MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0

Prepared for

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SUMMARY

This report presents modifications in the geochemical speciation model MINTEQA2 and its associated user interface, PRODEFA2, for version 4.0. The previous release, version 3.11, incorporated changes that were never formally described in model documentation. Important version 3.11 changes that apply to version 4.0 are also described in this document. The basic model theory described in the version 3.0 model documentation is still valid and provides a basic description of the model. The information in this document is intended to supplement that provided in the version 3.0 user manual.

Significant changes in the MINTEQA2/PRODEFA2 model since the publication of the version 3.0 user manual include: Incorporation of the Gaussian model for computing trace metal complexation with dissolved organic matter, modifications to minimize the occurrence of violations of Gibbs phase rule, modifications to allow direct simulation of a titration in one model run, modifications to allow selected output to be written for easy importing to a spreadsheet, modifications to improve model execution speed and convergence, and modifications to improve the thermodynamic database used by the model, including the addition of beryllium (II), cobalt (II and III), molybdenum (VI), and tin (II and IV) compounds. Also, errors in thermodynamic constants associated with certain metal-organic reactions in earlier versions have been corrected in version 4.0, thermodynamic constants for inorganic species have been reviewed and updated, and all reference citations for equilibrium constants have been included in the revised database. In addition, the model has been made Y2K compliant. These and other revisions are described in this document.

CHAPTER 1

INTRODUCTION AND BACKGROUND

MINTEQA2 is a equilibrium speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model is useful for calculating the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressure. A comprehensive database is included that is adequate for solving a broad range of problems without need for additional user-supplied equilibrium constants. The model employs a pre-defined set of components that includes free ions such as Na^+ and neutral and charged complexes (*e.g.*, $H_4SiO_4^0$, $Cr(OH)_2^+$). The database of reactions is written in terms of these components as reactants. An ancillary program, PRODEFA2, serves as an interactive pre-processor to help produce the required MINTEQA2 input files.

Several modifications important to the user have been made since the last publication of a MINTEQA2/PRODEFA2 user manual (Allison *et al.*,1991; version 3.0). This document is intended to supplement the basic information provided in the version 3.0 user manual. After a brief introduction and description of MINTEQA2, it describes significant changes since version 3.0.

1.1 MATHEMATICAL FORMULATION OF MINTEQA2

A system of *n* independent components that can combine to form *m* species is represented by a set of mass action expressions of the form

$$K_i = \{S_i\} \prod_{j=1}^{n} X_j^{-a_{ij}} \qquad (1)$$

where K_i is the formation constant for species *i*, $\{S_i\}$ is the activity of species *i*, X_j is the activity of component *j*, and a_{ij} is the stoichiometric coefficient of component *j* in species *i*. Rearranging to express the concentration C_i in terms of the activities of components gives

$$C_i = \frac{K_i}{\gamma_i} \prod_{j=1}^{n} X_j^{a_{ij}} \qquad (2)$$

where γ_i represents the activity coefficient of species *i*.

In addition to the mass action expressions, the set of *n* independent components is governed by *n* mass balance equations of the form

$$Y_j = \sum_{i=1}^{n} a_{ij} C_i - T_j \qquad (3)$$

where T_j is the known total concentration of component *j* (an input parameter). Thus, Y_j is the difference between the calculated total concentration and the known total concentration of component *j*. The mathematical solution of the equilibrium problem is the set of component activities that give species concentrations from equation (2) which produce a component mass imbalance of zero in equation (3) for each and every component. The equilibrium problem is solved iteratively—the X_j values are deemed correct and the problem is solved when the Y_j values are reduced to an acceptably small value for every component. If this is not the case, new estimates are made for component activities X_j, and the calculations are repeated in a new iteration beginning at Equation (2).

MINTEQA2 uses the Newton-Raphson approximation method to estimate the new X_j at each iteration. This method utilizes a Jacobian matrix whose elements represent the partial derivatives of each component mass balance difference Y_j with respect to every other component activity X_k where both *j* and *k* range from 1 to the number of components (*n*). Each gradient element of the Jacobian is given by

$$u_{j,k} = \frac{\partial Y_j}{\partial X_k} = \sum_{i=1}^{n} a_{ij} \frac{\partial C_i}{\partial X_k} \qquad (4)$$

In summary, the mathematical solution to the equilibrium problem is that set of component activities **X** (using bold symbols to indicate matrix notation for brevity) which results in the set of concentrations **C** such that each individual of the set of mass balance differences **Y** is equal to zero. In practice, it is only necessary to find **X** such that each individual of **Y** is made less than some tolerance value. The general procedure is to first guess **X**, then calculate **C** and **Y**. If any individual of **Y** exceeds (in absolute terms) its prescribed tolerance value, a new estimate is made for **X**, then **C** and **Y** are recalculated, and the test is repeated. This iterative procedure is continued until all the individuals of **Y** are less than the tolerance value. The tolerance value or convergence criterion for MINTEQA2 is pre-set to 10^{-4} times $|T_j|$ for each component *j*.

1.2 SUMMARY OF SIGNIFICANT MODIFICATIONS SINCE VERSION 3.0

Significant modifications made to MINTEQA2/PRODEFA2 since the publication of the version 3.0 user manual are described below. Particular attention is given to the model revisions that extend modeling capabilities and to relating theory that the user might want or need to know. The user interface (PRODEFA2) has been modified to accommodate the changes in MINTEQA2. For most modifications, the presentation of menus and options in PRODEFA2 is such as to eliminate the need for extensive "how to use" information. Specific changes to source code for important modifications are described elsewhere (Allison, 1997).

The following model revisions since version 3.0 are introduced below and discussed in more detail in succeeding chapters: Incorporation of the Gaussian model for computing trace metal complexation with dissolved organic matter, modifications to assist in avoiding violations of Gibbs phase rule, modifications to allow direct simulation of a titration in one model run, modifications to allow selected output to be written for easy importing to a spreadsheet, modifications to improve model execution speed and convergence, and modifications to improve the thermodynamic database used by the model, including the addition of beryllium (II), cobalt (II and III), molybdenum (VI), and tin (II and IV) compounds. Also, errors in thermodynamic constants associated with certain metal-organic reactions in earlier versions have been corrected in version 4.0, thermodynamic constants for inorganic species have been reviewed and updated, and reference citations for equilibrium constants have been included in the revised database. The model has been made Y2K compliant. These and other revisions are described in this document.

1.2.1 Gaussian Model for Dissolved Organic Matter

MINTEQA2 version 4.0 includes the implementation of a competitive Gaussian model for computing the complexation of metals by dissolved organic matter (DOM). The Gaussian DOM model is that described in Perdue and Lytle (1983) and further developed by Dobbs *et al.* (1989a, 1989b), Susetyo *et al.* (1990), and Grimm *et al*. (1991). Its earlier implementation in MINTEQA2 version 3.11 is described in Allison and Perdue (1994). Understanding the chemical reactions between DOM and trace metals is important because of the potential impact on trace metal mobility and toxicity. Dissolved organic matter strongly complexes many trace metals (*e.g*., copper and lead). Aquatic systems contain DOM at nominal concentrations ranging from very minor amounts up to about 50 mg/L in surface waters (Sunda and Hanson, 1979; Stumm and Morgan, 1996). Concentrations in localized surface environments and in soil or sediment porewaters may be significantly higher. Oxide and clay solid phases in soils and sediments tend to adsorb many trace metals in groundwater systems, but the presence of DOM, even at low concentrations, may reduce the amount sorbed and increase the total dissolved (mobile) trace metal concentration. The aquatic toxicity of some trace metals is related to the concentration of the free ion (Sunda and Guillard, 1976; Morel and Hudson, 1985; Stumm and Morgan, 1996). There is evidence that complexation of metals by DOM may serve to reduce metal uptake by fish (Playle *et al*., 1993; Janes and Playle, 1995). Several humic substance interaction models have been proposed in recent years (Bartschat *et al*., 1992; Tipping and Hurley,

1992; Tipping, 1993; Koopal *et al.*, 1994; Benedetti *et al.*, 1995, Milne *et al.*, 1995). However, few have been made readily accessible within the framework of a widely used speciation model.

1.2.2 Changes to Minimize Violations of Gibb's Phase Rule

Modifications have been made in MINTEQA2 version 4.0 to assist the user in avoiding violations of Gibbs phase rule during model execution. Some violations of the phase rule are a natural and unavoidable consequence of the user's specification of the equilibrium problem. For example, if the user specifies a particular solid phase as present at equilibrium, but, in fact that phase is not the thermodynamically stable phase, a violation of the phase rule will occur. Of course, this is not actually an error condition— it is geochemical information that should cause the user to re-think the specification of the equilibrium phase. This type of result may still occur in version 4.0. However, in previous versions, a violation of the phase rule also can occur when the user has not specified equilibrium constraints. This can happen during the model's attempt to arrive at the correct set of equilibrium phases, with the result that execution ends with an error. In earlier versions, the remedy was to attempt (by a combination of trail and error and geochemical judgement) to select those solids that should be allowed to precipitate and those that should be excluded. This procedure can be frustrating, especially for the inexperienced user. Version 4.0 includes logic to allow the model to test for possible phase rule violations and make solid phase selections to arrive at the correct set of equilibrium solids phases.

1.2.3 Other Changes in Model Code

Other improvements and modifications in MINTEQA2/PRODEFA2 since version 3.0 include changes to implement sparse matrix techniques to improve the execution speed, changes to reduce the occurrence of non-convergence, modifications to allow the user to model a titration of a system with any chosen species as the titrant (except DOM or sorption species), modifications to allow key output to be written to a separate file for import to a spreadsheet, and correction of known errors in earlier versions. These are discussed in separate sections below.

1.2.4 Database Changes

There have been two separate efforts to improve the thermodynamic database of MINTEQA2 since version 3.0. The version 3.0 database included 31 organic acids and several hundred species representing reactions between these ligands and trace metals. Unfortunately, some of the thermodynamic data included in the version 3.0 database was not properly reduced and re-formulated (Serkiz, *et al.*, 1996). These data have since been reviewed and corrected; this is reflected in the version 4.0 database. Also, a more general effort to improve the entire database has recently been completed and the result is presented here (Chapter 5). In this latter effort, reactions for the metals cobalt (II and III), molybdenum (VI; as MoO_4^{2-}), and tin (II and IV) with those ligands already in the

database have been added. Additionally, recent compilations of stability constants available from the National Institute of Standards and Technology (NIST), the International Union of Pure and Applied Chemistry (IUPAC), and other sources have been used to verify and update existing data and to augment the data with new reaction (especially for beryllium and strontium). Reference citations have been provided where possible. In addition, longer species names have been used to eliminate ambiguity in species identity.

CHAPTER 2

THE GAUSSIAN MODEL FOR DISSOLVED ORGANIC MATTER

2.1 BACKGROUND

The competitive Gaussian model of cation binding with dissolved organic matter (DOM) is an extension of the statistical proton binding model presented by Posner (1964) and further developed by Perdue and Lytle (1983), Perdue *et al.* (1984), and Dobbs *et al.*(1989a). In this model, the concentrations of individual ligands of the complex DOM mixture are normally distributed with respect to their log K values. Parameters μ and σ are the mean and standard deviation of the normally distributed log K values.

Recent models for metal-humic interaction may be categorized on the basis of two main features: (1) the manner in which heterogeneity among humic substance ligand sites is represented, and (2) whether electrostatic interactions between solute ions and ligand binding sites are explicitly parameterized. When the latter are not explicitly parameterized, no attempt is made in fitting the model to experimental data to derive parameters from which electrostatic attractions may be estimated, and no attempt is made to account for such electrostatic effects in implementing the model (predictively) within a general speciation model. Instead, the electrostatic attractions that may conceptually be included in the model are regarded as implicitly accounted for in the representation of site heterogeneity. Two methods are commonly used in representing site heterogeneity. In discrete ligand models (also called multi-ligand or N-site models) a small number of ligands (sites) are chosen whose combined effective complexation behavior represents that of the humic substance mixture (Mantoura *et al*., 1975; Buffle *et al*., 1977; Bresnahan *et al*., 1978; Dzombak *et al*., 1986; Cabaniss and Shuman, 1988a). In continuous distribution models, a continuous statistical or mathematical function is used to represent a continuum of sites (Posner, 1964; Perdue and Lytle, 1983; Shuman *et al.*, 1983; Dobbs *et al.*, 1989a). Models that belong to the discrete or the continuous genre may include an explicit representation of electrostatic effects on binding. The explicit incorporation of electrostatic interactions separately from the representation of site heterogeneity was proposed by Ephraim and Marinsky (1986) in an effort to account for observed variation in the degree of binding with the ionic strength of the solution. Much model development effort in recent years has focused on how to represent site heterogeneity and electrostatic (ionic strength) effects (de Wit *et al.*, 1990; Tipping and Hurley, 1992; Bartschat *et al*., 1992; Kinniburgh *et al.*, 1996). The hope has been that if binding site heterogeneity and ionic strength effects are properly represented in a predictive humic interaction model, then that model can be extrapolated

to systems other than that from which it was derived.

2.1.1 Discrete Ligand Models

In the discrete ligand approach, a small set of ligands (usually five or fewer) are designated to represent binding sites, and their relative concentrations and binding affinities are empirically scaled to reproduce observed binding. The chemical natures of the ligand sites are not explicitly stated in most discrete ligand models— the members of the set are simply identified by number or letter (*e.g.*, L_1, L_2, *etc.*). The relative concentration fraction of each ligand and the ligand log *K* for binding a particular cation are determined by means of fitting experimental titration data to the chosen ligand set by non-linear regression. Alternatively, real ligands may be chosen to collectively represent DOM. In the latter case, the selection of the real ligands may be predicated on an assessment of the actual functional group content of the DOM and on the site binding affinities (Stumm and Morgan, 1970; Bartschat *et al.*, 1992). Regardless of whether real or theoretical ligands are used, the discrete ligand method is amenable to other than 1:1 cation-to-ligand stoichiometries. Cabaniss and Shuman (1988a) derived a five-site model for copper binding that incorporated monoprotic and diprotic sites, but was 1:1 in copper-to-ligand ratio. In fitting data to discrete ligand models, cation-to-ligand stoichiometry becomes another fitting parameter, and in the absence of clear justification to the contrary, it usually is treated as 1:1 (Cabaniss and Shuman, 1988a).

The binding constants derived from the data-fitting regression in the discrete ligand approach are always conditional constants. The degree to which they are useful in systems other than that from which they were derived is somewhat dependent on the sophistication of the model fitting exercise. Constants reported in the literature have been based on models that range from simple representations in which the competition between protons and metal ions for binding sites is ignored and no attempt is made to account for ionic strength effects, to more complicated representations that attempt to include both pH and ionic strength dependence (Cabaniss and Shuman, 1988a and 1988b; Dzombak *et al.*, 1986).

The small number of ligands in a discrete representation of DOM provides a straightforward framework for representing DOM reactions within a general speciation model— each ligand of the set is defined as a component and reactions are defined between each ligand component and the metal of interest (Fish *et al.*, 1986). For a discrete representation that includes 1:1 metal-to-ligand stoichiometry and pH dependence, representative reactions for binding with protons and metal might be:

$$H + L_i \rightleftharpoons HL_i \tag{5}$$

and

$$M + L_i \rightleftharpoons ML_i \tag{6}$$

Mass law expressions for the above reactions are amenable for direct use in speciation models:

$$\{HL_i\} = K_{HL_i}\{H\}\{L_i\} \quad (7)$$

and

$$\{ML_i\} = K_{ML_i}\{M\}\{L_i\} \quad (8)$$

where quantities in braces represent activities. Any one of the ligand species (L_i, HL_i, or ML_i) may be chosen as the component representing the ligand in the speciation model; the choice dictates the form in which reactions (5) and (6) will be expressed. If HL_i is chosen as the component, reaction (6) would be rewritten as an exchange reaction

$$HL_i + M \rightleftharpoons ML_i + H \quad (9)$$

and its mass law expression would be changed accordingly.

Equations (7) and (8) are in the usual form implemented in speciation models such as MINTEQA2—activities of the ligand species are expressed in terms of a thermodynamic equilibrium constant and component activities. However, the equilibrium constants that result from fitting experimental data are not true thermodynamic constants. This is especially true for DOM, because the commonly used equations for estimating activity coefficients may not apply to DOM ligand sites. The Debye-Hückel equation and related equations such as the extended Debye-Hückel equation, the Davies equation, and the Guntelberg equation (see Stumm and Morgan, 1996) are based on the Debye-Hückel limiting law for single ions in solution. It is not clear that such expressions provide useful activity coefficient estimates for ligand sites that are present as part of a larger polymeric molecule. Discrete and continuous distribution models found in the literature have handled this difficulty by ignoring the distinction between activity and concentration (*i.e.*, by assuming activity coefficients of unity), by utilizing an expression such as the Davies equation even though it may not be appropriate, or by incorporating an explicit representation of electrostatic interactions. The first two alternatives are easily implemented in most speciation models; the third can also be implemented in a manner that follows the methodology already used in electrostatic models for oxide and other mineral surfaces (Westall and Hohl, 1980; Dzombak and Morel, 1990). Recent discrete ligand models include Model V (Tipping and Hurley, 1992) and models proposed by Tao (1992) and Westall *et al*. (1995). The model of Westall *et al*. (1995) uses four ligand sites with fixed log K_H values of 4, 6, 8, and 10. Fitting this model to titration data involves solving for the corresponding ligand concentrations and log *K* values for the metal of interest. The discrete model proposed by Tao (1992) employs a small number of ligands whose log *K* values are the same for all species bound. The only fitting parameters are the site concentrations of the discrete ligands.

2.1.2 Continuous Distribution Models

Continuous distribution models attempt to represent the heterogeneity of sites in DOM by means of a functional relationship between site abundance and binding affinity. Gamble (1970) laid the groundwork for the development of continuous ligand models by presenting a method for estimating the spectrum of acid-base dissociation constants in a material characterized by a continuum of such constants. Although his methods did not lead to a predictive model, others have extended the concept of a continuum of binding energies to the treatment of metal binding with humic substances (Shuman *et al*., 1983; Perdue and Lytle, 1983). A general definition of a continuous distribution model (adapted from Parrish and Perdue (1989) and Koopal *et al*. (1994)) is

$$\theta_t = \int \theta_L \, f(\log K) \, d(\log K) \tag{10}$$

where θ_t is the fraction of total ligand sites that are free or the fraction occupied by protons or the fraction occupied by metal in accordance with the definition of the local isotherm, θ_L, and $f(\log K)$ expresses the probability of occurrence of a binding site as a function its log K value. Perdue and Lytle (1983) presented an implementation of Equation (10) in which θ_L is a Langmuir-type expression for the complexed metal. In their single-metal system at constant pH, θ_L was given by

$$\theta_L = \frac{K\,[M]}{1 + K\,[M]} \tag{11}$$

(square brackets denote concentration), and $f(\log K)$ is a normal probability function characterized by a mean log K (μ) and standard deviation in log K (σ). Thus, Equation (10) becomes:

$$\theta_t \equiv \frac{[ML]}{T_L} = \frac{1}{\sigma\sqrt{2\pi}} \int \frac{K\,[M]}{1 + K\,[M]} \, e^{-\frac{1}{2}\left(\frac{\log K - \mu}{\sigma}\right)^2} \, d(\log K) \tag{12}$$

where T_L represents the total concentration of binding sites in molar units.

