mineral	2	92gre/fug	X	X	0	0	X	0
UC14		mineral	2	92gre/fug	X	X	0	0	X	0
UC14(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UC15		mineral	2	92gre/fug	X	X	0	0	X	0
UC15(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UC16		mineral	2	92gre/fug	X	X	0	X	X	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UC16(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UC1F3		mineral	2	92gre/fug	X	X	0	0	X	0
UC1I3		mineral	2	92gre/fug	X	X	0	0	X	0
UF(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UF2(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UF3		mineral	2	92gre/fug	X	X	0	0	X	0
UF3(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UF4		mineral	2	92gre/fug	X	X	0	0	X	0
UF4		mineral	3	80lem/tre	0	0	0	0	0	0
UF4(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UF4:2.5H2O		mineral	2	92gre/fug	X	X	0	0	X	0
UF5(alpha)		mineral	2	92gre/fug	X	X	0	0	X	0
UF5(beta)		mineral	2	92gre/fug	X	X	0	0	X	0
UF5(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UF6		mineral	2	92gre/fug	X	X	0	X	X	0
UF6(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UH3(beta)		mineral	2	92gre/fug	X	X	0	0	X	0
UI(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UI2(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UI3		mineral	2	92gre/fug	X	X	0	0	X	0
UI3(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UI4		mineral	2	92gre/fug	X	X	0	0	X	0
UI4(g)		mineral	2	92gre/fug	X	X	0	0	X	0
UN		mineral	2	92gre/fug	X	X	0	0	X	0
UN1.466(beta)		mineral	0	92gre/fug	0	0	0	0	0	0
UN1.59(alpha)		mineral	2	92gre/fug	X	X	0	0	X	0
UN1.606(alpha)		mineral	0	92gre/fug	0	0	0	0	0	0
UN1.674(alpha)		mineral	0	92gre/fug	0	0	0	0	0	0
UN1.73(alpha)		mineral	2	92gre/fug	X	X	0	0	X	0
UO(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(AsO3)2		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(IO3)2		mineral	1	92gre/fug	X	X	0	0	X	0
UO2(NO3)2		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(NO3)2:2H2O		mineral	1	92gre/fug	X	X	0	X	X	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO2(NO3)2:3H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(NO3)2:6H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(NO3)2:H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(OH)2		mineral	0	chemval*	0	0	0	0	0	0
UO2(OH)2		mineral	3	chemval*	0	0	0	0	0	0
UO2(OH)2(beta)		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(OH)2(beta)		mineral	3	80lem/tre	0	0	0	0	0	0
UO2(OH)2(gamma)		mineral	0	92gre/fug	0	0	0	0	0	0
UO2(OH)2(gamma)		mineral	3	80lem/tre	0	0	0	0	0	0
UO2(PO3)2		mineral	2	92gre/fug	X	X	0	X	X	0
UO2(am)		mineral	1	781an	0	0	0	0	0	0
UO2(am)		mineral	1	92gre/fug	X	X	0	0	X	0
UO2(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UO2.25		mineral	2	92gre/fug	X	X	0	0	X	0
UO2.25(beta)		mineral	2	92gre/fug	X	X	0	0	0	0
UO2.3333(alpha)		mineral	0	92gre/fug	0	0	0	0	0	0
UO2.3333(beta)		mineral	2	92gre/fug	X	X	0	0	X	0
UO2.6667		mineral	2	92gre/fug	X	X	0	0	X	0
UO2.86:.5H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UO2.86:1.5H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UO2Br2		mineral	2	92gre/fug	X	X	0	X	X	0
UO2Br2:3H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2Br2:H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2BrOH:2H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2CO3		mineral	0	chemval*	0	0	0	0	0	0
UO2CO3		mineral	1	92gre/fug	X	X	0	0	X	0
UO2CO3		mineral	3	chemval*	0	0	0	0	0	0
UO2C1		mineral	2	92gre/fug	X	X	0	0	X	0
UO2C12		mineral	2	92gre/fug	X	X	0	X	X	0
UO2C12(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UO2C12:3H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2C12:H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2C1OH:2H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2F2		mineral	2	92gre/fug	X	X	0	X	X	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO2F2 (g)		mineral	2	92gre/fug	X	X	0	X	X	0
UO2F2:3H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO2FOH		mineral	1	92gre/fug	X	X	0	X	X	0
UO2FOH:2H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2FOH:H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2HPO4		mineral	3	84tri	0	0	0	0	0	0
UO2HPO4:4H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2OH		mineral	3	80all/kip	0	0	0	0	0	0
UO2SO3		mineral	2	92gre/fug	X	X	0	0	X	0
UO2SO4		mineral	0	chemval*	0	0	0	0	0	0
UO2SO4		mineral	2	92gre/fug	X	X	0	X	X	0
UO2SO4		mineral	3	chemval*	0	0	0	0	0	0
UO2SO4:2.5H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2SO4:3.5H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2SO4:3H2O		mineral	1	92gre/fug	X	X	0	X	X	0
UO2SO4:H2O		mineral	1	64owe/may	X	X	0	X	0	0
UO2SeO3		mineral	0	92gre/fug	0	0	0	0	0	0
UO2SeO4		mineral	0	92gre/fug	0	0	0	0	0	0
UO2TeO3		mineral	0	92gre/fug	0	0	0	0	0	0
UO3(alpha)		mineral	0	chemval*	0	0	0	0	0	0
UO3(alpha)		mineral	2	92gre/fug	X	X	0	X	X	0
UO3(alpha)		mineral	3	chemval*	0	0	0	0	0	0
UO3(am)		mineral	0	92gre/fug	0	0	0	0	0	0
UO3(beta)		mineral	2	92gre/fug	X	X	0	X	X	0
UO3(delta)		mineral	0	92gre/fug	0	0	0	0	0	0
UO3(epsilon)		mineral	0	92gre/fug	0	0	0	0	0	0
UO3(g)		mineral	2	92gre/fug	X	X	0	X	X	0
UO3(gamma)		mineral	0	chemval*	0	0	0	0	0	0
UO3(gamma)		mineral	2	89cox/wag	X	X	0	X	0	0
UO3(gamma)		mineral	3	chemval*	0	0	0	0	0	0
UO3:.393H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UO3:.648H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UO3:.85H2O(alpha)		mineral	0	92gre/fug	0	0	0	0	0	0
UO3:.9H2O(alpha)		mineral	2	92gre/fug	X	X	0	X	X	0

SPECIES		DATA		EQ3/6 DATAFILES						
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
UO3:2H2O		mineral	0	chemval*	0	0	0	0	0	0
UO3:2H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UO3:2H2O		mineral	3	chemval*	0	0	0	0	0	0
UO4:2H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UO4:4H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UOBr2		mineral	2	92gre/fug	X	X	0	0	X	0
UOBr3		mineral	2	92gre/fug	X	X	0	0	X	0
UOCl		mineral	2	92gre/fug	X	X	0	0	X	0
UOCl2		mineral	2	92gre/fug	X	X	0	0	X	0
UOCl3		mineral	2	92gre/fug	X	X	0	0	X	0
UOF2		mineral	2	92gre/fug	X	X	0	0	X	0
UOF2:H2O		mineral	2	92gre/fug	X	X	0	X	X	0
UOF4		mineral	2	92gre/fug	X	X	0	X	X	0
UOF4 (g)		mineral	2	92gre/fug	X	X	0	0	X	0
UOFOH		mineral	2	92gre/fug	X	X	0	X	X	0
UOFOH:.5H2O		mineral	0	92gre/fug	0	0	0	0	0	0
UOTe		mineral	2	92gre/fug	X	X	0	0	X	0
UP		mineral	2	92gre/fug	X	X	0	X	X	0
UP2		mineral	2	92gre/fug	X	X	0	X	X	0
UP2O7		mineral	2	92gre/fug	X	X	0	X	X	0
UP2O7:20H2O		mineral	1	92gre/fug	X	X	0	0	X	0
UPO5		mineral	2	92gre/fug	X	X	0	0	X	0
US		mineral	2	92gre/fug	X	X	0	0	X	0
US1.9		mineral	2	92gre/fug	X	X	0	0	X	0
US2		mineral	2	92gre/fug	X	X	0	0	X	0
US3		mineral	2	92gre/fug	X	X	0	0	0	0
USb		mineral	2	92gre/fug	X	X	0	0	0	0
USb2		mineral	2	92gre/fug	X	X	0	0	X	0
USe		mineral	2	92gre/fug	X	X	0	0	X	0
USe2(alpha)		mineral	2	92gre/fug	X	X	0	0	X	0
USe2(beta)		mineral	2	92gre/fug	X	X	0	0	X	0
USe3		mineral	2	92gre/fug	X	X	0	0	X	0
Umangite	Cu3Se2	mineral	2	74mil	X	X	0	0	0	0
Uramphite	(NH4)(UO2)(PO4):3H2O	mineral	1	78lan	0	0	0	0	0	0



SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
Uraninite	UO2	mineral	0	chemval*	0	0	0	0	0	0
Uraninite	UO2	mineral	2	89cox/wag	X	X	0	X	0	0
Uraninite	UO2	mineral	3	chemval*	0	0	0	0	0	0
Uranocircite	Ba(UO2)2(PO4)2	mineral	1	78lan	X	X	0	X	0	0
Uranophane	Ca(UO2)2(SiO3)2(OH)2	mineral	1	78lan	X	X	0	X	0	0
V		mineral	1	79rob/hem	X	X	0	0	0	0
V2O4		mineral	1	82wag/eva	X	X	0	0	0	0
V3O5		mineral	1	82wag/eva	X	X	0	0	0	0
V4O7		mineral	1	82wag/eva	X	X	0	0	0	0
Vaesite	NiS2	mineral	1	78vau/cra	X	X	0	0	0	0
Vaterite	CaCO3	mineral	0	79rob/hem	0	0	0	0	0	0
Villiaumite	NaF	mineral	0	79rob/hem	0	0	0	0	0	0
Vivianite	Fe3(PO4)2·8H2O	mineral	1	87woo/gar	X	X	0	X	0	0
W		mineral	1	79rob/hem	X	X	0	0	0	0
Wairakite	CaAl2Si4O10(OH)4	mineral	1	supcrt92**	X	X	X	0	0	0
Weeksite	K2(UO2)2Si6O15·4H2O	mineral	1	82hem	X	X	0	0	0	0
Whitlockite	Ca3(PO4)2	mineral	1	79rob/hem	X	X	0	X	0	0
Wilkmanite	Ni3Se4	mineral	1	78vau/cra	X	X	0	0	0	0
Witherite	BaCO3	mineral	1	supcrt92**	X	X	X	0	0	0
Wollastonite	CaSiO3	mineral	1	supcrt92**	X	X	X	0	0	0
Wurtzite	ZnS	mineral	1	supcrt92**	X	X	X	0	0	0
Wustite	Fe.9470	mineral	1	82wag/eva	X	X	0	0	0	0
Xe(g)		mineral	1	supcrt92**	X	X	X	0	0	0
Xe(g)		mineral	2	89cox/wag	0	0	0	0	0	0
Xonotlite	Ca6Si6O17(OH)2	mineral	1	82sar/bar	X	X	0	0	0	0
Y		mineral	1	79rob/hem	X	X	0	X	0	0
Yb		mineral	1	79rob/hem	X	X	0	0	0	0
Zincite	ZnO	mineral	1	supcrt92**	0	0	0	0	0	0
Zincite	ZnO	mineral	2	89cox/wag	X	X	0	X	0	0
Zircon	ZrSiO4	mineral	1	79rob/hem	X	X	0	0	0	0
Zn		mineral	2	89cox/wag	X	X	0	X	0	0
Zn(g)		mineral	2	89cox/wag	X	X	0	X	0	0
Zn3(AsO4)2		mineral	1	82wag/eva	X	X	0	X	0	0
ZnCr2O4		mineral	1	76del/hal	X	X	0	X	0	0

SPECIES			DATA		EQ3/6 DATAFILES					
NAME	COMPOSITION	TYPE	TYPE	LIT. SOURCE	COM	ALT	SUP	PIT	NEA	HMW
ZnF2		mineral	1	82wag/eva	X	X	0	X	0	0
ZnSeO3:H2O		mineral	1	82wag/eva	X	X	0	0	0	0
Zoisite	Ca2Al3(SiO4)3OH	mineral	1	supcrt92**	X	X	X	0	0	0
Zr		mineral	1	79rob/hem	X	X	0	0	0	0
o-Phthalic acid	C8H6O4	mineral	2	70kar/kar	X	X	0	0	0	0

FOOTNOTES:

- \* Species contained in the chemval database are a special case in that the properties stored (logK data for electron-bearing dissociation reactions and standard molal enthalpies of these reactions) are unique for GEMBOCHS (and EQ3/6). Hence, the misleading appearance of a zero data type for the reaction enthalpy data. Chemval species are only output to a separate dedicated file.
- \*\* The reference for supcrt92 is Johnson, Oelkers, and Helgeson (1992) [92joh/oel].
- \*\*\* The standard molal thermodynamic properties of these solid solutions are computed using various site mixing models together with data for their end-member components.

Table B2: GEMBOCHS references

SQUIBB REF	AUTHOR	TITLE	PUBLISHER	VOL.	PAGES
70abb	Abbasov, A.S.	Evaluation of the thermodynamic properties of some III-V compounds	Teddington, Natl. Phys. Lab., DSC Rep. 8		12p
76abr/ber	Abrahams, S.C., Bernstein, J.L., and Nassau, K.	Transition metal iodates. VII. crystallographic and nonlinear optic survey of the 4f-iodates	J. Solid State Chem.	16	173-184
63ada/kel	Adami, L., and Kelley, K.	Heats of formations of two crystalline hydrates of ferrous sulfate	U.S. Bur. Mines Rep. Inv. 6260		7
67ahr	Ahrland, S.	Enthalpy and entropy changes by formation of different types of complexes	Helv. Chim. Acta	50	306-318
71ahr/kul1	Ahrland, S., and Kullberg, L.	Thermodynamics of metal complex formation in aqueous solution. I. A potentiometric study of fluoride complexes of hydrogen, uranium(VI), and vanadium(IV)	Acta Chem. Scand.	25	3457-3470
71ahr/kul2	Ahrland, S., and Kullberg, L.	Thermodynamics of metal complex formation in aqueous solution. II. A calorimetric study of flouride complexes of hydrogen, uranium(VI), and vanadium(IV)	Acta Chem. Scand.	25	3471-3483
80all/kip	Allard, B., Kipatsi, H., and Liljenzin, J.O.	Expected species of Uranium, Neptunium and Plutonium in neutral aqueous solutions	J. Inorg. Nuql. Chem.	42	1015-1027
77and/new	Anderson, P.A.M., Newton, R.C., and Kleppa, O.J.	The enthalpy change of the andalusite-sillimanite reaction and the Al <sub>2</sub> SiO <sub>5</sub> diagram	Amer. J. Sci.	277	585-593