Analytical solutions exist for Equation (10) for some choices of θ_L and $f(\log K)$. Koopal *et al*. (1994) examined several limiting cases obtained analytically when θ_L is a Langmuir expression (*e.g.*, Equation (11)), and $f(\log K)$ is a Gaussian-like function given by Sips (1948). The resulting analytical solution for mono-component binding is

$$\theta_t = \frac{(K'\,[M])^m}{1 + (K'\,[M])^m} \tag{13}$$

where K' is the median binding constant of the Sips distribution and m represents the distribution width. This expression corresponds to the Freundlich equation if $(K_{Freundlich})^{1/m}$ is substituted for K'.

It also corresponds to the Henderson-Hasselbalch equation for *m* values between 0 and 1 and to the Hill equation for *m* >1 (Koopal *et al*. (1994). The background of these developments is in colloidal and surface chemistry, so binding between the heterogenous substrate and protons or metal ions is referred to as adsorption rather than complexation. However, humic substances are appropriately studied as colloids, and the assumption is commonly made in modeling the equilibrium chemistry of adsorption reactions that they may be treated as completely analogous to coordination reactions in solution (Morel, 1983). Therefore, no distinction will be made herein between complexation and adsorption reactions in discussion of binding with humic substances.

2.1.3 The Gaussian DOM Model

The Gaussian DOM model is an instance of a continuous distribution model. In particular, the Gaussian model whose implementation is discussed here is that proposed by Dobbs *et al*. (1989a,b), which is an extension the Gaussian model proposed by Posner (1964) and developed by Perdue and Lytle (1983) and Perdue et *al*. (1984). The work of Dobbs *et al*. (1989a,b) extended the model to include pH-dependency and competition among multiple components that bind with DOM. In the Gaussian model, DOM is treated as exhibiting a normal probability distribution of site abundance in respect to site binding affinity. The total concentration of a particular binding site *i* (*i.e*., a ligand within the DOM mixture) with a binding affinity represented by the logarithm of an equilibrium constant for binding (log K_i) is determined from the expression:

$$\frac{T_{L_i}}{T_L} = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{1}{2}\left(\frac{\log K_i - \mu}{\sigma}\right)^2} \qquad (14)$$

where T_L and T_{Li} are the sum total concentration of binding sites and the total for ligand *i*, respectively, and the parameters μ and σ are the mean log *K* and standard deviation in log *K*, respectively. In terms of Equation (10), the local isotherm expression is of standard Langmuirian form given by

$$\theta_L = \frac{K_{ML_i}[M]}{1 + K_{HL_i}[H] + K_{ML_i}[M]} \qquad (15)$$

for a single metal, and the function *f*(log *K*) is given by the right side of Equation (14). Figure 2.1 shows such a distribution of sites. The total metal bound is obtained by calculating the amount bound by those ligands whose log *K*'s are within a vanishingly small log *K* interval, and integrating over log *K*. When θ_L and *f*(log *K*) are represented as described, there is no analytical solution for Equation (10). This presents difficulties for incorporation in a speciation model because the integral in Equation (10) must be evaluated numerically.

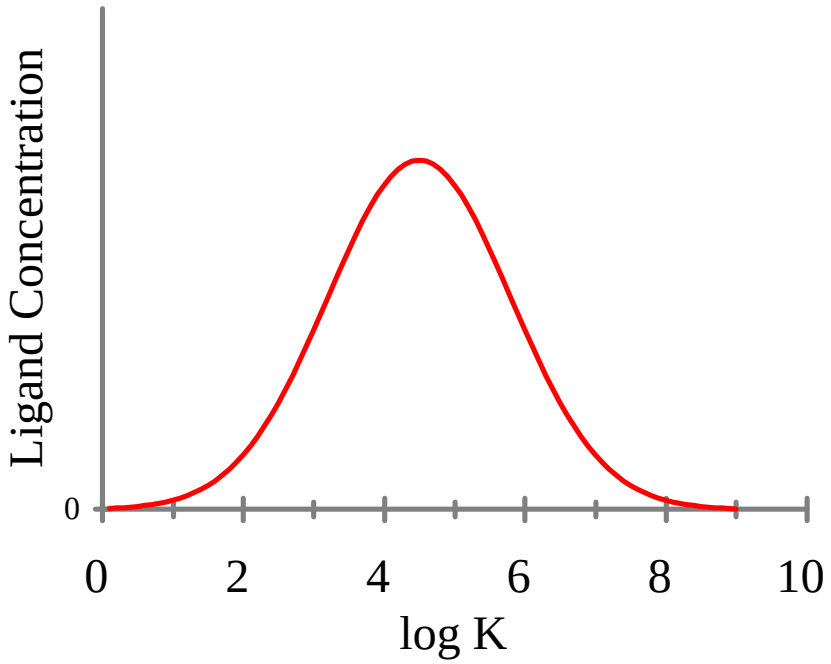

Figure 2.1 Illustrating Normal Probability of Occurrence (Concentration) of Ligands Versus Log *K* within the DOM Mixture. (Mean Log *K* (μ) =4.5).

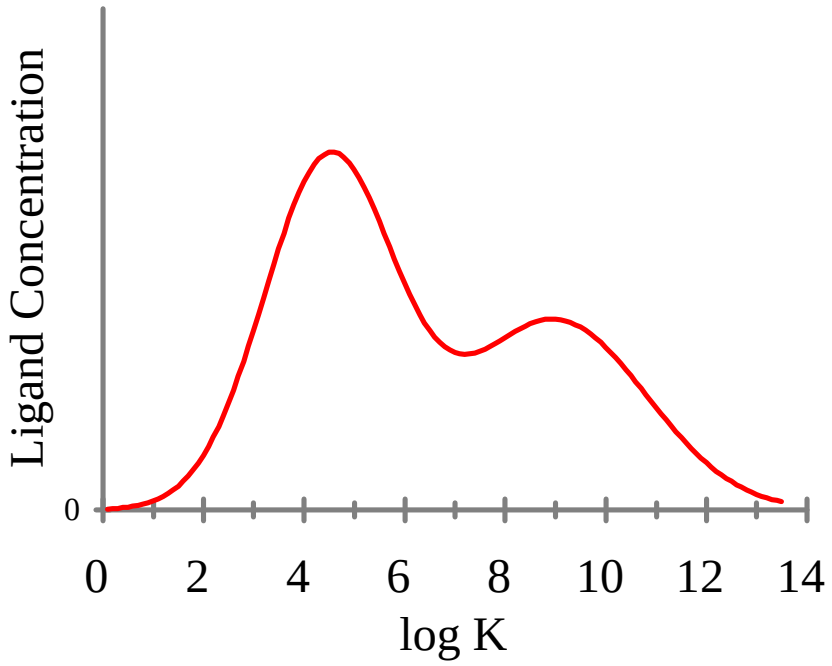

Figure 2.2 Bimodal Distribution of Relative Site Concentration Versus Log *K*.

The implementation of the Gaussian DOM model in MINTEQA2 is such as to allow treatment of a bimodal or tri-modal site distribution. The Gaussian distribution represented in Figure 2.1 is treated as describing the site abundance versus site affinity relationship for a particular functional group or site-type rather than the entire universe of sites available in the DOM. Figure 2.2 illustrates a bimodal site distribution. In MINTEQA2 there may be up to six Gaussian site-types, each characterized by a mean log *K* and standard deviation in log *K* for each metal (including protons), and by a site acidity (*i.e.*, abundance of binding sites per unit mass of DOM). Dissolved organic matter is widely regarded as containing several types of acidic functional groups with carboxylic groups being the most abundant. Other, weakly acidic groups are difficult to quantify and may include phenols, weaker carboxyl groups, and alcohols (Perdue, 1985). In his analysis of acid-base titrations of Suwannee river DOM for Gaussian model fitting parameters, Serkiz (1991) postulated two site-types. Tipping (1994) also used two site-types (carboxylic and phenolic) in his Model V representation of humic substances, as did Benedetti *et al*. (1995) in their implementation of the NICA model. In the bimodal representation of the Gaussian DOM model, the total site concentration associated with the organic matter is apportioned between the two site-types, and each site-type conforms to a Gaussian distribution as defined by Equation (14).

The competitive Gaussian model of cation-DOM binding whose incorporation in MINTEQA2 is discussed here is that described by Dobbs *et al.* (1989a). In this model, the concentrations of individual ligands of the complex DOM mixture are normally distributed with respect to their log *K* values (see Equation (14)). Parameters μ and σ are the mean and standard deviation of the normally distributed log *K* values. The model description below applies to the entity that is assumed to exhibit the normal site distribution. In accordance with the user's wishes, this could mean the entire set of DOM binding sites, or a subset of those sites (such as the carboxylic sites, or the phenolic sites). To simplify the presentation, reference will be made to only one such distribution (*i.e*, to the unimodal case). The reader is reminded that the model is capable of dealing with bimodal and tri-modal site distributions, but the second and third Gaussian distributions (should they be included) would each be calculated as additional unimodal distributions exactly as described below. As output, the user would be presented with the metal bound to each site-type at equilibrium. If more than one site-type are used in a particular model exercise, the only connection between the site-types in the calculation is that they may compete for the binding cations.

In the competitive Gaussian model, an individual ligand site L_i from the multiple ligand population may undergo reaction with protons or metals. The various metals for which reactions are provided compete with each other and with protons for binding sites. The equilibrium distribution of metal-DOM complexes is dictated by the relative log *K* values and relative free activities of all competing reactants. If we assume that all sites are equally available for all competing reactants, the reactions for protonation and metal complexation and their corresponding mass action expressions are

$$H + L_i \rightleftharpoons HL_i \; ; \qquad K_{HL_i} = \frac{[HL_i]}{[H]\,[L_i]} \frac{\gamma_{HL}}{\gamma_H\,\gamma_L} \tag{16}$$

$$M + L_i \rightleftarrows ML_i \; ; \qquad K_{ML_i} = \frac{[ML_i]}{[M]\,[L_i]} \frac{\gamma_{ML}}{\gamma_M \gamma_L} \tag{17}$$

where γ's denote activity coefficients, square brackets indicate concentration, and ion charges are omitted for simplicity. The index *i* is unnecessary on γ because we assume that the activity coefficients among individual ligands within the DOM mixture are identical. Note that both reactions assume 1:1 stoichiometry between the complexing cation and the ligand. This is not necessary from a computational viewpoint, and provision is made in the implementation for whatever ligand-to-metal stoichiometric ratio the user may desire. But as it is not possible to experimentally determine reaction stoichiometries in a complex mixture of ligand sites, 1:1 stoichiometry has traditionally been assumed in metal-humic models and will be observed here for simplicity. An important assumption relevant to the Gaussian DOM model as developed in Dobbs *et al.* (1989a) is that the ratio of the equilibrium constants $K_{\mathrm{ML_i}}/K_{\mathrm{HL_i}}$ is constant for all *i*. This means that the standard deviation σ is the same for binding protons as for metal ions— the protons and metals are bound at the same set of sites, but the sites have different affinities for different cations. This requirement pertained to the method whereby experimental data were analyzed for binding constants of competing metals in their work. It is not required by the mathematical formulation of the model.

In a system having a single metal species, the total concentration of the *i*th ligand in the DOM mixture is

$$T_{L_i} = [L_i] + [HL_i] + [ML_i] \tag{18}$$

The fraction of the *i*th ligand that is protonated is

$$\frac{[HL_i]}{T_{L_i}} = \frac{[HL_i]}{[L_i] + [HL_i] + [ML_i]} \tag{19}$$

Substituting mass action expressions that correspond with reaction Equations (16) and (17) into the right-hand side of Equation (19) and multiplying both sides by T_{L_i} gives an expression for the concentration of protonated *i*th ligand in terms of the free hydrogen and free metal concentrations and the thermodynamic equilibrium constants:

$$[HL_i] = \frac{T_{L_i} K_{HL_i} \Gamma_{HL}^{-1} [H]}{1 + K_{HL_i} \Gamma_{HL}^{-1} [H] + K_{ML_i} \Gamma_{ML}^{-1} [M]} \quad (20)$$

where Γ_{HL} and Γ_{ML} represent the ratio of activity coefficients for the protonation and metal complexation reactions given in Equations (16) and (17), respectively. With the assumption of 1:1 stoichiometry between the ligand and any species that complexes with it, a similar expression gives the concentration of the *i*th ligand complexed with the metal

$$[ML_i] = \frac{T_{L_i} K_{ML_i} \Gamma_{ML}^{-1} [M]}{1 + K_{HL_i} \Gamma_{HL}^{-1} [H] + K_{ML_i} \Gamma_{ML}^{-1} [M]} \quad (21)$$

Substituting for T_{L_i} via Equation (14) gives an expression for the concentration of metal-complexed *i*th ligand in terms of free concentrations, thermodynamic constants, and parameters of the Gaussian DOM distribution:

$$[ML_i] = \frac{T_L}{\sigma\sqrt{2\pi}} \frac{K_{ML_i} \Gamma_{ML}^{-1} [M]}{1 + K_{HL_i} \Gamma_{HL}^{-1} [H] + K_{ML_i} \Gamma_{ML}^{-1} [M]} e^{-\frac{1}{2}\left(\frac{\log K_{ML_i} - \mu_{ML}}{\sigma}\right)^2} \quad (22)$$

To obtain the total concentration of ligand bound with metal, [ML], it is necessary to sum Equation (22) over all *i*:

$$[ML] = \frac{T_L}{\sigma\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{K_{ML_i} \Gamma_{ML}^{-1} [M]}{1 + K_{HL_i} \Gamma_{HL}^{-1} [H] + K_{ML_i} \Gamma_{ML}^{-1} [M]} e^{-\frac{1}{2}\left(\frac{\log K_{ML_i} - \mu_{ML}}{\sigma}\right)^2} d(\log K) \quad (23)$$

A similar expression gives the total protonated ligand, [HL].

Equation (23) can be generalized to express the total concentration, [ML], of any cation-ligand complex in a system involving competitive complexation with N cations (M_1, M_2, ..., M_N). The concentration of cation ligand complex [M_1L] is

$$[M_1L] = \frac{T_L}{\sigma\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{K_{M_1L}\Gamma_{M_1L}^{-1}[M_1]}{1 + K_{HL}\Gamma_{HL}^{-1}[H] + \sum_{n=1}^{N} K_{M_nL}\Gamma_{M_nL}^{-1}[M_n]} e^{-\frac{1}{2}\left(\frac{\log K_{M_1L} - \mu_{M_1L}}{\sigma}\right)^2} d(\log K) \qquad (24)$$

2.2 IMPLEMENTATION OF THE GAUSSIAN DOM MODEL IN MINTEQA2

The Gaussian DOM model has been implemented by altering the MINTEQA2 source code and associated databases. The implementation is generic in the sense that the user may select from among six DOM components that behave in accordance with the Gaussian model. Any one of the DOM components may be used to represent a unimodal distribution about a single site of carboxylic or phenolic type, or as an unspecified type. Two components are used for bimodal distributions and three for tri-modal. The user defines the nature of the functional groups that the selected components represent by specifying names and Gaussian parameters (site acidity (c), μ, and σ) as desired. The inorganic components are entered in terms of their total concentrations as usual. The modified MINTEQA2 recognizes the special DOM components and retrieves proton and metal-complexation reactions from a user-prepared database file. These reactions provide μ and σ for use internally in a special routine that performs the calculation indicated in Equation (24) and computes the contribution of Gaussian DOM species to gradient expressions. (Note: An example database file, GAUSSIAN.DBS, is provided with the MINTEQA2 model. It contains reactions for DOM with protons and with several metals with μ, σ, and site acidities as reported in Susetyo et al., 1991).

The Fortran source code modifications in MINTEQA2 for implementing the Gaussian DOM model include logic to substitute Equation (24) for Equation (2) whenever a species involving DOM is encountered. Each component species in MINTEQA2 is identified by an assigned three-digit identifying number (*e.g.*, 150 for Ca^{2+}, 330 for H^+), and each species other than a component species by a seven-digit identifying number. The six component species provided for DOM have identifying numbers 144 through 149. Reactions involving the DOM components (such as are shown in Equations (16) and (17)) are written separately for each site-type. The seven-digit identifying numbers are assigned such that they lie with the range 1440000 to 1499999. For any species with an identifying number in this range, Equation (24) is implemented rather than Equation (2) via a call to subroutine COMPOSIT.

Equation (24) is implemented in subroutine COMPOSIT via Gaussian quadrature integration as described by Parrish and Perdue (1989). Specifically, the transformation of variables $z = (\log K - \mu)/\sigma$ is used to make the substitutions $10^{\mu+\sigma z} = K$ and $\sigma\, dz = d(\log K)$. The transformed equation is

$$[M_1L] = T_L \int_{-\infty}^{\infty} h(z)\, f(z)\, dz \qquad (25)$$

where $f(z) = (2\pi)^{-½} \exp(-z^2/2)$, and $h(z)$ is the Langmuirian term from Equation (24). For a particular metal M_1, $h(z)$ is expressed

$$h_1(z) = \frac{\Gamma_{M_1L}^{-1}[M_1]\, 10^{\mu_{M_1L} + \sigma z}}{1 + \Gamma_{HL}^{-1}[H]\, 10^{\mu_{HL} + \sigma z} + \sum_{n=1}^{N} \Gamma_{M_nL}^{-1}[M_n]\, 10^{\mu_{M_nL} + \sigma z}} \tag{26}$$

For a particular metal M_1, the integral in Equation (25) is evaluated using the Gauss-Hermite quadrature (Abramowitz and Stegun, 1972):

$$[M_1L] \approx T_L \sum_{i=1}^{J} w_i\, h_1(z_i) \tag{27}$$

where w_i and z_i are tabulated weights and points of the quadrature. Similar expressions are used for other members of the set of competing metals. The quality of the approximation improves with an increasing number of points J. MINTEQA2 implements Equation (27) with $J = 32$ points— larger values of J produce changes that are less than the precision of the MINTEQA2 calculations. Equations (26) and (27) are the implementing equations for the Gaussian DOM model in MINTEQA2.