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68arn	Arnek, R.	Thermochemical studies of hydrolytic reactions	Acta Chem. Scand.	4	1102-1106
82arn/sig	Arnorsson, S., Sigurdsson, S., and Svavarsson, H.	The chemistry of geothermal waters in Iceland. I. Calculation of aqueous speciation from 0 to 370degC	Geochim. Cosmochim. Acta	46	1513-1532
75aru	Aruga, R.	Thermodynamics of ion pairing of nitrate and chlorate with metal ions in aqueous solution	J. Chem. Soc. Dalton Trans.		2534-2538
68azi/lyl	Aziz, A., Lyle, S., and Naqvi, S.	Chemical equilibria in americium and curium sulphate and oxalate systems and an application of a liquid scintillation counting method	J. Inorg. Nucl. Chem.	30	1013-1018
69azi/lyl1	Aziz, A., and Lyle, S.	Equilibrium constants for aqueous fluoro complexes of scandium, yttrium, americium(III) and curium(III) by extraction into di-2-ethylhexyl phosphoric acid	J. Inorg. Nucl. Chem.	31	3471-3480
69azi/lyl2	Aziz, A., and Lyle, S.J.	Applications of the fluoride-sensitive electrode to the study of metal-fluoride ion association constants	Analyt. Chim. Acta	47	49-56
59bab/mch	Babushkin, W.I., and Mchedlov-Petrosyan, O.P.	Thermodynamics of the reactions in the systems: Ca(OH)2-SiO2-H2O, B-C2S-H2O and C3S-H2O under normal and hydrothermal conditions	Silikattechnik	10	605-609
76bae/mes	Baes, C.F.Jr., and Mesmer, R.E.	The hydrolysis of cations	Wiley-Interscience, New York		489p

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76bag/ram1	Bagawde, S.V., Ramakrishna, V.V., and Patil, S.K.	Aqueous TTA complexing of Np(IV) and Pu(IV)	J. Inorg. Nucl. Chem.	38	2085-2089
76bag/ram2	Bagawde, S.V., Ramakrishna, V.V., and Patil, S.K.	Complexing of tetravalent plutonium in aqueous solutions	J. Inorg. Nucl. Chem.	38	1339-1345
71bai/lar	Bailey, A.R., and Larson, J.W.	Heats of dilution and the thermodynamics of dissociation of uranyl and vanadyl sulfates	J. Phys. Chem.	75	2368-2372
79bal/jen	Ball, J.W., Jenne, E.A., and Nordstrom, D.K.	WATEQ2 - A computerized chemical model for trace and major element speciation and mineral equilibria of natural waters, in Jenne, E.A., ed., Chemical modeling in aqueous systems: Speciation, sorption, solubility, and kinetics	ACS Symp. Ser. 93, Amer. Chem. Soc., Washington		815-835
80bal/nor	Ball, J.W., Nordstrom, D.K., and Jenne, E.A.	Additional and revised thermochemical data and computer code for WATEQ2 - A computerized chemical model for trace and major element speciation and mineral equilibria of natural waters	U.S.G.S. Water Res. Inv. 78-116		109p
65bar	Barany, R.	Heats of formation of goethite ferrous vanadate, and manganese molybdate	U.S. Bur. Mines Rep. Inv. 6618		10
65bar/ada	Barany, R., and Adami, L.H.	Heats of formation of anhydrous ferric sulfate and indium sulfate	U.S. Bur. Mines Rep. Inv. 6687		8p

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81bar/lan	Barnes, H.L. and Langmuir, D.	Thermochemical data for substances at 25degC and 1 atm total pressure	Unpub. Bur. Mines Rep.		
60bar	Barton, P., and Bethke, P.	Thermodynamic properties of some synthetic zinc and copper minerals	Amer. J. Sci.	258-	21-34
70bas/smi	Baskin, Y., and Smith, S.D.	Enthalpy of formation data on compounds of uranium with groups Va and VIa elements	J. Nucl. Matl.	37	209-222
77bas	Bassett, R.L.	The geochemistry of boron in thermal waters	Unpub. Ph.D. Diss., Stanford Univ., Stanford, CA		290p
80bas	Bassett, R.L.	A critical evaluation of the thermodynamic data for boron ions, ion pairs, complexes, and polyanions in aqueous solution at 298.15 k and 1 bar	Geochim. Cosmochim. Acta	44	1151-1160
72bat/luk	Batsanova, L.R., and Lukina, L.V.	Structure of "hydrated" rare earth element trifluorides	Russ. J. Inorg. Chem.	17(5)	629-631
81bau	Bauman, J.E.	Thermodynamic measurements of carbonate equilibria involving metal ions, in Gokcen, N.A., Mrazek, R.V., and Pankratz, L.B., eds., Techniques for measurement of thermodynamic properties	U.S. Bur. Mines Rep. Inv. 8853		268-274

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79bel/dob	Belyaev, Y.I., Dobretsov, V.N., and Ustinov, V.A.	Enthalpy and heat capacity of Np2O5 over the temperature range 350-759K	Sov. Radiochem. (Engl. transl.)	21	386-387
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60ber/new	Berman, H.A., and Newman, E.S.	Heat of formation of calcium trisulfoaluminate at 25degC	Proc. 4th Intl. Symp. Chem. Cement		247-257
88ber	Berman, R.G.	Internally-consistent thermodynamic data for minerals in the system Na2O- K2O-CaO-MgO-FeO-Fe2O3-Al2O3- SiO2-TiO2-H2O-CO2	J. Petrol.	29	445-522
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82bil/sch	Bilinski, H., and Schindler, P.	Solubility and equilibrium constants of lead in carbonate solutions (25degC, I=0.3 mol/dm <sup>3</sup> )	Geochim. Cosmochim. Acta	46	921-928
73bil/stu	Bilinski, H., and Stumm, W.	Pb(II)-species in natural waters	Swiss Fed. Inst. Tech., EAWAG News no. 1		2-3
68bil/cot	Bills, F., and Cotton, F.	The heat of formation of germanium dioxide	J. Phys. Chem.	68	802-805
77bir/hel	Bird, D.K., and Helgeson, H.C.	Prediction of the chemical characteristics of geothermal reservoir fluids from authigenic mineral assemblages	Geol. Soc. Amer. Abs. Prog.	9	898-899
51boc	Bochirol, L.	Chaleur specifique vraie des ferrites de zinc, de nickel et de cobalt	Compt. Rend.	232	1474-1477
72bon/hef	Bond, A.M., and Hefter, G.	A study of the weak fluoride complexes of the divalent first row transition metal ions with a fluoride ion- selective electrode	J. Inorg. Nucl. Chem.	34	603-607
70bon/tay	Bond, A.M., and Taylor, R.J.	Polarographic studies of the fluoride complexes of Tin(II) in neutral and acidic media	J. Electroanal. Chem.	28	207-215



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93bou/kna	Bourcier, W.L., Knauss, K.G., and Jackson, K.J.	Aluminum hydrolysis constants to 250degC from boehmite solubility measurements	Geochim. Cosmochim. Acta	57	747-762
87bou/bar	Bourcier, W.L., and Barnes, H.L.	Ore solution chemistry. VII. Stabilities of chloride and bisulfide complexes of zinc to 350degC	Econ. Geol.	82	1839-1863
83bow/hel	Bowers, T.S., and Helgeson, H.C.	Calculation of the thermodynamic and geochemical consequences of nonideal mixing in the system H2O-CO2-NaCl on phase relations in geologic systems: equation of state for H2O-CO2-NaCl fluids at high pressures and temperatures	Geochim. Cosmochim. Acta	47	1247-1275
65bri	Bricker, O.	Some stability relations in the system Mn-O2-H2O at 25degC and one atmosphere total pressure	Amer. Mineral.	50	1296-1354
58bro/gia	Brodale, B., and Giaouque, W.	Low temperature heat capacity and entropy of sodium sulfate decahydrate	J. Amer. Chem. Soc.	80	2042-2044
68bro	Brown, D.	Halides of the transition elements: halides of the lanthanides and actinides	Wiley, New York		199p
69bun/fuc	Bunch, T.E., and Fuchs, L.H.	A new mineral: Brezinaite Cr3S4 and the Tucson meteorite	Amer. Mineral.	54	1503-18

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72bus/bev	Buses, R.H., Bevan, R.B.jr., and Gilbert R.A.	The heat capacity of potassium pertechnetate from 10 to 310K. Entropy and Gibbs energy. Entropy of the aqueous pertechnetate ion	J. Chem. Thermo.	4	77-84
50bus/cow	Busey, G.A., and Cowan, H.D.	Behavior of plutonium(III) chloride in titrations with base and acid	LANL, LANL-1105		27p
77bus/mes	Busey, R.H., and Mesmer, R.E.	Ionization equilibria of silica acid and polysilicate formation in aqueous sodium chloride to 300degC	Inorg. Chem.	16	2444-2450
62bus	Buslaev, Y.	Instability constants of complex zirconium flourides	Russ. J. Inorg. Chem.	7	619-620
81byr/kes	Byrne, R.H., and Kester, D.R.	Ultraviolet spectroscopic study of ferric equilibria at high chloride concentrations	J. Soln. Chem.	10	51-67
87can/byr	Cantrell, K.J., and Byrne, R.H.	Temperature dependence of europium carbonate complexation	J. Soln. Chem.	16	555-566

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60car/oll	Carrel, B., and Ollin, A.	Studies on the hydrolysis of metal ions. 31. The complex formation between Pb <sup>2+</sup> and OH in Na(OH.CIO <sub>4</sub> ) medium	Acta Chem. Scand.	14	1999-2008
88cha/new	Chandratillake, M.R. Newton, G.W.A., and Robinson, V.J.	Nuclear science and technology: Chemval project; comparison of thermodynamic databases used in geochemical modeling	W.S. Atkins Engr. Sci., Epsom, Surrey, UK		
74cha/cur	Chase, M.W., Curnutt J.L., Hu, A.T., Prophet, H., Syverud A.N., and Walker, L.C.	Janaf thermochemical tables, 1974 supplement	J. Phys. Chem. Ref. Data	3	311-480
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76cho/unr	Choppin, G., and Unrein, P.	Thermodynamic study of actinide fluoride complexation in Muller, W., and Linder, R., eds., Proc. 4th Intl. Transplutonium Symp.	Baden-Baden, Germany		97-107

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56chu 2	Chukhlantsev, V.G.	Solubility products of arsenates	Russ. J. Inorg. Chem.	1	1975-82
66cla	Clark, Jr., S.P. (ed.)	Handbook of physical constants	Geol. Soc. Amer., New Haven, CN		587p
82cob/mur	Cobble, J.W., Murray R.C., Turner, P.J., and Chen, K.	High-temperature thermodynamic data for species in aqueous solution	EPRI Rep. np-2400, Res. Proj. 1167-1		186p
76cod	Codata	Recommended key values for thermodynamics	J. Chem. Thermo.	8	603-605
77cod	Codata	Recommended key values for thermodynamics	J. Chem. Thermo.	9	705-706
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86coh/tay	Cohen, E.R., and Taylor, B.N.	The 1986 adjustment of the fundamental physical constants	CODATA Bull. 63		36p
71con/mcv	Connick, R., and McVey, W.	The aqueous chemistry of zirconium	J. Amer. Chem. Soc.	71	3182-3191
47coo	Cook, O.A.	High-temperature heat contents of V2O3, V2O4, and V2O5	J. Amer. Chem. Soc.	69	331-333
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78cor/oha	Cordfunke, E.H.P., and O'Hare, P.A.G.	The chemical thermodynamics of actinide elements and compounds. III. Miscellaneous actinide compounds	Intl. Atom. Ener. Agency, Vienna		13-52

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57cou/obr	Coughlin, J.P., and O'Brien, C.J.	High temperature heat content of calcium orthosilicate	J. Phys. Chem.	61	767-769
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79cox/har	Cox, J.D., Harrop, D., and Head, A.J.	The standard enthalpy of formation of ammonium nitrate and of the nitrate ion	J. Chem. Thermo.	11	811-814
88cox/wag	Cox, J.D., Wagman, D.D., and Medvedev, V.A.	Codata key values for thermodynamics	Hemisphere Pub., New York		271p
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78cre/sus	Crerar, D.A., Susak, N.J., and Borcsik, M.	Solubility of the buffer assemblage pyrite + pyrrhotite + magnetite in NaCl solutions from 200 to 350degC	Geochim. Cosmochim. Acta	42	1427-1437

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64cri/cob2	Criss, C.M., and Cobble, J.W.	The thermodynamic properties of high temperature aqueous solutions. V. The calculation of ionic heat capacities up to 200degC. Entropies and heat capacities above 200degC	J. Amer. Chem. Soc.	86	5390-5393
88db 1	Database development group	Database additions - Smectite end member volumes	LLNL Internal Memo		
88db 2	Database development group	Clinoptilolite endmembers and clinoptilolite solid solution	LLNL Internal Memo		
89db 1	Database development group	Database changes for the zeolite heulandite	LLNL Internal Memo		
89db 2	Database development group	Clinoptilolite -- O'Hare's single point data	LLNL Internal Memo		
89db 3	Database development group	Error report and resolution for zeolite gismondine	LLNL Internal Memo		
89db 4	Database development group	Error report and resolution for species Mn(OH)3	LLNL Internal Memo		
89db 6	Database development group	Zeolite thermodynamic data	LLNL Internal memo		
89db7	Database development group	Clinoptilite solid solution end member thermodynamic data	LLNL Internal Memo		
90db 1	Database development group	Iron chloride stability constants	LLNL Internal Memo		

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90db2	Database development group	Zeolite volumes	LLNL Internal Memo		
88db 3	Database development group iii/3	Errors in computation of estimated $\Delta H_{298}$ for montmor-x endmembers of smectite-di solid solution	LLNL Internal Memo		
88db 4	Database development group iii/4	Thermodynamic data for Cs-Smectite solid solution endmembers	LLNL Internal Memo		
88db 5	Database development group vi/1	Clinoptilolite endmembers and Clinoptilolite solid solutions	LLNL Internal Memo		
88db 6	Database development group xii/1	Database changes for aluminium hydrolysis constants	LLNL Internal Memo		
63dee/how	Deer, W.A., Howie, R.A., and Zussman, J.	Rock-forming minerals, vol. 4, framework silicates	Wiley, New York		435p
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80don/lan	Dongarra, G., and Langmuir, D.	The stability of $\text{UO}_2\text{OH}^+$ and $\text{UO}_2(\text{HPO}_4)_2^{--}$ complexes at 25degC	Geochim. Cosmochim. Acta	44	1747-1751