2.2.1 Calculation of Gradients

As discussed in Chapter 1, MINTEQA2 improves the activity estimate of each component with each iteration by computing the change in component mass balance, Y_j, as a function of the change in the activities of every component. As can be seen in Equation (4), this requires computing the partial derivative of the concentration of each species with respect to the activity of each component that has non-zero stoichiometry in that species. MINTEQA2 calculates $\partial[\mathrm{ML}]/\partial X_k$ where X_k is the activity of some component having non-zero stoichiometry in the DOM species ML via

$$\frac{\partial[ML]}{\partial X_k} = T_L \frac{\partial}{\partial X_k}\left(\sum_{i=1}^{J} w_i h(z_i) \right) \tag{28}$$

Distributing the partial derivative over the expanded sum gives

$$\frac{\partial[ML]}{\partial X_k} = T_L \left(\frac{\partial}{\partial X_k}\left(\frac{w_1 h_{num}(z_1)}{h_{denom}(z_1)} \right) + \frac{\partial}{\partial X_k}\left(\frac{w_2 h_{num}(z_2)}{h_{denom}(z_2)} \right) + \cdots + \frac{\partial}{\partial X_k}\left(\frac{w_J h_{num}(z_J)}{h_{denom}(z_J)} \right) \right) \tag{29}$$

where h_{num} and h_{denom} are the numerator and denominator portions of the expression for $h(z)$ given in Equation (26). For a particular metal-ligand complex M_1L, each partial derivative in Equation (29) has the form

$$w_i \frac{\partial}{\partial \{M_1\}} \left(\frac{\{M_1\} 10^{\mu'_{M_1L} + \sigma z_i}}{1 + \{H\} 10^{\mu'_{HL} + \sigma z_i} + \sum_{n=1}^{N} \{M_n\} 10^{\mu'_{M_nL} + \sigma z_i}} \right) \tag{30}$$

in which the activity coefficient term (Γ) has been included as an adjustment to the equilibrium constant (μ') and in expressing the activity of the complexing component (indicated by braces { } rather than square brackets [ ]). Each partial derivative may be evaluated using the quotient rule

$$\frac{\partial h(z)}{\partial X_k} = \frac{1}{h_{denom}} \frac{\partial h_{num}}{\partial X_k} - \frac{h_{num}}{h^2_{denom}} \frac{\partial h_{denom}}{\partial X_k} \tag{31}$$

In practice, the second term on the right in Equation (31) may be neglected because h^2_{denom} is very large. As a result, the contribution to the gradient for component M_1 complexing the organic DOM ligand can be approximated by

$$\frac{\partial [M_1L]}{\partial \{M_1\}} = \sum_{i=1}^{J} w_i \left(\frac{10^{\mu'_{M_1L} + \sigma z_i}}{1 + \{H\} 10^{\mu'_{HL} + \sigma z_i} + \sum_{n=1}^{N} \{M_n\} 10^{\mu'_{M_nL} + \sigma z_i}} \right) \tag{32}$$

The quantity calculated from this gradient expression gives the expected change in the computed concentration of M_1L as a function of a change in the activity of M_1. Within the framework of the broader speciation model calculations, this quantity is combined with similar gradient contributions from other (inorganic) species in which M_1 has non-zero stoichiometry to estimate the simultaneous change in all component activities that will result in a mass imbalance of zero.

2.2.2 Modifications in MINTEQA2 Source Code

Fortran 77 source code listings presenting the major modifications needed to calculate the concentrations of DOM species in accord with Equation (24) are presented in Allison (1997). Fortran code for the calculation of partial derivatives of DOM species with respect to relevant component activities as depicted in Equation (32) is also included. The source code for MINTEQA2 is included among the files distributed with version 4.0 of the model.

2.3 OTHER MODIFICATIONS FOR THE GAUSSIAN DOM MODEL

The menus and user prompts of PRODEFA2 were altered to query the user for appropriate input information when one or more of the DOM components are selected. In particular, the user is prompted to enter the dissolved organic carbon (DOC) concentration in mg/L. This form of specifying the concentration of dissolved humic substance was chosen because DOC is the usual analytical measurement. The mass fraction of carbon in the organic matter (expressed as a percentage) is also requested, as is the number average molecular weight in Daltons if the option to calculate organic molecular charge as a function of speciation is chosen. As discussed below, this is an optional alternative to using a fixed organic molecular charge.

2.3.1 Treatment of Charge and Activity Coefficients for Organic Species

It has long been noted that proton and metal titrations of DOM are influenced by the ionic strength (I) of the solution (Perdue, 1985). Ionic strength impacts the activity coefficients of all charged solution species. Various empirically derived equations may be used to estimate activity coefficients from ionic strength and species-specific parameters. The most widely used estimator of activity coefficients is the Davies equation, in which the only species-specific parameter is the ionic charge. One obvious difficulty in calculating activity coefficients for DOM species is that of establishing the appropriate value for charge. Susetyo *et al*. (1990) analyzed results from europium titrations of DOM using one site-type (carboxylic) in the Gaussian DOM model. Their results indicated that the use of a constant average charge of -2.8 for the free organic anion site was effective in predicting the change in speciation due to ionic strength changes over a range in I of approximately zero to 0.1 M.

Serkiz (1991) also assumed a constant value to represent the number-average charge of the humic substance organic anion in his acid-base titration study of Suwannee river DOM. He derived a best-fit number-average charge of the uncomplexed organic anion via a series of Gaussian model fitting exercises. Each Gaussian fit was performed on the same titration data ([DOC] = 1000 mg/L and added background electrolyte ranging from zero to 0.5 M) using a different imposed number-average charge (Z_n). The smallest mean squared error in the Gaussian fitting parameters was obtained with Z_n = -4.5. Although -4.5 represented the best average value of the free organic anion charge over the pH range of the titrations, Serkiz noted the need for more rigorous treatment that would account for the change in organic anion charge as a function of speciation as the titration proceeds.

Perdue (1997) has proposed a method of calculating the number-average charge of the humic substance organic anion as a function of speciation. Specifically,

$$Z_n = RZ_s + (R - 1)\frac{[HL]_s + 2[ML]_s}{C_s} \qquad (33)$$

where Z_n is the number-average charge of the organic anion in eq/mol, Z_s is the charge of a ligand binding site within the DOM mixture (assumed equal to -1 eq/mol for all ligands) and C_s is the molar concentration of binding sites (mol sites/L). (The derivation of this equation (by E.M. Perdue) is shown in Allison (1997) along with the Fortran source code representing the MINTEQA2 implementation.) The parameter R is the ratio C_s/C_n where C_n is the molar concentration of humic substance computed from the DOC concentration in mg/L, the percent organic carbon (C%) in the organic matter, and the number-average molecular weight (M_n):

$$C_n = \frac{[DOC]}{10\ C\%\ M_n} \tag{34}$$

The concentration quantities in square brackets with *s* subscripts in Equation (33) are the concentrations of protonated and metal-complexed sites. Thus, all quantities subscripted with *n* refer to properties of the humic substance molecule (whose definition is based on a number-average molecular weight), and all quantities subscripted with an *s* refer to properties of the of the binding sites associated with the humic molecule.

As can be seen by examination of Equation (33), for a given concentration of a particular humic substance, the average charge on the humic substance molecule (Z_n) varies with the speciation (*i.e.*, with pH and total metal concentration). The implementation of this charge calculation required the development of two new subroutines in MINTEQA2 and a reorganization of the logic that controls the calculation of ionic strength, activity coefficients, and adjusted equilibrium constants. In particular, the model was changed so that it re-calculates activity coefficients with each iteration, even if the ionic strength is constrained to a user-supplied value. This is made necessary by the interdependence of charge, activity coefficients, and speciation.

The program options for establishing the charge of DOM sites include the speciation-dependent method represented by Equation (33), or the use of a constant charge specified by the user. In either case, the charge on any DOM species other than the free (uncomplexed) anion is calculated by the usual charge balance equation as applied to chemical reactions. For example, if the free organic anion charge is -3.8, the charge on a species such as CuL_2 would be -5.6 (where Cu is the cupric ion).

CHAPTER 3

MODIFICATIONS IN MINTEQA2 TO MINIMIZE VIOLATIONS OF GIBBS PHASE RULE

MINTEQA2 version 4.0 has been modified to reduce to occurrence of violations of Gibbs phase rule during execution. The phase rule is an expression that relates the number of independent components (*C*), the number of phases (*P*), and the number of degrees of freedom (*F*) in an equilibrium system. In systems of variable temperature and pressure, the phase rule is expressed

$$F = C + 2 - P \tag{35}$$

For systems relevant to calculations with MINTEQA2, the temperature and pressure are constant and the phase rule becomes

$$F = C - P \tag{36}$$

In terms of speciation modeling in an aqueous system, this rule is violated when the number of equilibrium constraints (*e.g.*, user-specified equilibrium pH, gas partial pressure, *etc*.) exceeds the number of independent components. Two types of phase rule violations can occur in speciation programs such as MINTEQA2: global and local. A global violation occurs when the number of degrees of freedom calculated on the basis of all equilibrium constraints (represented by pure phases, *(P*) and all independent components (*C*) becomes zero. Consider for example the system represented by the components Ca^{2+}, Mg^{2+}, CO_3^{2-}, and H^+. (H_2O is understood to be both a pure phase and component in all aqueous speciation problems; it therefore has no impact on the number of degrees of freedom, and will be omitted from further discussion. Also, charges will be omitted hereafter except where clarity of meaning demands). Suppose that the model is configured to determine the speciation, including the equilibrium solid phases, given that total concentrations of Ca and Mg are specified (3 and 1 mM, respectively), and that equilibrium values are specified for the solution pH (11.5) and the partial pressure of CO_2(g) (P_{CO2} = 0.0003 atm). The problem is solved iteratively using mass action and mole balance equations as described in Chapter 1. Upon the determination of component activities satisfying equilibrium conditions for the solution phase, all possible solid phases are checked for supersaturation with respect to the solution, and all existing solid phases are checked for undersaturation with respect to the solution. The problem as specified above will result in the precipitation of calcite ($CaCO_3$). After depleting the aqueous concentrations of Ca and CO_3,

iterations will resume. The problem will terminate with a global phase rule violation immediately upon precipitating a second solid, no matter its composition. (The actual solid that precipitates is magnesite ($MgCO_3$)). The reason for this is that upon formation of the second precipitate, the number of constraining phases is equal to the number of components (four each). This is not a phase rule violation in the strict sense. It appears as such to the speciation model because all variables are constrained— there are no unknowns to be solved for. A global phase rule violation can be overcome by adding another component. Typically, a model execution that ends in this way is re-done after adding a small amount of an inert component such as nitrate (NO_3^-). If a third solid phase precipitates, this process may need to be repeated. The newly developed routines test for an impending phase rule violation of either type. Upon detecting a global violation, a dummy component (chemically inert) is automatically inserted into the problem so that calculations may continue without user intervention.

The local phase rule violation occurs when the number of degrees of freedom defined by a restricted subset of system components and associated equilibrium constraints becomes less than zero. Consider again the components and initial constraining conditions specified above. Before iterations begin, there are four components and two constraining species (fixed pH and fixed P_{CO2}). Each of these constraints established the value of one component activity and reduces *F* by one. Specifically, let us assume that the fixed pH establishes the value of H^+ activity, and P_{CO2} establishes the value of CO_3^{2-} activity. When calcite precipitates, the activity of Ca^{2+} must become fixed. Assuming that an inert component has been inserted so that no global violation occurs, the precipitation of magnesite establishes the value of Mg^{2+} activity. The system-wide *F* is equal to one because of the inert component. Within the restricted subset of components defined by Mg, Ca, CO_3, and H, the number of degrees of freedom is zero due to the four equilibrium constraints (pH, P_{CO2}, calcite, and magnesite). This is not a phase rule violation because *F* equal to zero is permissible in a restricted subset of the system. However, suppose that as iterations proceed, a third solid precipitates, specifically, one that consists only of components defined by the restricted subset. The addition of the third solid will certainly reduce the system-wide *F* to zero and cause a global phase rule violation. However, it will be observed that upon the addition of a second inert component, a local phase rule violation will result. This is because the addition of a second inert component does not address the key issue: the third solid phase composed only of two or more of the four components cannot establish the activity of any component because all four of those component activities are already fixed by the four previous constraints. This is a violation of the phase rule in the strictest sense. It can only mean that one of the two solids already precipitated is not a member of the true equilibrium solid phase assemblage. In cases where the user has imposed an equilibrium solid phase (not an issue in this example, but possible), it may mean that the specified solid cannot (according to thermodynamics) be a member of the true equilibrium solid phase assemblage.

Previously, a local phase rule violation could be overcome only by trial and error— the program is restarted with the specification that calcite is to be excluded from consideration as an equilibrium solid. Frequently, the result will be that an isomorph of calcite (*e.g.*, aragonite) will precipitate instead, and the same phase rule violation will occur when magnesite precipitates. After several aborted runs, a set of precipitates will be found that do not give a phase rule violation (magnesite and

dolomite ($CaMg(CO_3)_2$) for this example). Unfortunately, the results of this "successful" model run may be misleading. For instance, in our example the correct equilibrium solid phases are calcite and dolomite, not magnesite and dolomite. This can be confirmed by examining the saturation state (log ion activity product) of calcite in the "successful" run. The final equilibrium solution phase will be supersaturated with respect to calcite.

The new program logic has been implemented to eliminate all local phase rule violations that are not a direct consequence of user imposed equilibrium solid phases. This is accomplished by keeping track of which component each constraining species fixes, and testing each new precipitate to see if a local phase rule violation will result. If so, the species that have previously fixed the component activities of the new precipitate are tested to see which one should dissolve. If the one that should dissolve was precipitated in a prior iteration, it is dissolved and shifted to the excluded category. If the one that should dissolve to make way for the new solid is a user-specified equilibrium solid phase, the phase rule violation is not preventable. In that case it is allowed to occur and the user is advised either to change the specification of the imposed equilibrium solid, or to shift the true thermodynamically stable phase to the excluded category so that computations may continue. A bonus to including more stringent bookkeeping concerning relationships between the constraining solid phases and the components whose activities they fix is that it becomes possible to allow the simultaneous precipitation of multiple unrelated solid phases each time the aqueous solution is equilibrated.

In the example problem involving Ca, Mg, CO_3, and H discussed above, a single model run using the new routines will result in the correct equilibrium solids (calcite and dolomite). In arriving at this solution, the program will correctly handle both global and local phase rule violations without user intervention.

3.1 SOURCE CODE MODIFICATIONS

Subroutines PREP2, PRECIPIT, PHASECHK, and DISSOLVE constitute the major source code modifications to implement the phase rule checking procedures. Subroutine PREP2 establishes relationships among components and their controlling phases. It also shifts certain isomorphic forms of user-specified solids to the excluded category. Subroutine PRECIPIT determines which solid phases to precipitate and manages the simultaneous precipitation of multiple solids. Subroutine PHASECHK determines whether a phase rule violation will result from a precipitation event. Subroutine DISSOLV2 determines which previously precipitated solid should be dissolved when there is an impending local phase rule violation. These subroutines are presented in Allison (1997) and also are distributed with MINTEQA2 version 4.0.

CHAPTER 4

OTHER MODIFICATIONS IN MINTEQA2/PRODEFA2

Other improvements and modifications in MINTEQA2/PRODEFA2 since version 3.0 include changes to improve the execution speed and to reduce the occurrence of non-convergence in MINTEQA2, modifications to allow titration of a user-specified system with any chosen species as the titrant (except DOM or sorption species), modifications to allow key output to be written to a separate file for import to a spreadsheet, modifications to allow the user to provided customized filenames for database files, and correction of known errors in earlier versions. A minor modification in the subroutine that prints the date and time in the output file was made to insure the correct printing of full four-digit years for Y2K compliance. Significant changes are discussed more fully in separate sections below.

4.1 IMPROVEMENT IN EXECUTION SPEED

In MINTEQA2, mass law equations and equations for computing the partial derivatives of component mole balance equations with respect to component activities are implemented generally. The Fortran DO loops that implement these equations operate over indices that range from one to the number of components (*n*) and one to the number of species (*m*). The array of stoichiometric coefficients has dimensions *n* x *m*. When *n* and *m* are large, say *n* = 20 and *m* = 250, most of the coefficients will be zero. This arises from the fact that, with the exception of H^+ and H_2O, no component is likely to occur in more than a dozen or so species. In the mass law and partial derivative computations, the immediate result is that the program spends more time multiplying by zero and summing with zero than in calculating with the meaningful non-zero coefficients. Because the single largest computational burden is in calculating the partial derivatives for use in improving component activity estimates, and because this calculation must be done at each iteration, substantial time savings can be realized by eliminating multiplications by zero and subsequent additions of the result. This has been accomplished by designing and loading pointer arrays that contain the row and column addresses of all non-zero stoichiometric coefficients. The pointer arrays are loaded at the beginning of each speciation problem and each time a solid precipitates. They are used in calculating mass action equations and to calculate partial derivatives. The degree to which the execution speed has been increased is a function of the size of the speciation problem— the larger the problem, the greater the benefit. A problem with three components and less than ten species is not much effected. A typical groundwater speciation problem with 20 or so components and 200 to 300 species will execute almost ten times faster than without the pointer modifications. The number of iterations

required is not affected by the use of pointer arrays, but because the relevant equations are implemented with each iteration, problems that take more iterations benefit more from this modification.

Use of this modification requires no action of the part of the user and no changes in any input data. The source code modifications to implement these changes are described in Allison (1997).

4.2 MODIFICATIONS TO MINIMIZE NON-CONVERGENCE

Changes have been made in version 4.0 to reduce the number of iterations required to solve the equilibrium problem and to reduce the occurrence of non-convergence (failure to obtain a mathematical solution via Newton-Rapshon iterations). Logic has been added that puts a temporary hold on the computed ionic strength when the number of iterations without obtaining convergence exceeds 12. This option is operative only for model runs in which the user has specified that the equilibrium ionic strength is to be computed. In that case, the equilibrium problem is more difficult to solve because each time the concentrations of all species are re-computed, the computed ionic strength also changes, and thus the activity coefficients of all charged species change. The change in activity coefficients is expressed as a change in the equilibrium constants of the species, and thus, the concentrations must be re-computed, which in turn results in a change in the ionic strength, etc. In some circumstances, this can result in a very slow convergence or even non-convergence in the Newton-Raphson iterations. This modification remedies this problem by temporarily establishing a hold on the ionic strength (so that it is treated as invariant) if 12 iterations have occurred without convergence. With the ionic strength fixed, the problem can be more easily solved. Once a mathematical solution is obtained, the hold on the ionic strength is released and a few extra iterations are forced to insure that equilibrium with an unconstrained computation of ionic strength is achieved.

The use of the modification described above is user-controlled. PRODEFA2 provides prompts from EDIT LEVEL 1 that allow the user to specify the maximum number of to be allowed before execution is stopped. This option provides for 200 iterations, which should be sufficient for most problems. In cases where convergence is not obtained in 100 iterations, the user may select 500 iterations with the convergence-assist option activated.

Another significant revision in the version 4.0 includes the development of selection rules for choosing the component to be eliminated upon the precipitation of a solid phase. When a multi-component solid phase is imposed by the user or when a solid phase precipitates during the calculations, the number of degrees of freedom in the numerical solution is reduced by one. This reduction corresponds to the elimination of one component activity as an unknown in the equilibrium problem. For multi-component solid phases, this requires that the model select which component of the solid should be eliminated. Chemically and mathematically, no choice is more correct than another. However, because of limitations in the precision of calculations, there may be a “computationally” more correct choice. MINTEQA2 version 3.11 and previous versions made the selection of which component to eliminate based on the order of the components in the input file.

Since the order of the components in the input file is arbitrary, sometimes the "computationally correct" choice was not made. In such a case, the Newton-Raphson routine was unable to reach a solution (i.e., a failure to converge is reported by the model). The modification in version 4.0 includes the development of five new rules for selecting the component to eliminate and logic that enables the model to detect non-convergence and reconfigure the equilibrium problem using a different selection rule if non-convergence occurs.