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73don	Donnay, J.D.H., and Ondik, H.M. (eds.)	Crystal data determinative tables, 3rd ed., vol II: Inorganic compounds	U.S. Dept. Comm., NBS, JCPDS		
67dou/dit	Douglas, T.B., and Ditmars, D.A.	Measured relative enthalpy of anhydrous crystalline aluminum trifluoride, AlF <sub>3</sub> from 273 to 1173K and derived thermodynamic properties from 273 to 600K	U.S. Natl. Bur. Stds. J. Res.	71	185-193
79dou/den	Dousma, J., Den Ottelander, D., and De Bruyn, P.L.	The influence of sulfate ions on the formation of iron(III) oxides	J. Inorg. Nucl. Chem.	41	1565-1568
81dru	Drummond, S.E.	Boiling and mixing of hydrothermal fluids: Chemical effects on mineral precipitation	Unpub. Ph.D. Diss., Pennsylvania State Univ., State College PA		
61dut/gup	Dutt, N.K., and Gupta, A.	Fluorarsenates and their analogues with sulphates. Part III. Stability of fluorarsenate ion and its comparison with fluorphosphate ion	J. Indian Chem. Soc.	38	249-252
83ede/buc	Edelstein, N., Bucher, J., Silva, R., and Nitsche, H.	Thermodynamic properties of chemical species in nuclear waste	LBL Rep. LBL-4325		125p
61ega/wak	Egan, E.P., Wakefield, Z.T., and Luff, B.B.	Low temperature heat capacity, entropy and heat of formation of crystalline and colloidal ferric phosphate dihydrate	J. Phys. Chem.	65	1265-1270



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75elg/wed	Elgquist, B., and Wedborg, M.	Stability of ion pairs from gypsum solubility; Degree of ion pair formation between the major constituents of seawater	Marine Chem.	3	215-225
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76eme	Emerson, S.	Early diagenesis in anaerobic lake sediments: Chemical equilibria in interstitial waters	Geochim. Cosmochim. Acta	40	925-934
66eyr	Eyring, L. (ed.)	Progress in the science and technology of the rare earths, vol. 2	Pergamon, Oxford		p97
1887fab	Fabre, M.C.	Recherches thermiques sur les seleniures	Annuls. Chem. Phys.	10	472-550
87fei/sax	Fei, Y., and Saxena, S.K.	An equation for the heat capacity of solids	Geochim. Cosmochim. Acta	51	251-254
76fer/stu	Ferrante, B., Stuve, J., and Richardson, D.	Thermodynamic data for synthetic dawsonite	U.S. Bur. Mines Rep. Inv. 8129		13
83fer/gre	Ferri, D., Grenthe, I., Hietanen, S., and Salvatore, F.	Studies on metal Carbonate equilibria. 5. The cerium(III) carbonate complexes in aqueous perchlorate media	Acta Chem. Scand.		
76flo/osb	Flotow, H.E.; Osborn D.W., Fried, S.M., and Malm, J.G.	Heat capacity of 242-PuO <sub>2</sub> from 12 to 350K and of 244-PuO <sub>2</sub> from 4 to 25K. Entropy, enthalpy, and gibbs energy of formation of PuO <sub>2</sub> at 298.15K	J. Chem. Phys.	63	1224-1229

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63gal/stu	Galal-Gorchev, H., and Stumm, W.	The reaction of ferric iron with orthophosphate	J. Inorg. Nucl. Chem.	25	567-574
65gar/chr	Garrels, R.M., and Christ, C.L.	Solutions, Minerals, and Equilibria	Freeman Cooper, San Francisco		450
87gar/par	Garvin, D., Parker, V.B., and White, jr., H.J.	CODATA thermodynamic tables: Selections for some compounds of calcium and related mixtures: A prototype set of tables	Hemisphere Pub., New York		356p
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61gre	Green, J.H.S.	Thermodynamic properties of organic oxygen compounds	Quart. Rev.		125-153
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87haz/rob	Hazelton, H.T., Robie, R.A., and Hemingway, B.S.	Heat capacities of synthetic hedenbergite, ferrobustamite and CaFeSi2O6 glass	Geochim. Cosmochim. Acta	51	2211-2218
69hel	Helgeson, H.C.	Thermodynamics of hydrothermal systems at elevated temperatures and pressures	Amer. J. Sci.	267	729-804
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58hep	Hepler, L.G.	Thermodynamics of aqueous hydrogen chromate and dichromate ions. Heats of formation of chromates and dichromates	J. Amer. Chem. Soc.	80	6181-3
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68hub/hea	Huber, E., Head, E., and Holley, C.	The heats of formation of zirconium diboride and dioxide	J. Phys. Chem.	68	3040-3042
73hul/tur	Hull, H., and Turnbull, A.	A thermochemical study of monohydrocalcite	Geochim. Cosmochim. Acta	37	685-694
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63ing	Ingri, N.	Equilibrium studies of polyanions. 11. Polyborates in 3.0 m Na(Br), 3.0 m Li(Br) and 3.0 m K(Br), a comparison with data obtained in 3.0 m Na(ClO <sub>4</sub> )	Acta Chem. Scand.	17	581-589
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69iza/eat1	Izatt, R.M., Eatough D., Christensen, J.J., and Bartholomew, C.H.	Calorimetrically determined logK, delH <sub>0</sub> , and delS <sub>0</sub> values for the interaction of sulphate ion with H <sup>+</sup> , Na <sup>+</sup> , and K <sup>+</sup> in the presence of tetra-n- alkyl-ammonium ions	J. Chem. Soc. A		45-47
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84jac/hel	Jackson, K.J., and Helgeson, H.C.	Chemical and thermodynamic constraints on the hydrothermal transport and deposition of Tin. I. Calculation of the solubility of cassiterite at high pressures and temperatures	Geochim. Cosmochim. Acta	49	22p
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86jen	Jenkins, R. (ed.)	Mineral powder diffraction file	JCPDS Intl. Cent. Diffraction Data, Swarthmore, PA		
82joh/flo	Johnson, G.K., Flotow, H.E., O'Hare P.A.G., and Wise, W.S.	Thermodynamic studies of zeolites: Analcime and dehydrated analcime	Amer. Mineral.	67	736-748
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92joh/tas	Johnson, G.K., Tasker, I.R., Flotow H.E, Ohare, P.A.G, et al.	Thermodynamic studies of mordenite, dehydrated mordenite, and gibbsite	Amer. Mineral.	77	85-93

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90joh	Johnson, J.W.	Regression fit parameters that provide smooth metastable extrapolation of one-bar steam properties predicted by the Haar et al. (1984) equation of state to temperatures < the saturation temperature (99.632 degC)	Pers. calc., LLNL, Livermore, CA		
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65kel/cru	Kelemen, F., Cruceanu, E., and Miculescu, D.	Untersuchung einiger thermischer eigenschaften der verbindungen HgSe, HgTe and ZnTe	Phys. Stat. Solidi.	11	865-872
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46kel/sho	Kelley, K.K., Shomate, C.H., Young F.E., Naylor, B.F., Salo, A.E., and Huffman, E.H.	Thermodynamic properties of ammonium and potassium alums and related substances, with reference to extraction of alumina from clay and alunite	U.S. Bur. Mines Tech. Paper 688		104p
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86lai/azn	La Iglesia, A., and Aznar, A.J.	A method of estimating the gibbs energies of formation of zeolites	Zeolites	6	26-69
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93sch/sho	Schulte, M.D., and Shock, E.L.	Aldehydes in hydrothermal solution: Standard partial molal thermodynamic properties and relative stabilities at high temperatures and pressures	Geochim. Cosmochim. Acta	57	3835-3846
69ser/kho	Sergeyeva, E.I., and Khodakovskiy, I.L.	Physicochemical conditions of formation of native arsenic in hydrothermal deposits	Geokhim.	7	846-859
74sew	Seward, T.M.	Determination of the first ionization constant of silicic acid from quartz solubility in borate buffer solutions to 350degC	Geochim. Cosmochim. Acta	38	1651-1664
76sew	Seward, T.M.	The stability of chloride complexes of silver in hydrothermal solutions up to 350degC	Geochim. Cosmochim. Acta	40	1329-1341
84sew	Seward, T.M.	The formation of lead(II) chloride complexes to 300degC: A spectrophotometric study	Geochim. Cosmochim. Acta	48	121-134
72sha/ste	Shalinets, A., and Stepanov, A.	Investigation of complex formation of the trivalent actinide and lanthanide elements by the method of electromigration. XVII. Hydrolysis	Radiokhimiya	14	290-293

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79rob/hem	Robie, R.A., Hemingway, B.S., and Fisher, J.R.	Thermodynamic properties of minerals and related substances at 298.15K and 1 bar (10**5 Pascals) pressure and at higher temperatures	U.S.G.S. Bull. 1452 (with corrections)	1452	1456p
40rot/wir	Roth, W., Wirths, G. and Berendt, H.	Zentralblatt fur mineralogie, geologie und palaontologie	Z. Mineral. Geol.	11	225-227
87rua/sew	Ruaya, J.R., and Seward, T.M.	The ion-pair constant and other thermodynamic properties of HCl up to 350degC	Geochim. Cosmochim. Acta	51	121-130
83rya/rai	Ryan, J.L., and Rai, D.	The solubility of uranium(IV) hydrous oxide in sodium hydroxide solutions and under reducing conditions	Polyhedron	2	947-952
82sar/bar	Sarkar, A.K., Barnes M.W., and Roy, D.M.	Longevity of borehole and shaft sealing materials: thermodynamic properties of cements and related phases applied to repository sealing	ONWI Tech. Rep. ONWI 201		52p
63sch/teb	Schafer, V.H., Tebben, A., and Gerhardt, W.	Equilibria with Ru, RuO2, RuO3(g), and RuO4(g)	Z. Anorg. Allg. Chem.	321	41-55
71sch	Schedin, U.	On the hydrolysis of plutonyl ion in sodium perchlorate medium	Acta Chem. Scand.	25	747-749
75sch	Schedin, U.	Studies on the hydrolysis of metal ions. 62. The plutonyl ion in sodium perchlorate medium	Acta Chem. Scand.	29	333-344
63sch/rei	Schindler, P., Reinert, M., and Gamsjager, H.	Zur thermodynamik der Metallcarbonate. Loslichkeitskonstanten and freie bildungsenthalpien von Cu2(OH)2CO3(malachit) und Cu3(OH)2(CO3)2 (azurit) bei 25 C	Helv. Chim. Acta	51	1845-1856

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89sho/hell1	Shock, E.L., and Helgeson, H.C.	Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Standard partial molal properties of organic species	Geochim. Cosmochim. Acta	54	915-945
89sho/hell2	Shock, E.L., and Helgeson, H.C.	Corrections to Shock and Helgeson (1988)	Geochim. Cosmochim. Acta	53	215
93sho/kor	Shock, E.L., and Koretsky, C.M.	Metal-organic complexes in geochemical processes: Calculation of standard partial molal thermodynamic properties of aqueous acetate complexes at high pressures and temperatures	Geochim. Cosmochim. Acta	57	4899-4922
93sho/mck	Shock, E.L., and McKinnon, W.B.	Hydrothermal processing of cometary volatiles-- Applications to Triton	Icarus	106	464-477
44sho	Shomate, C.H.	High-temperature heat contents of magnesium nitrate, calcium nitrite and barium nitrate	J. Amer. Chem. Soc.	66	928-929
45sho/nay	Shomate, C.H., and Naylor, B.F.	High-temperature heat contents of aluminum oxide, aluminum sulfate, potassium sulfate, ammonium sulfate and ammonium bisulfate	J. Amer. Chem. Soc.	67	72-75
64sil/mar	Sillen, L.G., and Martell, A.E.	Stability constants of metal-ion complexes	Chem. Soc. Spec. Pub. 17, London		
71sil/mar	Sillen, L.G., and Martell, A.E.	Stability constants of metal-ion complexes, supplement no. 1	Chem. Soc. Spec. Pub. 25, London		



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87she/chu	Sheka, I.A., Chumakova, L.S., Malinko, L.A., Koshel, A.V., and Antishko, A.N.	The hydrolysis of carbonate complexes of zirconium and hafnium in sulphate-carbonate solutions	Russ. J. Inorg. Chem.	32	1576-1582
59she/tim	Shevchenko, V.B., Timoshev, V.G., and Volkova, A.A.	Stability constants of nitrate complexes of trivalent plutonium in aqueous and tributyl phosphate solutions	Sov. J. Atom. Ener.	6	293-296
69shi/giv	Shiloh, M., Givon, M., and Marcus, Y.	A spectrophotometric study of the trivalent actinide complexes in solution. III. Americium with bromide, iodide nitrate and carbonate ligands [no title]	J. Inorg. Nucl. Chem.	31	1807-1814
90sho	Shock, E.L.		Pers. calc., Univ. Cal., Berkeley, CA		
92sho	Shock, E.L.	Stability of peptides in high temperature aqueous solutions	Geochim. Cosmochim. Acta	56	3481-3491
93sho	Shock, E.L.	Hydrothermal dehydration of aqueous organic compounds	Geochim. Cosmochim. Acta	57	3341-3349
89sho/hel	Shock, E.L., Helgeson, H.C., and Sverjensky, D.A.	Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Standard partial molal properties of inorganic neutral species	Geochim. Cosmochim. Acta	53	2157-2183
88sho/hel	Shock, E.L., and Helgeson, H.C.	Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Correlation algorithms for ionic species and equation of state predictions to 5kb and 1000degC	Geochim. Cosmochim. Acta	52	2009-2036

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81str/ten	Strunz, H., and Tennyson, C.	Symmetry and twinning in boltwoodite	Sov. Phys. Cryst.	26(6)	732-735
70stu/hil	Stull, D.R., Hildenbran, L., Oetting, F.L., and Sinke, G.C.	Low temperature heat capacities of 15 inorganic compounds	J. Chem. Eng. Data	15	52-56
82sul/woo	Sullivan, J.C., Woods, M., Bertrand, P.A., and Choppin, G.R.	Thermodynamics of plutonium(VI) interaction with bicarbonate	Radiochim. Acta	31	45-50
84sve	Sverjensky, D.A.	Prediction of gibbs free energies of calcite type carbonates and the equilibrium distribution of trace elements between carbonates and aqueous solutions	Geochim. Cosmochim. Acta	48	1127-1134
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70swe/bae	Sweeton, F.H., and Baes, C.F., jr.	The solubility of magnetite and hydrolysis of ferrous ion in aqueous solutions at elevated temperatures	J. Chem. Thermo.	2	479-500