Rule 1- Select the candidate component with the smallest total concentration
Rule 2- Select the candidate component involved in the greatest number of equilibrium constraints
Rule 3- Select the candidate component involved in the fewest number of equilibrium constraints
Rule 4- Select the candidate component with the smallest magnitude free activity
Rule 5- Select the candidate component with the largest magnitude free activity

The selection rules are prioritized in the order shown above. Each execution begins with rule 1 as the basis for selecting which component to eliminate. If non-convergence is detected, the problem is reconfigured using rule 2. Continued non-convergence results in another reconfiguration using rule 2, and so on.

4.3 MODIFICATIONS FOR MODELING TITRATIONS

Version 3.11 included a limited titration capability in that the fixed (equilibrium) activity or total concentration of a single component could be designated as varying over a set of values supplied by the user. This option has been expanded in version 4.0 to allow any species that can be formed by MINTEQA2 components (except sorption or DOM components) to serve as the titrant. Even species that are not in the thermodynamic database (e.g., HCl) may be so designated, albeit with the assumption of total dissociation in aqueous solution. In addition to acids and bases that totally dissociate, any aqueous or solid species in the database (except sorption or DOM species) may be designated as the titrant. A titration over a series of fixed pH or pe values is also permitted.

This option is implemented in PRODEFA2 such that menu prompts guide the user in designating the titrant and the values of total concentration or equilibrium activity to be used at each titration point.

4.4 MODIFICATIONS FOR SPECIALIZED OUTPUT

Version 4.0 retains the capability of allowing the user to select up to six components or species whose equilibrium concentrations will be written to an ASCII text file in tabular form for import by a spreadsheet program. The equilibrium mass distribution among dissolved, sorbed, and precipitated phases may be written for components. Alternatively, the equilibrium concentration of any species (including component species) may be written. This use of this option is via menus and prompts in

PRODEFA2. It can be used together with the titration option to generate data for plotting, (e.g., the equilibrium concentration of HCO_3^- versus pH).

4.5 MODIFICATIONS FOR CUSTOMIZED DATABASE FILENAMES

This modification is intended to make it easy to use customized database files and to keep up with which database was used in generating an particular output file. Occasionally, a user may develop a database file using customized thermodynamic data. (Of course, this file must conform to MINTEQA2 format requirements; see Chapter 5). In earlier versions, the main thermodynamic database in MINTEQA2 must be named "THERMO.UNF". The "UNF" extension designates a file that is internally unformatted. The unformatted file is generated by the program UNFRMT using the corresponding ASCII text file "THERMO.DBS". Version 4.0 still requires the database to be an unformatted file and the generation of this file is still handled by UNFRMT. However, the database may be named whatever the user wishes. The PRODEFA2 program displays the current setting of filenames that MINTEQA2 will use. The user may change these names so that other files will be used instead. The selected files whose names are displayed by PRODEFA2 will be used the next time MINTEQA2 is executed and their names will appear in the main MINTEQA2 output file identifying them as the source of the thermodynamic data used in the model run.

4.6 CORRECTION OF KNOWN ERRORS IN EARLIER VERSIONS

Two known errors in version 3.11 are corrected in version 4.0:

1) In some circumstances, the standard deviation in log K for species used in the Gaussian DOM model could be treated as an enthalpy value and used to correct the mean log K for temperature. Because the standard deviation is a relatively small value (2.5 or less), this would not produce significant error in speciated results. This error has been corrected in version 4.0.

2) An error in the algorithm that calculates total carbonate from a user supplied alkalinity could cause erroneous results for cases where the equilibrium pH is less that 1.0. This error has been corrected in version 4.0.

CHAPTER 5

MODIFICATIONS TO THE THERMODYNAMIC DATABASE

The thermodynamic database used by MINTEQA2/PRODEFA2 has been revised to correct and update thermodynamic constants, to add environmentally relevant species and their associated reactions for beryllium (Be), cobalt (Co), molybdenum (Mo), and tin (Sn), and to provide reference citations for equilibrium constants for all species. In addition, the format of the database has been changed to accommodate longer species names.

With the release of version 3.0, the thermodynamic database for MINTEQA2 included 31 organic ligands and associated reactions to represent complexation with trace metals. Unfortunately, some equilibrium constants were not properly adjusted or re-formulated for use with MINTEQA2 components as reactants. Use of the database for affected ligands could lead to erroneous results (Serkiz *et al.*, 1996). In version 4.0, all species involving the 31 organic ligand components have been reviewed and corrected if needed. One organic component, identified as component number 960, "TRIBUTPH" was found to have no corresponding species and was removed from the database. Of the 450 species involving the other 30 organic ligand components, 370 have been retained, most with updated thermodynamic constants or other parameters. Eighty of the original 450 have been deleted due to an absence of data within the necessary range of ionic strength (I) and temperature (T) (0.0 to 1.0 M for I and 20-30 ^{o}C for T). More than 200 new species involving these organic ligands have been added to the database.

In addition to the correction of errors in the metal-organic complexes, the revised database for version 4.0 includes reactions for aqueous species of Be(II), Co(II and III), Mo(VI) and Sn (II and IV). Also, compilations of stability constants have been used to verify and update the thermodynamic constants for inorganic species. Where possible, the source of the thermodynamic data has been cited in the version 4.0 database. The format of the database has been changed to accommodate the reference citations and to allow longer species names

5.1 DATA SOURCES

Several recognized compilations of thermodynamic constants were used as data sources for the review and update of equilibrium constants and enthalpy of reaction values. Values were also obtained from journal articles. The sources were accorded priority according to their order in the list below. If data were not found, the next source in the list was consulted, etc.

5.1.1 Prioritized List of Sources

1. *Critical Stability Constants of Metal Complexes Database* (CRITICAL) published by the National Institute of Standards and Technology (NIST Standard Reference Database 46). Multiple versions of this database were used beginning with version 2.0 (released in late 1995), and ending with version 4.0 (released in late 1997). The correction and update of the v3.11 metal-organic reactions was completed first. This update employed version 2.0 of the NIST CRITICAL database. The update of the general inorganic species began while version 3.0 of CRITICAL was the current NIST product. Version 4.0 of CRITICAL was released during the course of updating the inorganic species and was used to finish the project. A comparison of log *K* values for a sampling of the metal-organic complexes from CRITICAL revealed no differences between version 4.0 and version 2.0 constants. The improvements in version 3.0 and 4.0 are primarily the presence of more reactions and improved program functionality rather than updated constants. In the final MINTEQA2 database, the source reference code for each species updated with the CRITICAL database indicates the version from which the data were obtained ("NIST46.2", "NIST46.3", "NIST46.4", respectively for CRITICAL versions 2.0, 3.0, and 4.0). These source designations are used in the database and in the table of values (Appendix A) accompanying this report.

2. *Stability Constants Database* (SC-DATABASE) published by the International Union of Pure and Applied Chemistry (IUPAC) and Academic Press. Two different versions of this database were used. In the correction of thermodynamic constants for metal-organic complexes, version 2.62 (released in 1996) was used. In the database review for inorganic species, version 3.02 (released in early 1998) was used. In the final MINTEQA2 database, the source reference code for each species updated with SC-DATABASE indicates the version from which the data were obtained ("SCD2.62" and "SCD3.02", respectively for versions 2.62 and 3.02). The reference cited in the actual MINTEQA2 database indicates the journal article reference within SC-DATABASE for version 3.02 citations. These source designations are used in the database and in this report.

3. Nordstrom *et al.*(1990) presented data intended to update and document data appearing in the U.S. Geological Survey equilibrium model WATEQ. Many of the reactions updated in that model also appear in the MINTEQA2 database, so those updates were incorporated. Data from this source are indicated with the source reference code "Nord90" in the database and in this report.

4) Relevant data from journal articles and other compilations. Use of data from journal articles was indicated by a code with the year followed by the first two authors initials (surnames) and a suffixed letter to insure uniqueness (e.g., 1993 DKa). The complete reference is given in the bibliography with the code used in the database.

5. Gibbs free energy of formation ($\Delta_f G^o$) and enthalpy of formation ($\Delta_f H^o$) values from four different sources were used to compute the Gibbs free energy of reaction and enthalpy of reaction. The

former was used to compute the log *K* for the reaction. The four data sources (in the preferred priority) were: 1) *CODATA Key Values for Thermodynamics* published by the Committee on Data for Science and Technology (CODATA) in 1989; 2) NIST *JANAF Thermochemical Tables 1985*, Standard Reference Database 13, version 1.0. Released in electronic format in 1993, the last update of the actual data in this database was 1985; 3) The NIST *Chemical Thermodynamics Database*, Standard Reference Database 2, version 1.1. This is the electronic form of the older National Bureau of Standards thermodynamic database. Version 1.1 was released in 1992, but the latest revisions to the data are from 1989; and 4) Standard Potentials in Aqueous Solution (Bard *et al.*, 1985). Data obtained from these four sources are denoted by the codes "CODATA89", "NIST13.1", "NIST2.1.1", and "Bard85", respectively, in the source indication for the MINTEQA2 database and in this report.

5.2 DATA REDUCTION

Data reduction tasks are often required before adding thermodynamic data for a new or existing reaction to the MINTEQA2 database: 1) The log *K* of the defining reaction must be extrapolated to zero ionic strength and adjusted to correspond to a temperature of 25 °C, and 2) The defining reaction must be formulated so that it is expressed in terms of MINTEQA2 components. For data given at other values or *I* or *T*, the correction to zero ionic strength and 25 °C should always be done prior to reformulating the reaction in terms of MINTEQA2 components. This is because the process of reformulation may involve adding one or more reactions to the defining reaction. If the log *K* correction is not done prior to reformulation and if the log *K* values corresponding to these added reactions are already corrected to I=0 and T=25, the resulting composite constant will be a hybrid that does not correspond to the values of *I* and *T* of the original reaction or to I= 0 and T=25. Therefore, correction of the original reaction log *K* values to I=0 and T=25 was always performed first.

If the log *K* and enthalpy of reaction for a MINTEQA2 reaction were not available from reviewed compilations, these values were computed from $\Delta_f G^o$ and $\Delta_f H^o$ values.

5.2.1 Ionic Strength and Temperature Corrections of Log *K*

When new reactions are added to the database, log *K* values reported at I>0 must be corrected using estimates of activity coefficients (γ) for reactants and products. It is reasonable to use the same method to estimate the activity coefficients in this data correction step as is used in MINTEQA2 to adjust the constants during calculations. The most universally applicable estimator available in MINTEQA2 is the Davies equation:

$$\log \gamma_i = -0.51 z_i^2 \left[\frac{\sqrt{I'}}{1 + \sqrt{I'}} - 0.3 I' \right]$$

where the subscript *i* refers to each of the reactants and products in the reaction, z_i is the ionic charge of each reactant or product, and I' is the ionic strength reported for the experimental data. Once computed, the activity coefficients are used in the following relationship to correct the equilibrium constant to I=0:

$$K_{I=0} = K_{I'} \frac{\prod_i \gamma^{\nu}_{i,products}}{\prod_i \gamma^{\nu}_{i,reactants}}$$

where ν represents the reactant or product stoichiometric coefficient.

The correction to 25° C was accomplished by use of the standard enthalpy of reaction (ΔH_r^o) and the van't Hoff equation. For some reactions, ΔH_r^o is simply not available and zero is entered for enthalpy in the MINTEQA2 database. In such cases, the reported equilibrium constant is incorporated without correction. MINTEQA2 also uses the van't Hoff equation to adjust equilibrium constants during speciation calculations for those reactions having non-zero enthalpy when the user specifies a system temperature other than 25° C. When ΔH_r^o is given in kJ mol^{-1}, the van't Hoff equation is:

$$\log K_{25} = \log K_T + \Delta H_r^o (25 - T) (0.000588)$$

where T is the temperature at which log K is reported in degrees Celsius.

5.2.2 Expressing the Reaction in Terms of MINTEQA2 Components

All reactions in MINTEQA2 must be written as formation reactions from the MINTEQA2 components. For solid species, the log K and standard enthalpy of reaction, ΔH_r^o, needed in MINTEQA2 may be of opposite sign to that reported in the literature (usually reported as a solubility product constant). Also, both solid and dissolved reactions obtained from the literature and their associated thermodynamic constants may need to be added or subtracted from other reactions as required to reformulate the reaction in terms of MINTEQA2 components. An example is the species $CuHEDTA^-$ given in the NIST CRITICAL database by the reaction:

$$CuEDTA^{2-} + H^+ \rightleftharpoons CuHEDTA^- \qquad \log K = 3.1 \text{ @ } I = 0.1 \text{ M}$$

After correction to ionic strength zero, a log K value of 3.5 is obtained. This reaction still cannot be used in MINTEQA2 because $CuEDTA^{2-}$ is not a MINTEQA2 component. To reformulate the reaction for MINTEQA2, the reaction for the formation of $CuEDTA^{2-}$ from the components Cu^{2+} and $EDTA^{4-}$ must be added to this reaction:

$CuEDTA^{2-} + H^{+} \rightleftharpoons CuHEDTA^{-}$ $\log K = 3.5$ (i)

$Cu^{2+} + EDTA^{4-} \rightleftharpoons CuEDTA^{2-}$ $\log K = 20.54$ (ii)

$Cu^{2+} + H^{+} + EDTA^{4-} \rightleftharpoons CuHEDTA^{-}$ $\log K = 24.0$ (iii)

The last reaction (iii) and its associated thermodynamic constants are now correctly expressed in terms of MINTEQA2 components and are in the appropriate form for the MINTEQA2 thermodynamic database.

5.2.3 Other Data Reduction Methods

If the log *K* and enthalpy of reaction for a MINTEQA2 reaction were not available from reviewed data sources, the following relationships were used to compute these values from $\Delta_f G^o$ and $\Delta_f H^o$ values:

$$\Delta G_r^o = \sum_i \nu_i \Delta_f G_{i,products}^o - \sum_i \nu_i \Delta_f G_{i,reactants}^o$$

$$\log K = \frac{-\Delta G_r^o}{2.303 R T}$$

where *R* is the universal gas constant, and

$$\Delta H_r^o = \sum_i \nu_i \Delta_f H_{i,products}^o - \sum_i \nu_i \Delta_f H_{i,reactants}^o$$

5.3 QUALITY ASSURANCE EFFORTS

Apart from the accuracy of information recorded and presented in CRITICAL, SC-DATABASE, and other data sources, the process of querying a data compilation, recording the retrieved information, reducing the data in some fashion, entering the result in another database requires attention to details and repeated checking for accuracy to insure a final product that is free of secondary errors. The following steps were taken to minimize errors in the final MINTEQA2 thermodynamic database:

1) Data obtained from compilations of log *K* and enthalpy were recorded on data entry sheets with the exact reaction as given in the source and the pertinent ionic strength and temperature. During the data gathering stage, no attempt was made to correct the data for ionic strength or temperature, or to reformulate reactions in terms of MINTEQA2 components. After recording,

the information was double-checked against the source for accuracy.

2) The information recorded on each data entry sheet was entered in a data storage and manipulation program, MINCHEK, via on-screen prompts having the same format as the data entry sheet. After entering, the displayed data was compared against the data entry sheet for accuracy.

3) The $\Delta_f G^o$ and $\Delta_f H^o$ values from the JANAF and NIST2 databases were read directly into the data storage program from the computer databases of the sources themselves.

4) After all data was collected and entered, the data reduction module in MINCHEK was used to correct the log *K* values for ionic strength, temperature corrections were computed and applied, and the data were reformulated such that all reactions were expressed in terms of MINTEQA2 components. The latter step was accomplished by adding reactions and their log *K* and ΔH_R values as required. All data reduction steps were computed and applied internally by MINCHEK. Gram-formula weights and species charge were computed automatically by MINCHEK for each species from the stoichiometry, gram-formula weight (or atomic weight), and charge of each reactant (component).

5) The corrected, reformulated data were displayed on-screen for selection. For the most part, the prioritization of the data sources as described above resulted in only a single new value of a data element. However, sometimes more that one reasonable value was obtained, and the value to be used was selected from among these multiple data elements. Multiple data elements were displayed together on one screen along with the "old" version 3.11 values.

6) After log *K* and ΔH_R values were selected in MINCHEK for each species, the new MINTEQA2 database was automatically written in the required format, including reference citations for the data source. New unformatted database files (*.UNF files) were created by the UNFRMT program for use with MINTEQA2.

7) A table showing "old" and updated values of log *K* and ΔH_R side-by-side for each species was examined to find instances of large disparity. These were individually examined to be sure the updated data were correct.

5.4 REVIEW AND CORRECTION OF METAL-ORGANIC SPECIES

The v3.11 database had 31 organic ligand components and 450 species. The updated database has 30 organic components and over 500 species. No species were actually present in the v3.11 database for the component number 960, Trbutph (Tributylphosphate). Inasmuch as there were no current species, and no reactions could be found in CRITICAL or SC-DATABASE for this ligand, this component was deleted.

5.4.1 Component and Species Names for Organic Species

Component numbers for organic ligands are the same as in v3.11. Also, seven-digit species identifying numbers of species present in v3.11 have not been changed unless they were found to be in error. However, most organic ligand component names and metal-organic species names have been changed for clarity. The component name field in COMP.DBS is only eight characters wide and the species name field formerly allowed only 12 characters in THERMO.DBS. The expansion of this field to 21 characters in version 4.0 allows complete and understandable names to be used. These are combined in the usual way with parentheses and a following number to indicate a stoichiometric subscript. The species charge is not given in the names of metal-organic species as it is for aqueous inorganic species. Square brackets have been used to separate the metal and organic ligand portions of the species names. The identifying number, name, and charge of each organic ligand component is given in Table 5.1. The carboxylic and di-carboxylic ligands are referenced by their fully protonated names in CRITICAL and SC-DATABASE and most other literature references. However, the reactions and associated equilibrium constants are often written with the de-protonated form representing the ligand. For example, in both CRITICAL and SC-DATABASE, one must enter the search name Benzoic Acid for the purposes of referencing the available data. But, once retrieved, the data is presented with the de-protonated form, benzoate, as the actual ligand. Likewise, MINTEQA2 uses the deprotonated form of this monoprotic acid, benzoate, as the component. The component field in MINTEQA2 will not accommodate the full names of some organic ligands, so these are abbreviated in the component database.

Table 5.1 Organic Ligands and the Associated MINTEQA2 Component ID No., Name, and Charge.