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76smi/mar	Smith, R.M., and Martell, A.E.	Critical Stability Constants, Vol. 4: Inorganic Complexes	Plenum, New York	4	257p
88smy/bis	Smyth, J.R., and Bish, D.L.	Crystal structures and cation sites of the rock-forming minerals	Allen Unwin, Boston		
61som/pli	Sommer, L., and Pliska, K.	Iron(III) acetate complexes	Coll. Czech. Chem. Comm.	26	2754-2773
41sou	Southard, J.C.	A modified calorimeter for high temperatures. The heat content of silica, wollastonite and thorium dioride above 25degC	J. Amer. Chem. Soc.	63	3142-3150
42sou/moo	Southard, J.C., and Moore, G.E.	High temperature heat content of Mn <sub>3</sub> O <sub>4</sub> , MnSiO <sub>3</sub> and Mn <sub>3</sub> C	J. Amer. Chem. Soc.	64	1769-1770
71spe	Spencer, P.J.	Thermodynamic properties of alkali metal alloys	Natl. Phys. Lab., Div. Chem. Stds.		37p
73spe	Spencer, P.J.	The thermodynamic properties of silicates	Natl. Phys. Lab., Div. Chem. Stds.		35p
89spy/ree	Spycher, N.F., and Reed, M.A.	As(III) and Sb(III) sulfide complexes: An evaluation of stoichiometry from existing experimental data	Geochim. Cosmochim. Acta	53	2185-2194

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84tri	Tripathi, V.S.	Uranium(VI) transport modeling: Geochemical data and submodels	Unpub. Ph.D. Diss., Stanford Univ., Stanford, CA		297p
74tru/jon	Truesdell, A.H., and Jones, B.F.	WATEQ, a computer program for calculating chemical equilibria of natural waters	U.S.G.S. J. Res.	2	233-248
71tum	Tumnavuori, J.	Spectrophotometric determination of the stability constants of complexes formed by copper(II) and nitrite ions in sodium perchlorate solutions at 25degC	Suomen Kem. B	44	222-228
61tur	Turnbull, A.	Thermochemistry of zirconium halides	J. Phys. Chem.	65	1652-1961
73tur	Turnbull, A.G.	A thermochemical study of vaterite	Geochim. Cosmochim. Acta	37	1593-1601
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86ull/sch	Ullman, W.J., and Schreiner, F.	Calorimetric determination of the enthalpies of U(VI)-, Np(VI)-, and Pu(VI)-SO-24 complexes in aqueous solution at 25degC	Radiochim. Acta	40	179-184
65bur/lil	Urkov, K.A., Lilic, L.S., and Sillen, L.G.	The nickel ion, Ni <sup>2+</sup> , in 3m (Na)ClO <sub>4</sub> medium	Acta Chem. Scand.	19	14-29

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87tas/oha	Tasker, I.R., O'Hare P.A.G., Lewis, B.M., Johnson, G.K., and Cordfunke, E.H.P.	Thermochemistry of uranium compounds. XVI. Calorimetric determination of the standard molar enthalpy of formation at 298.15K, low temperature heat capacity, and high-temperature enthalpy increments of UO <sub>2</sub> (OH)·2H <sub>2</sub> O (Schoepite)	LLNL, UCRL-21055		17p
62tay/smi	Taylor, A.R., jr., and Smith, D.F.	Thermodynamic properties of strontium bromide and strontium nitrate	U.S. Bur. Mines Dept. Inv. 5967		12p
67ter/rat	Terpilowski, J., and Ratajczak, E.	Wlasnosci thermodynamiczne selenku cynku	Roczn. Chem.	41	429-432
51tod	Todd, S.S.	Low-temperature heat capacities and entropies at 298.16K of crystalline calcium orthosilicate, zinc orthosilicate and tricalcium silicate	J. Amer. Chem. Soc.	73	3277-3278
69tor/sho	Torgeson, D., and Shomate, C.	Heats of formation of 3CaO·B <sub>2</sub> O <sub>3</sub> , 2CaO·B <sub>2</sub> O <sub>3</sub> , CaO·B <sub>2</sub> O <sub>3</sub> and CaO·B <sub>2</sub> O <sub>3</sub>	J. Amer. Chem. Soc.	69	2103-2105
81tre/che	Tremaine, P.R., Chen J.D., Wallace, G.J., and Boivin, W.A.	Solubility of uranium(IV) oxide in alkaline aqueous solutions to 300degC	J. Soln. Chem.	10	221-230

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68wag/eva	Wagman, D.D., Evans, W.H., Parker, V.B., Halow, I., Bailey, S.M., and Shumm, R.H.	Selected values of chemical thermodynamic properties	U.S. Natl. Bur. Stds. Tech. Note 270 3		264p
82wag/eva	Wagman, D.D., Evans, W.H., Parker, V.B., Schumm, R.H., Halow, I., Bailey, S.M., Churney, K.L., and Nuttall, R.L.	The NBS tables of chemical thermodynamic properties, selected values for inorganic and c1 and c2 organic substances in SI units	J. Phys. Chem. Ref. Data, V. 11, supp. 2		392p
81wag/eva	Wagman, D.D., Evans, W.H., Parker, V.B., Schumm, R.H., and Nuttall, R.	Selected values of chemical thermodynamic properties. Compounds of uranium, protactinium, thorium, actinium, and the alkali metals	U.S. Natl. Bur. Stds. Tech. Note 270 8		134p
77wag/sch	Wagman, D.D., Schumm R.H., and Parker, V.B.	A computer assisted evaluation of the thermochemical data of compounds of thorium	U.S. Natl. Bur. Stds. Int. Rep. 77-1300		93
62wal/art	Walsh, P.N., Art, E.W., and White, D.	The heat capacity of the silver chalcogenides. Ag1.99S, Ag1.99Se, and Ag1.88Te from 16 to 300K	J. Phys. Chem.	66	1546-1549
88wan 1	Wanner, H.	The NEA thermochemical data base project	OECD NEA Data Bank, F-91191, Gif-sur-Yvette, France		1-11

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78vau/cra	Vaughan, D.J., and Craig, J.R.	Mineral chemistry of metal sulfides	Cambridge Univ. Press, Cambridge, MA		
61vic/dou	Victor, A.C., and Douglas, T.B.	Thermodynamic properties of thorium dioxide from 298 to 1200K	U.S. Natl. Bur. Stds. J. Res.	65a	105-111
63vic/dou	Victor, A.C., and Douglas, T.B.	Thermodynamic properties of magnesium oxide and beryllium oxide from 298 to 1200K	U.S. Natl. Bur. Stds. J. Res.	67a	325-329
75vol/yag	Volkov, A.I., Yaglov V.N., and Novikov, G.I.	Heats of formation of cobalt and nickel orthophosphates octahydrides	Vesti. Akad. Navuk. B. SSSR. Ser. Khim. Navuk.		124-125
70vor	Voronon, G.F.	Estimation of standard entropies of chemical compounds	Russ. Phys. Chem.	44	1717-1719
76wag/par	Wagman, D., Parker, W., and Schumm, R.	Chemical thermodynamic properties of compounds of sodium, potassium and rubidium	U.S. Natl. Bur. Stds.	76	
76wag/eva	Wagman, D.D, Evans, W.H., Parker, V.B., and Schumm, R.H.	Chemical thermodynamic properties of compounds of sodium, potassium and rubidium: An interim tabulation of selected values	U.S. Natl. Bur. Stds. Int. Rep. 76- 1034		
71wag/eva	Wagman, D.D., Evans, W.H., Parker, V.B., Halow, I., Bailey, S.M., Schumm, R.H., and Churney, K.L.	Selected values of chemical thermodynamic properties	U.S. Natl. Bur. Stds. Tech. Note 270 5		12-21

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85wol	Wolery, T.J.	Notes	Personal Written Communication		23p
87woo/gar	Woods, T.L., and Garrels, R.M.	Thermodynamic values at low temperature for natural inorganic materials: An uncritical summary	Oxford Univ. Press, Oxford		
79zot/kot	Zotov, A.V., and Kotova, Z.Y.	Spectroscopic determination of the first hydrolysis constant of Fe+++ in the interval 80-200degC	Geokhim.	5	768-773