Ligand	Component ID No.	Component Name	Charge
Benzoic acid	917	Benzoate	-1.0
Phenylacetic acid	918	Phenylacetate	-1.0
Isophthalic acid	920	Isophthalate	-2.0
Diethylamine	955	Diethylamine	0.0
Butylamine	956	Butylamine	0.0
Methylamine	958	Methylamine	0.0
Dimethylamine	959	Dimethylamine	0.0
Hexylamine	961	Hexylamine	0.0
Ethylenediamine	963	Ethylenediamine	0.0
Propylamine	964	Propylamine	0.0

Ligand	Component ID No.	Component Name	Charge
Isopropylamine	965	Isopropylamine	0.0
Trimethylamine	966	Trimethylamine	0.0
Citric acid	967	Citrate	-3.0
Nitrilotriacetic acid (NTA)	968	NTA	-3.0
Ethylenediaminetetra-acetic acid (EDTA)	969	EDTA	-4.0
Propionic acid	971	Propionate	-1.0
Butyric acid	972	Butyrate	-1.0
Isobutyric acid	973	Isobutyrate	-1.0
2-Methylpyridine	980	2-Methylpyridine	0.0
3-Methylpyridine	981	3-Methylpyridine	0.0
4-Methylpyridine	982	4-Methylpyridine	0.0
Formic acid	983	Formate	-1.0
Isovaleric acid	984	Isovalerate	-1.0
Valeric acid	985	Valerate	-1.0
Acetic acid	992	Acetate	-1.0
Tartaric acid	993	Tartrate	-2.0
Glycine	994	Glycine	-1.0
Salicylic acid	995	Salicylate	-2.0
Glutamic acid	996	Glutamate	-2.0
Phthalic acid	997	Phthalate	-2.0

5.4.2 Database Changes for Metal-Organic Species

Of the 450 metal-organic species present in the v3.11 database, 370 were retained after the review and 80 were deleted. A total of 192 new species were added in the updated database (not counting species added later for Be, Co, Mo, Sn, and Sr) . The equilibrium constant (log *K*), enthalpy of reaction (ΔH_r^o), species charge, gram-formula weight, and stoichiometry have been reviewed and corrected if needed. There were three possible reasons for deletion:

1) No reference was found to the species in CRITICAL or SC-DATABASE or other sources consulted.

2) Data was found, but was given for an ionic strength greater than 1.0 M. Log *K* values in the MINTEQA2 database are should be referenced to zero ionic strength. Frequently, data is given at ionic strength of 0.1 M or above. These log K values must be corrected to zero ionic strength using activity coefficients pertinent to the given ionic strength. All such activity coefficients used in this database review were computed from the Davies Equation. Coefficients become progressively less reliable above an ionic strength of 0.5 M. The cut-off for effective use of the Davies equation was treated as 1.0 M in updating and correcting the metal-organic species from the v3.11 database.

3) Data found in CRITICAL or SC-DATABASE, but was incongruous with other data.

5.5 REVIEW AND UPDATE OF OTHER DATABASE SPECIES

After the modifications described above, the inorganic species were reviewed and reactions were added for beryllium, cobalt (II and III), molybdenum (VI), tin (II and IV) and strontium. The version 3.11 database already had a few reactions for Be and Sr, but the databases were too incomplete to be useful. Data sources listed above were searched for reactions for these metals with all ligands in the MINTEQA2 database. In addition, the data sources were searched for thermodynamic data for all current reactions so that as many data elements as possible were verified or updated. Approximately 230 new inorganic species were added to the database. In addition, the v3.11 cyanide section of the database was completely replaced, certain silicate minerals not known to exhibit reversible solubility equilibria in natural waters were deleted according to recommendations in Nordstrom *et al.* (1990), various species for which equilibrium constants were not available were deleted in favor of allowing the user to make the judgement as to whether to include them.

The entire revised database is presented in Appendix A. The old (v3.11) data is displayed alongside the new data. Species that were not present in version 3.11 do not have old data displayed. The source of the log *K* or thermodynamic data from which log *K* was computed is also indicated. The source of the enthalpy of reaction is not listed in the table of Appendix A, but does appear in the MINTEQA2 database. The format of the version 4.0 database is given in Appendix B.

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APPENDIX A

THERMODYNAMIC DATABASE FOR MINTEQA2 V4.0

Enthalpy of reaction (del H) is in kJ/mol. Any species for which an "old" (v3.11) log K is not specified has been added in version 4.0. The cited source reference pertains to the log K of the reaction. Reference codes are explained in the reference section. The actual database gives a separate source citation for log K and enthalpy of reaction. A source of "MTQ3.11" means that the values are not updated from the version 3.11 database. This is almost always because reliable values were not found in the sources consulted.

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
3307301	S-2	-12.9180	-17.3000	50.6264	49.4000	LMa1987
3307601	Se-2	-14.9529	-15.0000	48.1160	48.1160	SCD3.02
8713300	Tl+3	4.7424	3.2910	0.0000	0.0000	NIST46.3
3600000	Hg (aq)	6.9316	6.5667	-69.4753	-45.7350	NIST2.1.1
3613300	Hg+2	6.0970	6.1940	-46.2750	-39.7200	NIST46.3
2113300	Cr+3	9.6200	9.5688	-84.2658	-129.6200	NIST46.3
3300020	OH-	-13.9980	-13.9970	55.8355	55.8100	NIST46.4
7903301	Sn+2		7.0940		0.0000	NIST46.4
7903302	SnOH+		3.6970		0.0000	NIST46.4
7903303	Sn(OH)3-		-9.4970		0.0000	NIST46.4
7903304	Sn2(OH)2+2		9.3940		0.0000	NIST46.4
7903305	Sn3(OH)4+2		14.3940		0.0000	NIST46.4
7903306	HSnO2-		-8.9347		0.0000	Bard85
7913301	Sn+4		21.2194		0.0000	Bard85
7913302	SnO3-2		-2.2099		0.0000	Bard85
6003300	PbOH+	-7.7100	-7.5970	0.0000	0.0000	NIST46.3
6003301	Pb(OH)2 (aq)	-17.1200	-17.0940	0.0000	0.0000	NIST46.3
6003302	Pb(OH)3-	-28.0600	-28.0910	0.0000	0.0000	NIST46.3
6003303	Pb2OH+3	-6.3600	-6.3970	0.0000	0.0000	NIST46.3
6003304	Pb3(OH)4+2	-23.8800	-23.8880	110.8760	115.2400	NIST46.3
6003305	Pb(OH)4-2	-39.6990	-39.6990	0.0000	0.0000	MTQ3.11
6003306	Pb4(OH)4+4		-19.9880		88.2400	NIST46.4
902700	BF(OH)3-	-0.3990	-0.3990	7.7404	7.7404	MTQ3.11
902701	BF2(OH)2-	7.6300	7.6300	6.8408	6.8408	MTQ3.11
902702	BF3OH-	13.6670	13.2200	-6.6107	-20.4897	NIST2.1.1
303300	AlOH+2	-4.9900	-4.9970	49.7854	47.8100	NIST46.3
303301	Al(OH)2+	-10.1000	-10.0940	0.0000	0.0000	NIST46.3
303303	Al(OH)3 (aq)	-16.0000	-16.7910	0.0000	0.0000	NIST46.3
303302	Al(OH)4-	-23.0000	-22.6880	184.3470	173.2400	NIST46.3
8703300	TlOH (aq)	-13.1717	-13.2070	58.3040	56.8100	NIST46.3
8713301	TlOH+2	3.5770	2.6940	0.0000	0.0000	NIST46.3
8713302	Tl(OH)2+	2.1183	1.8970	0.0000	0.0000	NIST46.3
8713303	Tl(OH)4-1	-10.2545	-11.6970	0.0000	0.0000	NIST46.3
9503300	ZnOH+	-8.9600	-8.9970	56.0614	55.8100	NIST46.3
9503301	Zn(OH)2 (aq)	-16.8990	-17.7940	0.0000	0.0000	NIST46.3
9503302	Zn(OH)3-	-28.3990	-28.0910	0.0000	0.0000	NIST46.3
9503303	Zn(OH)4-2	-41.1990	-40.4880	0.0000	0.0000	NIST46.3
1603300	CdOH+	-10.0800	-10.0970	54.8104	54.8100	NIST46.3
1603301	Cd(OH)2 (aq)	-20.3500	-20.2940	0.0000	0.0000	NIST46.3
1603302	Cd(OH)3-	-33.3000	-32.5050	0.0000	0.0000	NIST46.3
1603303	Cd(OH)4-2	-47.3500	-47.2880	0.0000	0.0000	NIST46.3
1603304	Cd2OH+3	-9.3900	-9.3970	45.6014	45.8100	NIST46.3
3613302	HgOH+	2.6974	2.7970	0.0000	-18.9100	NIST46.3
3613303	Hg(OH)3-1	-15.0042	-14.8970	0.0000	0.0000	NIST46.3
2313300	CuOH+	-8.0000	-7.4970	0.0000	35.8100	NIST46.3
2313301	Cu(OH)2 (aq)	-13.6800	-16.1940	0.0000	0.0000	NIST46.3
2313302	Cu(OH)3-	-26.8990	-26.8790	0.0000	0.0000	NIST46.3
2313303	Cu(OH)4-2	-39.6000	-39.9800	0.0000	0.0000	NIST46.3
2313304	Cu2(OH)2+2	-10.3590	-10.5940	73.3832	76.6200	NIST46.3
203300	AgOH (aq)	-12.0000	-11.9970	0.0000	0.0000	NIST46.3
203301	Ag(OH)2-	-24.0000	-24.0040	0.0000	0.0000	NIST46.3
5403300	NiOH+	-9.8600	-9.8970	51.9653	51.8100	NIST46.3
5403301	Ni(OH)2 (aq)	-19.0000	-18.9940	0.0000	0.0000	NIST46.3

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
5403302	Ni(OH)3-	-30.0000	-29.9910	0.0000	0.0000	NIST46.3
2003300	CoOH+	-9.6500	-9.6970	0.0000	0.0000	NIST46.4
2003301	Co(OH)2 (aq)	-18.8000	-18.7940	0.0000	0.0000	NIST46.4
2003302	Co(OH)3-	-31.5000	-31.4910	0.0000	0.0000	NIST46.4
2003303	Co(OH)4-2	-46.3000	-46.2880	0.0000	0.0000	NIST46.4
2003304	Co2OH+3	-11.2000	-10.9970	0.0000	0.0000	NIST46.4
2003306	Co4(OH)4+4	-30.5300	-30.4880	0.0000	0.0000	NIST46.4
2003305	CoOOH-		-32.0915		260.4540	NIST2.1.1
2013300	CoOH+2		-1.2910		0.0000	NIST46.4
2803300	FeOH+	-9.5000	-9.3970	55.2246	55.8100	NIST46.3
2803302	Fe(OH)2 (aq)	-20.5700	-20.4940	119.5160	119.6200	NIST46.3
2803301	Fe(OH)3-	-31.0000	-28.9910	126.7752	126.4300	NIST46.3
2813300	FeOH+2	-2.1900	-2.1870	43.5094	41.8100	NIST46.3
2813301	Fe(OH)2+	-5.6700	-4.5940	0.0000	0.0000	NIST46.3
2813302	Fe(OH)3 (aq)	-13.6000	-12.5600	0.0000	103.8000	Nord90
2813303	Fe(OH)4-	-21.6000	-21.5880	0.0000	0.0000	NIST46.3
2813304	Fe2(OH)2+4	-2.9500	-2.8540	56.4840	57.6200	NIST46.3
2813305	Fe3(OH)4+5	-6.3000	-6.2880	59.8312	65.2400	NIST46.3
4703300	MnOH+	-10.5900	-10.5970	60.2454	55.8100	NIST46.3
4703301	Mn(OH)3-	-34.8000	-34.8000	0.0000	0.0000	MTQ3.11
4703302	Mn(OH)4-2		-48.2880		0.0000	NIST46.4
4700020	MnO4-	-127.8240	-127.7945	738.9781	822.6699	NIST2.1.1
4700021	MnO4-2	-118.4400	-118.4218	627.6837	711.0699	NIST2.1.1
2113301	Cr(OH)+2	5.6200	5.9118	0.0000	-77.9100	NIST46.3
2113302	Cr(OH)3 (aq)	-7.1300	-8.4222	0.0000	0.0000	SCD3.02
2113303	Cr(OH)4-	-18.1500	-17.8192	0.0000	0.0000	SCD3.02
2113304	CrO2-	-17.7456	-17.7456	0.0000	0.0000	MTQ3.11
9003300	VOH+	-5.6400	-6.4870	0.0000	59.8100	NIST46.3
9013300	VOH+2	-2.3000	-2.2970	39.1204	43.8100	NIST46.3
9013301	V(OH)2+	-5.8300	-6.2740	0.0000	0.0000	NIST46.3
9013302	V(OH)3 (aq)	-11.0200	-3.0843	0.0000	0.0000	SCD3.02
9013304	V2(OH)2+4	-3.7500	-3.7940	0.0000	0.0000	NIST46.3
9013303	V2(OH)3+3	-7.5000	-10.1191	0.0000	0.0000	NIST46.3
9023300	V(OH)3+	-5.6700	-5.6970	0.0000	0.0000	NIST46.4
9023301	H2V2O4+2	-6.4400	-6.6940	0.0000	53.6200	NIST46.4
8913300	UOH+3	-0.6560	-0.5970	49.0156	47.8100	NIST46.3
8913301	U(OH)2+2	-2.2700	-2.2700	74.1823	74.1823	MTQ3.11
8913302	U(OH)3+	-4.9350	-4.9350	94.7467	94.7467	MTQ3.11
8913303	U(OH)4 (aq)	-8.4980	-8.4980	103.5958	103.5958	MTQ3.11
8913304	U(OH)5-	-13.1200	-13.1200	115.3738	115.3738	MTQ3.11
8913305	U6(OH)15+9	-17.2290	-17.1550	0.0000	0.0000	NIST46.3
8933300	UO2OH+	-5.0900	-5.8970	42.7437	47.8100	NIST46.3
8933301	(UO2)2(OH)2+2	-5.6450	-5.5740	42.8023	41.8200	NIST46.3
8933302	(UO2)3(OH)5+	-15.5930	-15.5850	104.9138	108.0500	NIST46.3
1103301	BeOH+		-5.3970		0.0000	NIST46.4
1103302	Be(OH)2 (aq)		-13.5940		0.0000	NIST46.4
1103303	Be(OH)3-		-23.1910		0.0000	NIST46.4
1103304	Be(OH)4-2		-37.3880		0.0000	NIST46.4
1103305	Be2OH+3		-3.1770		0.0000	NIST46.4
1103306	Be3(OH)3+3		-8.8076		0.0000	NIST46.4
4603300	MgOH+	-11.7900	-11.3970	66.6720	67.8100	NIST46.3
1503300	CaOH+	-12.5980	-12.6970	60.8144	64.1100	NIST46.3
8003300	SrOH+	-13.1780	-13.1770	60.6471	60.8100	NIST46.3
1003300	BaOH+	-13.3580	-13.3570	63.1575	60.8100	NIST46.3
3302700	HF (aq)	3.1690	3.1700	14.4766	13.3000	NIST46.3
3302701	HF2-	3.7490	3.7500	19.0372	17.4000	NIST46.3
3302702	H2F2 (aq)	6.7680	6.7680	0.0000	0.0000	MTQ3.11
7402700	SbOF (aq)	6.1864	6.1864	0.0000	0.0000	PNL89
7402702	Sb(OH)2F (aq)	6.1937	6.1937	0.0000	0.0000	PNL89
7702700	SiF6-2	30.1800	30.1800	-68.0318	-68.0000	Nord90
7902701	SnF+		11.5820		0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
7902702	SnF2 (aq)		14.3860		0.0000	NIST46.4
7902703	SnF3-		17.2060		0.0000	NIST46.4
7912701	SnF6-2		33.5844		0.0000	Bard85
6002700	PbF+	1.2500	1.8480	0.0000	0.0000	NIST46.3
6002701	PbF2 (aq)	2.5600	3.1420	0.0000	0.0000	NIST46.3
6002702	PbF3-	3.4200	3.4200	0.0000	0.0000	SCD3.02
6002703	PbF4-2	3.1000	3.1000	0.0000	0.0000	SCD3.02
902703	BF4-	20.2740	19.9120	-7.5103	-18.6700	NIST46.3
302700	AlF+2	7.0100	7.0000	0.0000	4.6000	NIST46.3
302701	AlF2+	12.7500	12.6000	83.6800	8.3000	NIST46.3
302702	AlF3 (aq)	17.0200	16.7000	10.4600	8.7000	NIST46.3
302703	AlF4-	19.7200	19.4000	0.0000	8.7000	NIST46.3
8702700	TlF (aq)	-0.4251	0.1000	0.0000	0.0000	NIST46.3
9502700	ZnF+	1.1500	1.3000	9.2885	11.0000	NIST46.3
1602700	CdF+	1.1000	1.2000	0.0000	5.0000	NIST46.3
1602701	CdF2 (aq)	1.5000	1.5000	0.0000	0.0000	MTQ3.11
3612701	HgF+	8.0848	7.7630	0.0000	-35.7200	NIST46.3
2312700	CuF+	1.2600	1.8000	6.7781	13.0000	NIST46.3
202700	AgF (aq)	0.3600	0.4000	-11.8407	12.0000	NIST46.3
5402700	NiF+	1.3000	1.4000	0.0000	7.1000	NIST46.3
2002700	CoF+	0.9000	1.5000	0.0000	9.2000	NIST46.4
2812700	FeF+2	6.1990	6.0400	11.2926	10.0000	NIST46.3
2812701	FeF2+	10.8000	10.4675	20.0832	17.0000	NIST46.3
2812702	FeF3 (aq)	14.0000	13.6170	22.5894	29.0000	NIST46.3
4702700	MnF+	0.8500	1.6000	0.0000	11.0000	NIST46.3
2112700	CrF+2	14.5424	14.7688	-70.2452	-70.2452	NIST46.3
9022700	VOF+	3.3400	3.7780	7.9496	7.9000	NIST46.3
9022701	VOF2 (aq)	5.7400	6.3520	14.6440	14.0000	NIST46.3
9022702	VOF3-	7.3000	7.9020	20.5016	20.0000	NIST46.3
9022703	VOF4-2	8.1100	8.5080	26.7776	26.0000	NIST46.3
9032700	VO2F (aq)	3.1200	3.2440	0.0000	0.0000	NIST46.3
9032701	VO2F2-	5.6700	5.8040	0.0000	0.0000	NIST46.3
9032702	VO2F3-2	6.9700	6.9000	0.0000	0.0000	NIST46.3
9032703	VO2F4-3	7.0700	6.5920	0.0000	0.0000	NIST46.3
8912700	UF+3	8.6590	9.3000	21.1292	21.1292	NIST46.3
8912701	UF2+2	14.4570	16.4000	30.1248	30.1248	NIST46.3
8912702	UF3+	19.1150	21.6000	29.9156	29.9156	NIST46.3
8912703	UF4 (aq)	23.6400	23.6400	19.2464	19.2464	MTQ3.11
8912704	UF5-	25.2380	25.2380	20.2924	20.2924	MTQ3.11
8912705	UF6-2	27.7180	27.7180	13.8072	13.8072	MTQ3.11
8932700	UO2F+	5.1050	5.1400	-1.8828	1.0000	NIST46.3
8932701	UO2F2 (aq)	8.9200	8.6000	-3.7656	2.0000	NIST46.3
8932702	UO2F3-	11.3640	11.0000	-3.5564	2.0000	NIST46.3
8932703	UO2F4-2	12.6070	11.9000	-4.6024	0.4000	NIST46.3
1102701	BeF+		5.2490		0.0000	NIST46.4
1102702	BeF2 (aq)		9.1285		-4.0000	NIST46.4
1102703	BeF3-		11.9085		-8.0000	NIST46.4
4602700	MgF+	1.8200	2.0500	19.5560	13.0000	NIST46.3
1502700	CaF+	0.9400	1.0380	15.8908	14.0000	NIST46.3
8002701	SrF+		0.5480		16.0000	NIST46.4
5002700	NaF (aq)	-0.7900	-0.2000	0.0000	12.0000	NIST46.3
7901801	SnCl+		8.7340		0.0000	NIST46.4
7901802	SnCl2 (aq)		9.5240		0.0000	NIST46.4
7901803	SnCl3-		8.3505		0.0000	NIST46.4
6001800	PbCl+	1.6000	1.5500	18.3259	8.7000	NIST46.3
6001801	PbCl2 (aq)	1.8000	2.2000	4.5187	12.0000	NIST46.3
6001802	PbCl3-	1.6990	1.8000	9.0793	4.0000	NIST46.3
6001803	PbCl4-2	1.3800	1.4600	14.7695	14.7695	SCD3.02
8701800	TlCl (aq)	0.6824	0.5100	-4.7990	-6.2000	NIST46.3
8701801	TlCl2-1	0.2434	0.2800	0.0000	0.0000	SCD3.02
8711800	TlCl+2	12.2342	11.0110	0.0000	0.0000	NIST46.3

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
8711801	TlCl2+	18.0402	16.7710	0.0000	0.0000	NIST46.3
8711802	TlCl3 (aq)	21.4273	19.7910	0.0000	0.0000	NIST46.3
8711803	TlCl4-1	24.2281	21.5910	0.0000	0.0000	NIST46.3
8711804	TlOHCl+	10.6290	10.6290	0.0000	0.0000	MTQ3.11
9501800	ZnCl+	0.4300	0.4000	32.5934	5.4000	NIST46.3
9501801	ZnCl2 (aq)	0.4500	0.6000	35.5640	37.0000	NIST46.3
9501802	ZnCl3-	0.5000	0.5000	39.9990	39.9990	MTQ3.11
9501803	ZnCl4-2	0.1990	0.1990	45.8566	45.8566	MTQ3.11
9501804	ZnOHCl (aq)	-7.4800	-7.4800	0.0000	0.0000	MTQ3.11
1601800	CdCl+	1.9800	1.9800	2.4686	1.0000	NIST46.3
1601801	CdCl2 (aq)	2.6000	2.6000	5.1882	3.0000	NIST46.3
1601802	CdCl3-	2.3990	2.4000	16.3176	10.0000	NIST46.3
1601803	CdOHCl (aq)	-7.4040	-7.4040	18.2213	18.2213	MTQ3.11
3611800	HgCl+	12.8500	13.4940	0.0000	-62.7200	NIST46.3
3611801	HgCl2 (aq)	19.2203	20.1940	0.0000	-92.4200	NIST46.3
3611802	HgCl3-1	20.1226	21.1940	0.0000	-94.0200	NIST46.3
3611803	HgCl4-2	20.5338	21.7940	0.0000	-100.7200	NIST46.3
3611804	HgClI (aq)	25.3532	25.5320	0.0000	-135.2999	NIST2.1.1
3611805	HgClOH (aq)	9.3170	10.4440	-52.2247	-42.7200	NIST46.3
2311800	CuCl+	0.4300	0.2000	36.1916	8.3000	NIST46.3
2311801	CuCl2 (aq)	0.1600	-0.2600	44.1830	44.1830	SCD3.02
2311802	CuCl3-	-2.2900	-2.2900	57.2790	57.2790	MTQ3.11
2311803	CuCl4-2 1	-4.5900	-4.5900	32.5515	32.5515	MTQ3.11
2301800	CuCl2-	5.5000	5.4200	-1.7573	-1.7573	NIST46.3
2301801	CuCl3-2	5.7000	4.7500	1.0878	1.0878	NIST46.3
2301802	CuCl (aq)		3.1000		0.0000	NIST46.4
201800	AgCl (aq)	3.2700	3.3100	-11.2131	-12.0000	NIST46.3
201801	AgCl2-	5.2700	5.2500	-16.4431	-16.0000	NIST46.3
201802	AgCl3-2	5.2900	5.2000	0.0000	0.0000	NIST46.3
201803	AgCl4-3	5.5100	5.5100	0.0000	0.0000	MTQ3.11
5401800	NiCl+	0.3990	0.4080	0.0000	2.0000	NIST46.3
5401801	NiCl2 (aq)	0.9600	-1.8900	0.0000	0.0000	SCD3.02
2001800	CoCl+	0.5300	0.5390	0.0000	2.0000	NIST46.4
2011800	CoCl+2		2.3085		16.0000	NIST46.4
2811800	FeCl+2	1.4800	1.4800	23.4304	23.0000	NIST46.3
2811801	FeCl2+	2.1300	2.1300	0.0000	0.0000	NIST46.3
2811802	FeCl3 (aq)	1.1300	1.1300	0.0000	0.0000	Nord90
4701800	MnCl+	0.6070	0.1000	0.0000	0.0000	NIST46.3
4701801	MnCl2 (aq)	0.0410	0.2500	0.0000	0.0000	Nord90
4701802	MnCl3-	-0.3050	-0.3100	0.0000	0.0000	Nord90
2111800	CrCl+2	9.3683	9.6808	-57.9358	-103.6200	NIST46.3
2111801	CrCl2+	8.6580	8.6580	-39.2208	-39.2208	MTQ3.11
2111802	CrOHCl2 (aq)	2.9627	2.9627	0.0000	0.0000	MTQ3.11
9021800	VOCl+	0.0200	0.4480	0.0000	0.0000	NIST46.3
8911800	UCl+3	1.3380	1.7000	41.5597	-20.0000	NIST46.3
8931800	UO2Cl+	0.2200	0.2100	5.1589	16.0000	NIST46.3
1101801	BeCl+		0.2009		0.0000	NIST46.4
7901301	SnBr+		8.2540		0.0000	NIST46.4
7901302	SnBr2 (aq)		8.7940		0.0000	NIST46.4
7901303	SnBr3-		7.4800		0.0000	NIST46.4
6001300	PbBr+	1.7700	1.7000	12.0499	8.0000	NIST46.3
6001301	PbBr2 (aq)	1.4400	2.6000	0.0000	-4.0000	NIST46.3
8701300	TlBr (aq)	0.9477	0.9100	-10.2968	-12.0000	NIST46.3
8701301	TlBr2-1	0.9719	-0.3840	12.5436	12.3600	NIST46.3
8701302	TlBrCl-1	0.8165	0.8165	0.0000	0.0000	MTQ3.11
8703802	TlIBr-1	2.1850	2.1850	0.0000	0.0000	MTQ3.11
8711300	TlBr+2	14.2221	12.8030	0.0000	0.0000	NIST46.3
8711301	TlBr2+	21.5761	20.7110	0.0000	0.0000	NIST46.3
8711302	TlBr3 (aq)	27.0244	27.0244	0.0000	0.0000	MTQ3.11
8711303	TlBr4-1	31.1533	31.1533	0.0000	0.0000	MTQ3.11
9501300	ZnBr+	-0.5800	-0.0700	0.0000	1.0000	NIST46.3

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
9501301	ZnBr2 (aq)	-0.9800	-0.9800	0.0000	0.0000	MTQ3.11
1601300	CdBr+	2.1700	2.1500	-3.3890	-3.0000	NIST46.3
1601301	CdBr2 (aq)	2.8990	3.0000	0.0000	-3.0000	NIST46.3
3611301	HgBr+	15.8347	15.8030	0.0000	-81.9200	NIST46.3
3611302	HgBr2 (aq)	23.6065	24.2725	-129.0011	-127.1200	NIST46.3
3611303	HgBr3-1	25.7857	26.7025	0.0000	-138.8200	NIST46.3
3611304	HgBr4-2	27.0633	27.9330	0.0000	-153.7200	NIST46.3
3611305	HgBrCl (aq)	22.0145	22.1811	0.0000	-113.7700	NIST2.1.1
3611306	HgBrI (aq)	27.1212	27.3133	0.0000	-151.2700	NIST2.1.1
3611307	HgBrI3-2	34.2135	34.2135	0.0000	0.0000	MTQ3.11
3611308	HgBr2I2-2	32.3994	32.3994	0.0000	0.0000	MTQ3.11
3611309	HgBr3I-2	30.1528	30.1528	0.0000	0.0000	MTQ3.11
3613301	HgBrOH (aq)	11.5980	12.4330	0.0000	0.0000	NIST46.3
201300	AgBr (aq)	4.2400	4.6000	0.0000	0.0000	NIST46.3
201301	AgBr2-	7.2800	7.5000	0.0000	0.0000	NIST46.3
201302	AgBr3-2	8.7100	8.1000	0.0000	0.0000	NIST46.3
5401300	NiBr+	0.5000	0.5000	0.0000	0.0000	MTQ3.11
2111300	CrBr+2	7.5519	7.5519	-46.9068	-46.9068	MTQ3.11
1101301	BeBr+		0.1009		0.0000	NIST46.4
6003800	PbI+	1.9400	2.0000	0.0000	0.0000	NIST46.3
6003801	PbI2 (aq)	3.1990	3.2000	0.0000	0.0000	NIST46.3
8703800	TlI (aq)	1.4279	1.4279	0.0000	0.0000	MTQ3.11
8703801	TlI2-1	1.8588	1.8588	0.0000	0.0000	MTQ3.11
8713800	TlI4-1	34.7596	34.7596	0.0000	0.0000	MTQ3.11
9503800	ZnI+	-2.9100	-2.0427	0.0000	-4.0000	NIST46.3
9503801	ZnI2 (aq)	-1.6900	-1.6900	0.0000	0.0000	MTQ3.11
1603800	CdI+	2.1500	2.2800	-9.9161	-9.6000	NIST46.3
1603801	CdI2 (aq)	3.5900	3.9200	0.0000	-12.0000	NIST46.3
3613801	HgI+	18.8949	19.6030	0.0000	-111.2200	NIST46.4
3613802	HgI2 (aq)	30.1081	30.8225	-186.2800	-182.7200	NIST46.4
3613803	HgI3-1	33.7935	34.6025	-200.5935	-194.2200	NIST46.4
3613804	HgI4-2	35.7858	36.5330	0.0000	-220.7200	NIST46.4
203800	AgI (aq)	6.6000	6.6000	0.0000	0.0000	NIST46.3
203801	AgI2-	10.6800	11.7000	0.0000	0.0000	NIST46.3
203802	AgI3-2	13.3700	12.6000	-113.0935	-122.0000	NIST46.3
203803	AgI4-3	14.0800	14.2290	0.0000	0.0000	NIST46.3
2113800	CrI+2	4.8289	4.8289	0.0000	0.0000	MTQ3.11
3307300	H2S (aq)	6.9940	7.0200	-22.1752	-22.0000	NIST46.3
6007300	Pb(HS)2 (aq)	15.2700	15.2700	0.0000	0.0000	MTQ3.11
6007301	Pb(HS)3-	16.5700	16.5700	0.0000	0.0000	MTQ3.11
8707300	TlHS (aq)	1.8178	2.4740	0.0000	0.0000	NIST46.3
8707301	Tl2HS+	7.6979	5.9740	0.0000	0.0000	NIST46.3
8707302	Tl2OH(HS)3-2	1.0044	1.0044	0.0000	0.0000	MTQ3.11
8707303	Tl2(OH)2(HS)2-2	-11.0681	-11.0681	0.0000	0.0000	MTQ3.11
9507300	Zn(HS)2 (aq)	14.9400	12.8200	0.0000	0.0000	DHa1993
9507301	Zn(HS)3-	16.1000	16.1000	0.0000	0.0000	MTQ3.11
9507302	ZnS(HS)2-2		6.1200		0.0000	DHa1993
9507303	Zn(HS)4-2		14.6400		0.0000	DHa1993
9507304	ZnS(HS)-		6.8100		0.0000	DHa1993
1607300	CdHS+	10.1700	8.0080	0.0000	0.0000	NIST46.3
1607301	Cd(HS)2 (aq)	16.5300	15.2120	0.0000	0.0000	NIST46.3
1607302	Cd(HS)3-	18.7100	17.1120	0.0000	0.0000	NIST46.3
1607303	Cd(HS)4-2	20.9000	19.3080	0.0000	0.0000	NIST46.3
3617300	HgS2-2	31.2398	29.4140	0.0000	0.0000	NIST46.4
3617301	Hg(HS)2 (aq)	43.8178	44.5160	0.0000	0.0000	NIST46.3
3617302	HgHS2-1		38.1220		0.0000	NIST46.4
2317300	Cu(HS)3-	25.8990	25.8990	0.0000	0.0000	MTQ3.11
207300	AgHS (aq)	14.0500	13.8145	0.0000	0.0000	NIST46.3
207301	Ag(HS)2-	18.4500	17.9145	0.0000	0.0000	NIST46.3
2807300	Fe(HS)2 (aq)	8.9500	8.9500	0.0000	0.0000	MTQ3.11
2807301	Fe(HS)3-	10.9870	10.9870	0.0000	0.0000	MTQ3.11

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
7317300	S2-2	-14.5280	-11.7828	47.6976	46.4000	NIST2.1.1
7317301	S3-2	-13.2820	-10.7667	43.5136	42.2000	NIST2.1.1
7317302	S4-2	-9.8290	-9.9608	40.5848	39.3000	NIST2.1.1
7317303	S5-2	-9.5950	-9.3651	38.9112	37.6000	NIST2.1.1
7317304	S6-2	-9.8810	-9.8810	0.0000	0.0000	MTQ3.11
7407300	Sb2S4-2	49.3005	49.3886	-316.6451	-321.7801	NIST2.1.1
2307300	Cu(S4)2-3	3.3900	3.3900	0.0000	0.0000	MTQ3.11
2307301	CuS4S5-3	2.6600	2.6600	0.0000	0.0000	MTQ3.11
207302	Ag(S4)2-3	0.9910	0.9910	0.0000	0.0000	MTQ3.11
207303	AgS4S5-3	0.6800	0.6800	0.0000	0.0000	MTQ3.11
207304	Ag(HS)S4-2	10.4310	10.4310	0.0000	0.0000	MTQ3.11
3307320	HSO4-	1.9870	1.9900	20.5434	22.0000	NIST46.3
4907320	NH4SO4-	1.1100	1.0300	0.0000	0.0000	NIST46.3
6007320	PbSO4 (aq)	2.7500	2.6900	0.0000	0.0000	NIST46.3
6007321	Pb(SO4)2-2	3.4700	3.4700	0.0000	0.0000	SCD3.02
307320	AlSO4+	3.0200	3.8900	8.9956	28.0000	NIST46.3
307321	Al(SO4)2-	4.9200	4.9200	11.8826	11.9000	Nord90
8707320	TlSO4-1	1.3853	1.3700	-0.9205	-0.8000	NIST46.3
9507320	ZnSO4 (aq)	2.3700	2.3400	5.6902	6.2000	NIST46.3
9507321	Zn(SO4)2-2	3.2800	3.2800	0.0000	0.0000	MTQ3.11
1607320	CdSO4 (aq)	2.4600	2.3700	4.5187	8.7000	NIST46.3
1607321	Cd(SO4)2-2	3.5000	3.5000	0.0000	0.0000	MTQ3.11
3617320	HgSO4 (aq)	7.4911	8.6120	0.0000	0.0000	NIST46.3
2317320	CuSO4 (aq)	2.3100	2.3600	5.1045	8.7000	NIST46.3
207320	AgSO4-	1.2900	1.3000	6.2342	6.2000	NIST46.3
5407320	NiSO4 (aq)	2.2900	2.3000	6.3597	5.8000	NIST46.3
5407321	Ni(SO4)2-2	1.0200	0.8200	0.0000	0.0000	SCD3.02
2007320	CoSO4 (aq)	2.3400	2.3000	5.8576	6.2000	NIST46.4
2807320	FeSO4 (aq)	2.2500	2.3900	13.5143	8.0000	NIST46.3
2817320	FeSO4+	3.9200	4.0500	16.3594	25.0000	NIST46.3
2817321	Fe(SO4)2-	5.4200	5.3800	19.2464	19.2000	Nord90
4707320	MnSO4 (aq)	2.2600	2.2500	9.0793	8.7000	NIST46.3
2117320	CrSO4+	10.9654	12.9371	-52.8021	-98.6200	NIST46.3
2117321	CrOHSO4 (aq)	8.2754	8.2871	0.0000	0.0000	NIST46.3
2117323	Cr2(OH)2SO4+2	16.1550	16.1550	0.0000	0.0000	MTQ3.11
2117324	Cr2(OH)2(SO4)2 (aq)	17.9288	17.9288	0.0000	0.0000	MTQ3.11
8917320	USO4+2	5.4610	6.6000	15.4808	8.0000	NIST46.3
8917321	U(SO4)2 (aq)	9.7490	10.5000	31.7984	33.0000	NIST46.3
8937320	UO2SO4 (aq)	2.7090	3.1800	21.3384	20.0000	NIST46.3
8937321	UO2(SO4)2-2	4.1830	4.3000	25.5224	38.0000	NIST46.3
9017320	VSO4+	1.4400	2.6740	0.0000	0.0000	NIST46.3
9027320	VOSO4 (aq)	2.4500	2.4400	15.5645	17.0000	NIST46.3
9037320	VO2SO4-	1.7100	1.3780	0.0000	0.0000	NIST46.3
1107321	BeSO4 (aq)		2.1900		29.0000	NIST46.4
1107322	Be(SO4)2-2		2.5960		0.0000	NIST46.4
4607320	MgSO4 (aq)	2.2500	2.2600	5.8534	5.8000	NIST46.3
1507320	CaSO4 (aq)	2.3090	2.3600	6.1505	7.1000	NIST46.3
8007321	SrSO4 (aq)		2.3000		8.0000	NIST46.4
4407320	LiSO4-	0.6400	0.6400	0.0000	0.0000	NIST46.3
5007320	NaSO4-	0.7000	0.7300	4.6861	1.0000	NIST46.3
4107320	KSO4-	0.8500	0.8500	9.4140	4.1000	NIST46.3
3307600	H2Se	3.8115	3.8900	3.3472	3.3000	NIST46.3
207600	Ag2Se	34.0677	34.9110	0.0000	0.0000	NIST46.3
207601	AgOH(Se)2-4	-18.6237	-20.5090	0.0000	0.0000	NIST46.3
4707600	MnSe (aq)	-6.7435	-5.3850	0.0000	0.0000	NIST46.3
3307611	SeO3-2	-8.4800	-8.4000	5.3555	5.0200	NIST46.3
3307610	H2SeO3 (aq)	2.6500	2.6300	7.0710	6.2000	NIST46.3
1607610	Cd(SeO3)2-2	-11.1890	-10.8840	0.0000	0.0000	NIST46.4
207610	AgSeO3-1	-5.5985	-5.5920	0.0000	0.0000	NIST46.3
207611	Ag(SeO3)2-3	-13.2000	-13.0400	0.0000	0.0000	NIST46.3
2817610	FeHSeO3+2	3.6100	3.4220	0.0000	25.0000	NIST46.3