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88wan 2	Wanner, H.	Guidelines for the review procedure and data selection	OECD NEA Data Bank, F-91191, Gif-sur-Yvette, France		1-5
88wan 3	Wanner, H.	Guidelines for the assignment of uncertainties	OECD NEA Data Bank, F-91191, Gif-sur-Yvette, France		1-14
56war/wel	Ward, M., and Welch, G.	The chloride complexes of trivalent plutonium, americium and curium	J. Inorg. Nucl. Chem.	2	95-402
90crc	Weast, R.C. (ed.)	CRC Handbook of Chemistry and Physics	CRC Press, Boca Raton, FL, 70th ed.		
64wel/kel	Weller, W.W., and Kelley, K.K.	Low-temperature heat capacities and entropies at 298.15K of sulfides of arsenic germanium and nickel	U.S. Bur. Mines Rep. Inv. 6511		7p
69wel	Wells, C.F.	Reaction of $Feaq^{2+}$ and $FeClaq^{+}$ with hydrogen peroxide in perchlorate media at 25degC	J. Chem. Soc. A		2741-2743
57wes/gre	Westrum, E.F., and Grenier, G.J.	Heat capacities and thermodynamic properties for crystalline and vitreous anhydrous sodium tetraborate from 6 to 350K	J. Amer. Chem. Soc.	79	1799-1802
62wes/gro	Westrum, E.F., and Gronvold, F.	Chemical thermodynamics of the actinide element chalcogenides	Intl. Atom. Ener. Agency, Vienna		3-37
71wil/jel	Wildervanck, J.C., and Jellinek, F.	proceedings of the symposium on thermodynamics of nuclear materials The dichalcogenides of technetium and rhenium	J. Less-Common Metals	24	73-81

## APPENDIX C

### GEMBOCHS MODIFICATIONS AND ADDITIONS: 2nd QUARTER, FY 1994

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During the second quarter of FY 1994, efforts were focused on completing development of two major software projects, augmenting GEMBOCHS with additional thermodynamic data, expanding the suite of datafiles generated for use with EQ3/6, and improving user access to EQ3/6 datafiles, which are described in the following paragraphs.

During the past year, considerable effort was devoted toward development of two critical software interfaces with GEMBOCHS. The first of these is the *jewel* program, a mouse-driven utility that facilitates point-and-click generation of thermodynamic datafiles for use with EQ3/6 (and other analogous modeling packages). More specifically, *jewel* reads reference-state and various coefficient data for a user-specific subset of GEMBOCHS species, extrapolates these data over the P-T range of interest using a variety of theoretical and empirical models, and outputs the requisite elevated P-T properties in a format suitable as input for various target modeling codes. *Jewel* can be used to generate a number of standard datafiles; more important is the program's extreme flexibility, which permits generation of customized datafiles based on major datasets, species subsets, bulk system composition, or any combination thereof. The *jewel* interface represents a dramatic improvement in both versatility and ease-of-use over its relatively inflexible, batch-mode predecessor. The code has been used and refined extensively over the past few months, and a user's manual is in the process of being completed.

The second interface under development is *facet*, another mouse-driven utility that permits review, revision, deletion, and addition of GEMBOCHS data. All updates to GEMBOCHS are incorporated using *facet*, which provides an auditing capability that explicitly documents all database modifications. Like *jewel*, *facet* represents a tremendous improvement over its predecessor, which required function-key navigation through a labyrinth of on-screen menus. Also in analogy with *jewel*, the *facet* development effort, including the documentation, is nearing completion and will be available in the near future. Recently, *facet* was used to upload reference-state standard molal thermodynamic data and equation-of-state parameters for a large number of aqueous species, including aqueous peptides, aldehydes, and metal acetate complexes (Shock, 1992, 1993; Schultz and Shock, 1993; Shock and Koretsky, 1993; Shock and McKinnon, 1993). These data improve significantly the ability to model aqueous organic/inorganic systems.

Also, a sixth member has been added to the standard suite of thermodynamic datafiles provided for use with EQ3/6. The new file, data0.alt, represents an alternate composite database in which aqueous Np, Pu, and Am species are represented exclusively by the compilation of reference-state dissociation constants given by Palmer et al. (1992). Otherwise, the file is identical to the composite datafile, data0.com, in which a smaller set of aqueous Np, Pu, and Am species is represented by data from a variety of published sources.

In an attempt to improve user accessibility to newly revised suites of GEMBOCHS datafiles for use with EQ3/6, an "anonymous" ftp account has recently been established on a local machine. This account permits off-site EQ3/6 users to-keep abreast of recent GEMBOCHS updates and to acquire the latest suites of EQ3/6 datafiles in timely fashion via electronic transfer. The R23 suite will be the first available via the "anonymous" account, sometime during April 1994. At that time, interested parties will be informed as to the particulars of remote access procedures.

APPENDIX D

GENISES ADDITIONS: 2nd QUARTER, FY 1994

<u>DATA TRACKING NO.</u>	<u>DATA ITEM DESCRIPTION</u>
LA0000000000051.001	LONG-TERM THERMAL STABILITY OF CLINOPTILOLITE: THE DEVELOPMENT OF A B PHASE
TM0000000000001.037	METEOROLOGICAL MONITORING PROGRAM SUMMARY REPORT DECEMBER 1985 THROUGH DECEMBER 1991 (YMP/93-12-MMPSR)
GS920483117412.014	SEISMICITY AND FOCAL MECHANISMS FOR THE SOUTHERN GREAT BASIN OF NEVADA AND CALIFORNIA IN 1990 (USGS OFR 92-367)
GS920783117412.022	SEISMICITY AND FOCAL MECHANISMS FOR THE SOUTHERN GREAT BASIN OF NEVADA AND CALIFORNIA IN 1991 (USGS OFR 92-340)
GS920983117412.032	SEISMICITY AND FOCAL MECHANISMS FOR THE SOUTHERN GREAT BASIN OF NEVADA AND CALIFORNIA: 1987 THROUGH 1989 (USGS OFR 91-572)
GS910808312232.002	BOREHOLE AND GEOHYDROLOGIC DATA FOR TEST HOLE USW UZ-6, YUCCA MOUNTAIN AREA, NYE COUNTY, NEVADA (USGS OFR 92-28)
GS930731174101.003	1983-1988 LEVELING RESULTS, 1983-1988 QUADRILATERAL RESULTS AND VARIOUS EARLIER DATA
GS920508314212.005	PRINCIPAL FACTS FOR 16,000 GRAVITY STATIONS IN THE NEVADA TEST SITE AND VICINITY (USGS OFR 89-682 A, B, &C)
GS920108314213.001	GEOPHYSICAL AND CORE MEASUREMENTS FROM FORTY BOREHOLES AT YUCCA MOUNTAIN
GS930208318523.001	TEMPERATURE, THERMAL CONDUCTIVITY, AND HEAT FLOW NEAR YUCCA MOUNTAIN, NEVADA: SOME TECTONIC AND HYDROLOGIC IMPLICATIONS (USGS OFR 87-649)

DATA TRACKING NO.

DATA ITEM DESCRIPTION

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GS930908314214.006    GEOLOGICAL AND MINERALOGICAL CONTROLS ON  
PHYSICAL PROPERTIES OF TUFFS AT YUCCA  
MOUNTAIN

GS930908314214.007    BULK POROSITY IN LITHOPHYSAL ZONES ABOVE THE  
STATIC WATER LEVEL AT YUCCA MOUNTAIN, NEVADA,  
CALCULATED FROM BOREHOLE GRAVITY AND GAMMA-  
GAMMA DENSITY LOGS