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
3307620	HSeO4-1	1.9058	1.7000	17.5728	23.0000	NIST46.4
9507620	ZnSeO4	2.2019	2.1900	0.0000	0.0000	NIST46.4
9507621	Zn(SeO4)2-2	-0.0704	2.1960	0.0000	0.0000	NIST46.4
1607620	CdSeO4 (aq)	2.2415	2.2700	0.0000	0.0000	NIST46.4
5407620	NiSeO4 (aq)	2.6387	2.6700	14.6440	14.0000	NIST46.4
2007621	CoSeO4 (aq)		2.7000		12.0000	NIST46.4
4707620	MnSeO4 (aq)	2.4188	2.4300	14.4766	14.0000	NIST46.4
3304900	NH3 (aq)	-9.2520	-9.2440	52.2163	-52.0000	NIST46.3
204901	AgNH3+		-5.9340		-72.0000	NIST46.4
204902	Ag(NH3)2+		-11.2680		-160.0000	NIST46.4
3614900	HgNH3+2	5.6139	5.7500	0.0000	0.0000	NIST46.3
3614901	Hg(NH3)2+2	5.0341	5.5060	0.0000	-246.7200	NIST46.3
3614902	Hg(NH3)3+2	-3.2493	-3.1380	0.0000	-312.7200	NIST46.3
3614903	Hg(NH3)4+2	-11.7307	-11.4820	0.0000	-379.7200	NIST46.3
2314901	CuNH3+2		-5.2340		-72.0000	NIST46.4
5404901	NiNH3+2		-6.5140		-67.0000	NIST46.4
5404902	Ni(NH3)2+2		-13.5980		-111.6000	NIST46.4
2004900	Co(NH3)+2	-7.2500	-7.1640	46.2750	-65.0000	NIST46.4
2004901	Co(NH3)2+2	-15.0100	-14.7780	0.0000	0.0000	NIST46.4
2004902	Co(NH3)3+2	-23.3600	-22.9220	0.0000	0.0000	NIST46.4
2004903	Co(NH3)4+2	-32.0100	-31.4460	0.0000	0.0000	NIST46.4
2004904	Co(NH3)5+2		-40.4700		0.0000	NIST46.4
2014901	Co(NH3)6OH+2		-43.7148		0.0000	NIST2.1.1
2014902	Co(NH3)5Cl+2		-17.9584		113.3800	NIST2.1.1
2014903	Co(NH3)6Cl+2		-33.9179		104.3400	NIST2.1.1
2014904	Co(NH3)6Br+2		-33.8884		110.5699	NIST2.1.1
2014905	Co(NH3)6I+2		-33.4808		115.4399	NIST2.1.1
2014906	Co(NH3)6SO4+		-28.9926		124.4999	NIST2.1.1
2114900	Cr(NH3)6+3	-32.5709	-32.8952	0.0000	0.0000	NIST46.3
2114901	Cr(NH3)5OH+2	-30.2759	-30.2759	0.0000	0.0000	MTQ3.11
2114904	Cr(NH3)6Cl+2	-31.7932	-31.7932	0.0000	0.0000	MTQ3.11
2114905	Cr(NH3)6Br+2	-31.8870	-31.8870	0.0000	0.0000	MTQ3.11
2114906	Cr(NH3)6I+2	-32.0080	-32.0080	0.0000	0.0000	MTQ3.11
4902113	cis-Cr(OH)2(NH3)4+	-29.8574	-29.8574	0.0000	0.0000	MTQ3.11
4902114	trans-Cr(OH)2(NH3)4+	-30.5537	-30.5537	0.0000	0.0000	MTQ3.11
1504901	CaNH3+2		-9.1440		0.0000	NIST46.4
1504902	Ca(NH3)2+2		-18.7880		0.0000	NIST46.4
8004901	SrNH3+2		-9.3440		0.0000	NIST46.4
1004901	BaNH3+2		-9.4440		0.0000	NIST46.4
8704910	TlNO2 (aq)	0.9969	0.8300	0.0000	0.0000	NIST46.3
204911	AgNO2 (aq)		2.3200		-29.0000	NIST46.4
204910	Ag(NO2)2-	2.2200	2.5100	0.0000	-46.0000	NIST46.3
2314911	CuNO2+		2.0200		0.0000	NIST46.4
2314912	Cu(NO2)2 (aq)		3.0300		0.0000	NIST46.4
2004911	CoNO2+		0.8480		0.0000	NIST46.4
7904921	SnNO3+		7.9420		0.0000	NIST46.4
6004920	PbNO3+	1.1700	1.1700	0.0000	2.0000	NIST46.3
6004921	Pb(NO3)2 (aq)		1.4000		-6.6000	NIST46.4
8704920	TlNO3 (aq)	0.3665	0.3300	-2.7196	-2.0000	NIST46.3
8714920	TlNO3+2	7.0073	7.0073	0.0000	0.0000	MTQ3.11
1604920	CdNO3+	0.3990	0.5000	-21.7568	-21.0000	NIST46.3
1604921	Cd(NO3)2 (aq)		0.2000		0.0000	NIST46.4
3614920	HgNO3+	6.4503	5.7613	0.0000	0.0000	NIST46.3
3614921	Hg(NO3)2 (aq)	4.7791	5.3800	0.0000	0.0000	NIST46.3
2314921	CuNO3+		0.5000		-4.1000	NIST46.4
2314922	Cu(NO3)2 (aq)		-0.4000		0.0000	NIST46.4
9504921	ZnNO3+		0.4000		-4.6000	NIST46.4
9504922	Zn(NO3)2 (aq)		-0.3000		0.0000	NIST46.4
204920	AgNO3 (aq)	-0.2900	-0.1000	0.0000	22.6000	NIST46.3
5404921	NiNO3+		0.4000		0.0000	NIST46.4
2004921	CoNO3+		0.2000		0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
2004922	Co(NO3)2 (aq)		0.5085		0.0000	NIST46.4
2814921	FeNO3+2		1.0000		-37.0000	NIST46.4
4704921	MnNO3+		0.2000		0.0000	NIST46.4
4704920	Mn(NO3)2 (aq)	0.6000	0.6000	-1.6569	-1.6569	NIST46.3
2114920	CrNO3+2	8.2094	8.2094	-65.4378	-65.4378	MTQ3.11
8934921	UO2NO3+		0.3000		-12.0000	NIST46.4
9034920	VO2NO3 (aq)	-0.4300	-0.2960	0.0000	0.0000	NIST46.3
1504921	CaNO3+		0.5000		-5.4000	NIST46.4
8004921	SrNO3+		0.6000		-10.0000	NIST46.4
1004921	BaNO3+		0.7000		-13.0000	NIST46.4
3301431	HCN (aq)	9.2356	9.2100	-43.5136	-43.6300	NIST46.4
1601431	CdCN+	5.3200	6.0100	0.0000	-30.0000	NIST46.4
1601432	Cd(CN)2 (aq)	10.3703	11.1200	-54.3920	-54.3000	NIST46.4
1601433	Cd(CN)3-	14.8341	15.6500	-90.3744	-90.3000	NIST46.4
1601434	Cd(CN)4-2	18.2938	17.9200	-98.5750	-112.0000	NIST46.4
3611431	HgCN+	24.1738	23.1940	-141.5447	-136.7200	NIST46.4
3611432	Hg(CN)2 (aq)	40.6513	38.9440	-239.4922	154.2800	NIST46.4
3611433	Hg(CN)3-	44.4042	42.5040	-271.2487	-262.7200	NIST46.4
3611434	Hg(CN)4-2	47.4094	45.1640	-292.5871	-288.7200	NIST46.4
2301432	Cu(CN)2-	24.0272	21.9145	-121.7544	-121.0000	NIST46.4
2301433	Cu(CN)3-2	28.6524	27.2145	-168.1968	-167.4000	NIST46.4
2301431	Cu(CN)4-3	30.3456	28.7145	-215.0576	-214.2000	NIST46.4
201432	Ag(CN)2-	20.3814	20.4800	-136.7122	-137.0000	NIST46.4
201433	Ag(CN)3-2	21.4002	21.7000	-140.1431	-140.0000	NIST46.4
201431	Ag(CN)OH-	-0.5600	-0.7770	0.0000	0.0000	NIST46.4
5401431	Ni(CN)4-2	30.1257	30.2000	-180.7070	-180.0000	NIST46.4
5401432	NiH(CN)4-	36.7482	36.0289	0.0000	0.0000	NIST46.4
5401433	NiH2CN4 (aq)	41.4576	40.7434	0.0000	0.0000	NIST46.4
5401434	NiH3(CN)4+	43.9498	43.3434	0.0000	0.0000	NIST46.4
2001431	Co(CN)3-		14.3120		0.0000	NIST46.4
2001432	Co(CN)5-3		23.0000		-257.0000	NIST46.4
2801431	Fe(CN)6-4	45.6063	35.4000	-358.9872	-358.0000	NIST46.4
2801432	HFe(CN)6-3	49.9969	39.7100	-352.1255	-356.0000	NIST46.4
2801433	H2Fe(CN)6-2	52.4450	42.1100	-347.6904	-352.0000	NIST46.4
2811431	Fe(CN)6-3	52.6283	43.6000	-293.2984	-293.0000	NIST46.4
2811432	Fe2(CN)6 (aq)	56.9822	47.6355	0.0000	-218.0000	NIST46.4
7901431	SnFe(CN)6-		53.5400		0.0000	Beck87
4901431	NH4Fe(CN)6-3	48.0684	37.7000	-353.5480	-354.0000	NIST46.4
8701432	TlFe(CN)6-3	48.7508	38.4000	-355.1379	-365.5000	NIST46.4
4601431	MgFe(CN)6-	55.3916	46.3900	-289.9930	-290.0000	NIST46.4
4601432	MgFe(CN)6-2	49.4251	39.2100	0.0000	-346.0000	NIST46.4
1501431	CaFe(CN)6-	55.4730	46.4300	-290.7880	-291.0000	NIST46.4
1501432	CaFe(CN)6-2	49.6898	39.1000	-347.6904	-347.0000	NIST46.4
1501433	Ca2Fe(CN)6 (aq)	50.9952	40.6000	-350.2008	-350.2008	NIST46.4
8001431	SrFe(CN)6-	55.6181	46.4500	-292.1687	-292.0000	NIST46.4
8001432	SrFe(CN)6-2		39.1000		-350.0000	NIST46.4
1001430	BaFe(CN)6-2	49.4032	39.1900	0.0000	-342.0000	NIST46.4
1001431	BaFe(CN)6-1	55.4356	46.4800	-291.5411	-292.0000	NIST46.4
5001431	NaFe(CN)6-3	47.9885	37.6000	-355.2216	-354.0000	NIST46.4
4101433	KFe(CN)6-3	48.1204	37.7500	-351.4560	-353.9000	NIST46.4
4101430	KFe(CN)6-2		45.0400		-291.0000	NIST46.4
3305800	HPO4-2	12.3460	12.3750	-14.7695	-15.0000	NIST46.3
3305801	H2PO4-	19.5530	19.5730	-18.9117	-18.0000	NIST46.3
3305802	H3PO4	21.7000	21.7210	0.0000	-10.1000	NIST46.3
2005800	CoHPO4 (aq)	15.4100	15.4128	0.0000	0.0000	NIST46.4
2805800	FeH2PO4+	22.2530	22.2730	0.0000	0.0000	NIST46.3
2805801	FeHPO4 (aq)	15.9500	15.9750	0.0000	0.0000	NIST46.3
2815801	FeH2PO4+2	24.9800	23.8515	0.0000	0.0000	NIST46.3
2815800	FeHPO4+	17.7800	22.2920	-30.5432	-30.5432	NIST46.3
2115800	CrH2PO4+2	31.9068	31.9068	0.0000	0.0000	MTQ3.11
8915800	UHPO4+2	24.4430	24.4430	31.3800	31.3800	MTQ3.11

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
8915801	U(HPO4)2 (aq)	46.8330	46.8330	7.1128	7.1128	MTQ3.11
8915802	U(HPO4)3-2	67.5640	67.5640	-32.6352	-32.6352	MTQ3.11
8915803	U(HPO4)4-4	88.4830	88.4830	-110.8760	-110.8760	MTQ3.11
8935800	UO2HPO4 (aq)	20.8140	19.6550	-8.7864	-8.7864	NIST46.3
8935801	UO2(HPO4)2-2	42.9880	42.9880	-47.6934	-47.6934	MTQ3.11
8935802	UO2H2PO4+	22.6430	22.8330	-15.4808	-15.4808	NIST46.3
8935803	UO2(H2PO4)2 (aq)	44.7000	44.7000	-69.0360	-69.0360	MTQ3.11
8935804	UO2(H2PO4)3-	66.2450	66.2450	-119.6624	-119.6624	MTQ3.11
8935805	UO2PO4-		13.2500		0.0000	NIST46.4
4605800	MgPO4-	6.5890	4.6540	12.9704	12.9704	SCD3.02
4605801	MgH2PO4+	21.0660	21.2561	-4.6861	-4.6861	NIST46.3
4605802	MgHPO4 (aq)	15.2200	15.1750	-0.9623	-3.0000	NIST46.3
1505800	CaHPO4 (aq)	15.0850	15.0350	-0.9623	-3.0000	NIST46.3
1505801	CaPO4-	6.4590	6.4600	12.9704	12.9704	SCD3.02
1505802	CaH2PO4+	20.9600	20.9230	-4.6861	-6.0000	NIST46.3
8005800	SrHPO4 (aq)		14.8728		0.0000	NIST46.4
8005801	SrH2PO4+		20.4019		0.0000	NIST46.4
5005800	NaHPO4-	12.6360	13.4450	0.0000	0.0000	NIST46.3
4105800	KHPO4-	12.6400	13.2550	0.0000	0.0000	NIST46.3
3300602	AsO3-3	-34.7440	-34.7440	84.7260	84.7260	MTQ3.11
3300601	HAsO3-2	-21.3300	-21.3300	59.4086	59.4086	MTQ3.11
3300600	H2AsO3-	-9.2280	-9.2900	27.4470	27.4100	NIST46.4
3300603	H4AsO3+	-0.3050	-0.3050	0.0000	0.0000	MTQ3.11
3300613	AsO4-3	-20.5970	-20.7000	14.3511	12.9000	NIST46.4
3300612	HAsO4-2	-9.0010	-9.2000	-3.8493	-4.1000	NIST46.4
3300611	H2AsO4-	-2.2430	-2.2400	-7.0710	-7.1000	NIST46.4
7400020	Sb(OH)4-1	-12.0429	-12.0429	69.8519	69.8519	PNL89
7403302	Sb(OH)2+	1.3853	1.3853	0.0000	0.0000	PNL89
7400021	HSbO2	-0.0073	-0.0105	-0.0628	-0.1300	NIST2.1.1
7403301	SbO2-	-11.8011	-11.8011	70.1866	70.1866	PNL89
7403300	SbO+	0.9228	0.9228	8.2425	8.2425	PNL89
7410021	SbO3-	2.9319	2.9319	0.0000	0.0000	PNL89
7413300	SbO2+	2.3895	2.3895	0.0000	0.0000	PNL89
3301400	HCO3-	10.3300	10.3290	-15.1335	-14.6000	NIST46.4
3301401	H2CO3 (aq)	16.6810	16.6810	-9.4014	-23.7600	NIST46.4
6001400	Pb(CO3)2-2	10.6400	9.9380	0.0000	0.0000	NIST46.3
6001401	PbCO3 (aq)	7.2400	6.4780	0.0000	0.0000	NIST46.3
6001402	PbHCO3+	13.2000	13.2000	0.0000	0.0000	MTQ3.11
9501401	ZnCO3 (aq)	5.3000	4.7600	0.0000	0.0000	NIST46.4
9501400	ZnHCO3+	12.4000	11.8290	0.0000	0.0000	NIST46.4
3611401	HgCO3 (aq)		18.2720		0.0000	NIST46.4
3611402	Hg(CO3)2-2		21.7720		0.0000	NIST46.4
3611403	HgHCO3+		22.5420		0.0000	NIST46.4
1601401	CdCO3 (aq)	5.3990	4.3578	0.0000	0.0000	NIST46.4
1601400	CdHCO3+	12.4000	10.6863	0.0000	0.0000	NIST46.4
1601403	Cd(CO3)2-2		7.2278		0.0000	NIST46.4
2311400	CuCO3 (aq)	6.7300	6.7700	0.0000	0.0000	NIST46.4
2311402	CuHCO3+	13.0000	12.1290	0.0000	0.0000	NIST46.4
2311401	Cu(CO3)2-2	9.8300	10.2000	0.0000	0.0000	NIST46.4
5401401	NiCO3 (aq)	6.8700	4.5718	0.0000	0.0000	NIST46.3
5401400	NiHCO3+	12.4700	12.4199	0.0000	0.0000	NIST46.3
2001400	CoCO3 (aq)		4.2280		0.0000	NIST46.4
2001401	CoHCO3+		12.2199		0.0000	NIST46.4
2801400	FeHCO3+		11.4290		0.0000	NIST46.4
4701400	MnHCO3+	11.6000	11.6290	0.0000	-10.6000	NIST46.4
8931400	UO2CO3 (aq)	10.0710	9.6000	3.5146	4.0000	NIST46.3
8931401	UO2(CO3)2-2	17.0080	16.9000	14.5603	16.0000	NIST46.3
8931402	UO2(CO3)3-4	21.3840	21.6000	-36.7355	-40.0000	NIST46.3
1101401	BeCO3 (aq)		6.2546		0.0000	NIST46.4
4601400	MgCO3 (aq)	2.9800	2.9200	8.4600	12.0000	NIST46.3
4601401	MgHCO3+	11.4000	11.3390	-10.1671	-10.6000	NIST46.3

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
1501400	CaHCO3+	11.3300	11.5990	7.4894	5.4000	NIST46.3
1501401	CaCO3 (aq)	3.1500	3.2000	16.8615	16.0000	NIST46.3
8001401	SrCO3 (aq)		2.8100		20.0000	NIST46.4
8001400	SrHCO3+		11.5390		10.4000	NIST46.4
1001401	BaCO3 (aq)		2.7100		16.0000	NIST46.4
1001400	BaHCO3+		11.3090		10.4000	NIST46.4
5001400	NaCO3-	1.2680	1.2700	37.2836	-20.3500	NIST46.3
5001401	NaHCO3 (aq)	10.0800	10.0790	0.0000	-28.3301	NIST46.3
3307701	H2SiO4-2	-21.6190	-23.0400	124.3234	61.0000	NIST46.4
3307700	H3SiO4-	-9.9300	-9.8400	37.3840	20.0000	NIST46.4
8937700	UO2H3SiO4+	-2.4000	-1.9111	0.0000	0.0000	NIST46.4
3300900	H2BO3-	-9.2400	-9.2360	13.4892	13.0000	NIST46.4
3300901	H5(BO3)2-		-9.3060		8.4000	NIST46.4
3300902	H8(BO3)3-		-7.3060		29.4000	NIST46.4
200901	AgH2BO3 (aq)		-8.0360		0.0000	NIST46.4
4600901	MgH2BO3+		-7.6960		13.0000	NIST46.4
1500901	CaH2BO3+		-7.4760		17.0000	NIST46.4
8000901	SrH2BO3+		-7.6860		17.0000	NIST46.4
1000901	BaH2BO3+		-7.7460		17.0000	NIST46.4
5000901	NaH2BO3 (aq)		-9.0360		0.0000	NIST46.4
2123300	HCrO4-	6.5089	6.5100	3.7656	2.0000	NIST46.4
2123301	H2CrO4 (aq)	5.6513	6.4188	0.0000	39.0000	NIST46.4
2123302	Cr2O7-2	14.5571	14.5600	-12.5311	-15.0000	NIST46.4
2121800	CrO3Cl-	7.3086	7.3086	0.0000	0.0000	MTQ3.11
2127320	CrO3SO4-2	8.9937	8.9937	0.0000	0.0000	MTQ3.11
2125800	CrO3H2PO4-	29.3634	29.3634	0.0000	0.0000	MTQ3.11
2125801	CrO3HPO4-2	26.6806	26.6806	0.0000	0.0000	MTQ3.11
5002120	NaCrO4-	0.6963	0.6963	0.0000	0.0000	MTQ3.11
4102120	KCrO4-	0.7990	0.5700	0.0000	0.0000	NIST46.4
3304801	HMoO4-		4.2988		20.0000	NIST46.4
3304802	H2MoO4 (aq)		8.1636		-26.0000	NIST46.4
3304803	Mo7O24-6		52.9900		-228.0000	NIST46.4
3304804	HMo7O24-5		59.3768		-218.0000	NIST46.4
3304805	H2Mo7O24-4		64.1590		-215.0000	NIST46.4
3304806	H3Mo7O24-3		67.4050		-217.0000	NIST46.4
304801	AlMo6O21-3		54.9925		0.0000	NIST46.4
204801	Ag2MoO4 (aq)		-0.4219		-1.1800	Bard85
9033303	VO4-3	-28.4000	-30.2000	81.7135	-25.0000	NIST46.4
9033302	HVO4-2	-15.1500	-15.9000	62.4671	0.0000	NIST46.3
9033301	H2VO4-	-7.0900	-7.3000	47.4047	0.0000	NIST46.3
9033300	H3VO4 (aq)	-3.3000	-3.3000	44.4759	44.4759	MTQ3.11
9030020	V2O7-4	-29.0800	-31.2400	0.0000	-28.0000	NIST46.3
9030021	HV2O7-3	-16.3200	-20.6700	0.0000	0.0000	NIST46.3
9030022	H3V2O7-	-3.7900	-3.7900	0.0000	0.0000	MTQ3.11
9030023	V3O9-3	-15.8800	-15.8800	0.0000	0.0000	MTQ3.11
9030024	V4O12-4	-20.7900	-20.5600	0.0000	-87.0000	NIST46.3
9030025	V10O28 -6	-17.5300	-24.0943	0.0000	0.0000	NIST46.4
9030026	HV10O28 -5	-11.3500	-15.9076	90.0397	90.0397	NIST46.4
9030027	H2V10O28-4	-7.7100	-10.7000	0.0000	0.0000	NIST46.3
3309171	H[Benzoate]	4.2000	4.2020	0.0000	0.0000	NIST46.2
6009171	Pb[Benzoate]	2.5000	2.4000	0.0000	0.0000	NIST46.2
309171	Al[Benzoate]	2.0500	2.0500	0.0000	0.0000	NIST46.2
309172	AlOH[Benzoate]	-0.5600	-0.5600	0.0000	0.0000	NIST46.2
9509171	Zn[Benzoate]	1.4000	1.7000	0.0000	0.0000	SCD2.62
1609171	Cd[Benzoate]	1.9000	1.8000	0.0000	0.0000	NIST46.2
1609172	Cd[Benzoate]2	1.6500	1.8200	0.0000	0.0000	SCD2.62
2319171	Cu[Benzoate]	2.1000	2.1900	0.0000	0.0000	NIST46.2
209171	Ag[Benzoate]	0.9100	0.9100	0.0000	0.0000	NIST46.2
5409171	Ni[Benzoate]	1.4000	1.8600	0.0000	0.0000	SCD2.62
2009171	Co[Benzoate]		1.0537		0.0000	NIST46.4
4709171	Mn[Benzoate]	2.0600	2.0600	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
4609171	Mg[Benzoate]	0.1000	1.2600	0.0000	0.0000	SCD2.62
1509171	Ca[Benzoate]	0.2000	1.5500	0.0000	0.0000	SCD2.62
3309181	H[Phenylacetate]	4.3100	4.3100	0.0000	0.0000	NIST46.2
9509181	Zn[Phenylacetate]	1.6700	1.5700	0.0000	0.0000	NIST46.2
2319181	Cu[Phenylacetate]	1.9700	1.9700	0.0000	0.0000	NIST46.2
2009181	Co[Phenylacetate]	0.0000	0.5910	0.0000	0.0000	NIST46.4
2009182	Co[Phenylacetate]2	0.0000	0.4765	0.0000	0.0000	NIST46.4
3309201	H[Isophthalate]	3.5000	4.5000	0.0000	0.0000	NIST46.2
3309202	H2[Isophthalate]	8.0000	8.0000	0.0000	0.0000	NIST46.2
6009201	Pb[Isophthalate]	2.1700	2.9900	0.0000	0.0000	NIST46.2
6009202	Pb[Isophthalate]2	3.3600	4.1800	0.0000	0.0000	NIST46.2
6009203	PbH[Isophthalate]	6.2800	6.6900	0.0000	0.0000	NIST46.2
1609201	Cd[Isophthalate]	1.3300	2.1500	0.0000	0.0000	NIST46.2
1609202	Cd[Isophthalate]2	2.1700	2.9900	0.0000	0.0000	NIST46.2
1609203	CdH[Isophthalate]	5.3200	5.7300	0.0000	0.0000	NIST46.2
1509200	Ca[Isophthalate]	2.0000	2.0000	0.0000	0.0000	NIST46.2
1009201	Ba[Isophthalate]	1.5500	1.5500	0.0000	0.0000	NIST46.2
3309551	H[Diethylamine]	10.7740	10.9330	0.0000	0.0000	NIST46.2
9509551	Zn[Diethylamine]	2.5100	2.7400	0.0000	0.0000	SCD2.62
9509552	Zn[Diethylamine]2	4.9600	5.2700	83.6800	0.0000	SCD2.62
9509553	Zn[Diethylamine]3	7.4900	7.7100	0.0000	0.0000	SCD2.62
9509554	Zn[Diethylamine]4	9.8300	9.8400	0.0000	0.0000	SCD2.62
1609551	Cd[Diethylamine]	2.6200	2.7300	0.0000	0.0000	SCD2.62
1609552	Cd[Diethylamine]2	4.8600	4.8600	0.0000	0.0000	SCD2.62
1609553	Cd[Diethylamine]3	6.3600	6.3700	0.0000	0.0000	SCD2.62
1609554	Cd[Diethylamine]4	7.3100	7.3200	0.0000	0.0000	SCD2.62
209551	Ag[Diethylamine]	3.9650	2.9800	0.0000	0.0000	NIST46.2
209552	Ag[Diethylamine]2	7.0200	6.3800	0.0000	0.0000	NIST46.2
5409551	Ni[Diethylamine]	2.7800	2.7800	0.0000	0.0000	SCD2.62
5409552	Ni[Diethylamine]2	4.9700	4.9700	0.0000	0.0000	SCD2.62
5409553	Ni[Diethylamine]3	6.7200	6.7200	0.0000	0.0000	SCD2.62
5409554	Ni[Diethylamine]4	7.9300	7.9300	0.0000	0.0000	SCD2.62
5409555	Ni[Diethylamine]5	8.8700	8.8700	0.0000	0.0000	SCD2.62
3309561	H[Butylamine]	10.6400	10.6400	-58.2831	0.0000	NIST46.2
3619561	Hg[Butylamine]	14.8400	14.8400	0.0000	0.0000	NIST46.2
3619562	Hg[Butylamine]2	24.2400	24.2400	0.0000	0.0000	NIST46.2
3619563	Hg[Butylamine]3	25.1000	25.1000	0.0000	0.0000	NIST46.2
3619564	Hg[Butylamine]4	26.1000	26.1000	0.0000	0.0000	NIST46.2
209561	Ag[Butylamine]	3.5500	3.4200	0.0000	0.0000	NIST46.2
209562	Ag[Butylamine]2	7.7700	7.4700	0.0000	0.0000	NIST46.2
3309581	H[Methylamine]	10.7200	10.6400	0.0000	0.0000	NIST46.2
1609581	Cd[Methylamine]	2.7500	2.7500	0.0000	0.0000	NIST46.2
1609582	Cd[Methylamine]2	4.8100	4.8100	-29.2880	0.0000	NIST46.2
1609583	Cd[Methylamine]3	5.9400	5.9400	0.0000	0.0000	NIST46.2
1609584	Cd[Methylamine]4	6.5500	6.5500	-58.5760	0.0000	NIST46.2
3619581	Hg[Methylamine]	14.7600	14.7600	0.0000	0.0000	NIST46.2
3619582	Hg[Methylamine]2	23.9600	23.9600	0.0000	0.0000	NIST46.2
3619583	Hg[Methylamine]3	24.3000	24.3000	0.0000	0.0000	NIST46.2
3619584	Hg[Methylamine]4	24.6000	24.6000	0.0000	0.0000	NIST46.2
2319581	Cu[Methylamine]	4.1100	4.1100	0.0000	0.0000	NIST46.2
2319582	Cu[Methylamine]2	7.5100	7.5100	0.0000	0.0000	NIST46.2
2319583	Cu[Methylamine]3	10.2100	10.2100	0.0000	0.0000	NIST46.2
2319584	Cu[Methylamine]4	12.0800	12.0800	0.0000	0.0000	NIST46.2
209581	Ag[Methylamine]	3.1800	3.0700	0.0000	0.0000	NIST46.2
209582	Ag[Methylamine]2	7.1400	6.8900	0.0000	0.0000	NIST46.2
5409581	Ni[Methylamine]	2.2300	2.2300	0.0000	0.0000	NIST46.2
3309591	H[Dimethylamine]	10.7740	10.7740	-50.2080	0.0000	NIST46.2
209591	Ag[Dimethylamine]2	5.3700	5.3700	-40.5848	0.0000	NIST46.2
5409591	Ni[Dimethylamine]	1.4700	1.4700	0.0000	0.0000	NIST46.2
3309611	H[Hexylamine]	10.6300	10.6300	0.0000	0.0000	NIST46.2
209611	Ag[Hexylamine]	3.6600	3.5400	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
209612	Ag[Hexylamine]2	7.3500	7.5500	0.0000	0.0000	NIST46.2
3309631	H[Ethylenediamine]	9.9600	9.9280	0.0000	0.0000	NIST46.2
3309632	H2[Ethylenediamine]	16.8500	16.7760	0.0000	0.0000	NIST46.2
6009631	Pb[Ethylenediamine]	7.0000	5.0400	0.0000	0.0000	NIST46.2
6009632	Pb[Ethylenediamine]2	8.4500	8.5000	0.0000	0.0000	NIST46.2
9509631	Zn[Ethylenediamine]	5.6500	5.6600	0.0000	0.0000	NIST46.2
9509632	Zn[Ethylenediamine]2	10.6200	10.6000	0.0000	0.0000	NIST46.2
9509633	Zn[Ethylenediamine]3	13.8300	13.9000	0.0000	0.0000	NIST46.2
1609631	Cd[Ethylenediamine]	5.6100	5.4100	0.0000	0.0000	NIST46.2
1609632	Cd[Ethylenediamine]2	10.3400	9.9000	0.0000	0.0000	NIST46.2
1609633	Cd[Ethylenediamine]3	12.2600	11.6000	0.0000	0.0000	NIST46.2
3619631	Hg[Ethylenediamine]	20.4000	20.4000	0.0000	0.0000	NIST46.2
3619632	Hg[Ethylenediamine]2	29.3000	29.3000	-173.2176	0.0000	NIST46.2
3619633	HgH[Ethylenediamine]	34.7000	34.7000	0.0000	0.0000	NIST46.2
2309631	Cu[Ethylenediamine]2	11.2000	11.2000	0.0000	0.0000	NIST46.2
2319631	Cu[Ethylenediamine]	10.4900	10.5000	0.0000	0.0000	NIST46.2
2319632	Cu[Ethylenediamine]2	19.6200	19.6000	0.0000	0.0000	NIST46.2
209631	Ag[Ethylenediamine]	4.7000	4.6000	0.0000	0.0000	NIST46.2
209632	Ag[Ethylenediamine]2	7.7000	7.5000	0.0000	0.0000	NIST46.2
209633	AgH[Ethylenediamine]	7.3100	11.9900	0.0000	0.0000	NIST46.2
209634	Ag2[Ethylenediamine]	1.4300	6.5000	0.0000	0.0000	NIST46.2
209635	Ag2[Ethylenediamine]	12.7300	12.7000	0.0000	0.0000	NIST46.2
209636	Ag[HEthylenediamine]	24.0000	24.0000	-150.2056	0.0000	NIST46.2
209637	AgH[Ethylenediamine]	8.4000	8.4000	-47.6976	0.0000	NIST46.2
5409631	Ni[Ethylenediamine]	7.2400	7.3200	0.0000	0.0000	NIST46.2
5409632	Ni[Ethylenediamine]2	13.3600	13.5000	0.0000	0.0000	NIST46.2
5409633	Ni[Ethylenediamine]3	17.5400	17.6000	0.0000	0.0000	NIST46.2
2009631	Co[Ethylenediamine]		5.5000		0.0000	NIST46.4
2009632	Co[Ethylenediamine]2		10.1000		0.0000	NIST46.4
2009633	Co[Ethylenediamine]3		13.2000		0.0000	NIST46.4
2019631	Co[Ethylenediamine]2		34.7000		0.0000	NIST46.4
2019632	Co[Ethylenediamine]3		48.6900		0.0000	NIST46.4
2809631	Fe[Ethylenediamine]	4.3600	4.2600	0.0000	0.0000	NIST46.2
2809632	Fe[Ethylenediamine]2	7.6500	7.7300	0.0000	0.0000	NIST46.2
2809633	Fe[Ethylenediamine]3	9.6800	10.1700	0.0000	0.0000	NIST46.2
4709631	Mn[Ethylenediamine]	2.6700	2.7400	0.0000	0.0000	NIST46.2
4709632	Mn[Ethylenediamine]2	4.2000	4.8000	0.0000	0.0000	NIST46.2
2119631	Cr[Ethylenediamine]2	22.5700	22.5700	0.0000	0.0000	NIST46.2
2119632	Cr[Ethylenediamine]3	29.0000	29.0000	0.0000	0.0000	NIST46.2
4609631	Mg[Ethylenediamine]	0.3700	0.3700	0.0000	0.0000	NIST46.2
1509631	Ca[Ethylenediamine]	0.1000	0.1100	0.0000	0.0000	NIST46.2
3309641	H[Propylamine]	10.8000	10.5660	0.0000	0.0000	NIST46.2
9509641	Zn[Propylamine]	2.4200	2.4200	0.0000	0.0000	SCD2.62
9509642	Zn[Propylamine]2	4.8500	4.8500	0.0000	0.0000	SCD2.62
9509643	Zn[Propylamine]3	7.3800	7.3800	0.0000	0.0000	SCD2.62
9509644	Zn[Propylamine]4	9.4900	9.4900	0.0000	0.0000	SCD2.62
1609641	Cd[Propylamine]	2.6200	2.6200	0.0000	0.0000	SCD2.62
1609642	Cd[Propylamine]2	4.6400	4.6400	0.0000	0.0000	SCD2.62
1609643	Cd[Propylamine]3	6.0300	6.0300	0.0000	0.0000	SCD2.62
209641	Ag[Propylamine]	3.4700	3.4500	0.0000	0.0000	NIST46.2
209642	Ag[Propylamine]2	7.5100	7.4400	0.0000	0.0000	NIST46.2
5409641	Ni[Propylamine]	2.8100	2.8100	0.0000	0.0000	SCD2.62
5409642	Ni[Propylamine]2	5.0200	5.0200	0.0000	0.0000	SCD2.62
5409643	Ni[Propylamine]3	6.7900	6.7900	0.0000	0.0000	SCD2.62
5409644	Ni[Propylamine]4	8.3100	8.3100	0.0000	0.0000	SCD2.62
3309651	H[Isopropylamine]	10.6700	10.6700	-58.3668	0.0000	NIST46.2
9509651	Zn[Isopropylamine]	2.3700	2.3700	0.0000	0.0000	SCD2.62
9509652	Zn[Isopropylamine]2	4.6700	4.6700	0.0000	0.0000	SCD2.62
9509653	Zn[Isopropylamine]3	7.1400	7.1400	0.0000	0.0000	SCD2.62
9509654	Zn[Isopropylamine]4	9.4400	9.4400	0.0000	0.0000	SCD2.62
1609651	Cd[Isopropylamine]	2.5500	2.5500	0.0000	0.0000	SCD2.62

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
1609652	Cd[Isopropylamine]2	4.5700	4.5700	0.0000	0.0000	SCD2.62
1609653	Cd[Isopropylamine]3	6.0700	6.0700	0.0000	0.0000	SCD2.62
1609654	Cd[Isopropylamine]4	6.9000	6.9000	0.0000	0.0000	SCD2.62
3619651	Hg[Isopropylamine]	14.8500	14.8500	0.0000	0.0000	NIST46.2
3619652	Hg[Isopropylamine]2	24.3700	24.3700	0.0000	0.0000	NIST46.2
209651	Ag[Isopropylamine]	3.1900	3.6700	0.0000	0.0000	NIST46.2
209652	Ag[Isopropylamine]2	6.8500	7.7700	0.0000	0.0000	NIST46.2
5409651	Ni[Isopropylamine]	2.7100	2.7100	0.0000	0.0000	SCD2.62
5409652	Ni[Isopropylamine]2	4.8600	4.8600	0.0000	0.0000	SCD2.62
5409653	Ni[Isopropylamine]3	6.5700	6.5700	0.0000	0.0000	SCD2.62
5409654	Ni[Isopropylamine]4	7.8300	7.8300	0.0000	0.0000	SCD2.62
5409655	Ni[Isopropylamine]5	8.4300	8.4300	0.0000	0.0000	SCD2.62
3309661	H[Trimethylamine]	9.8000	9.8000	0.0000	0.0000	NIST46.2
209661	Ag[Trimetylamine]	1.7010	1.7010	0.0000	0.0000	SCD2.62
3309671	H[Citrate]	6.3300	6.3960	0.0000	0.0000	NIST46.2
3309672	H2[Citrate]	11.0500	11.1570	0.0000	0.0000	NIST46.2
3309673	H3[Citrate]	14.1800	14.2850	0.0000	0.0000	NIST46.2
6009671	Pb[Citrate]	4.3400	7.2700	0.0000	0.0000	SCD2.62
6009672	Pb[Citrate]2	6.0800	6.5300	0.0000	0.0000	NIST46.2
309671	Al[Citrate]	9.9700	9.9700	0.0000	0.0000	NIST46.2
309672	Al[Citrate]2	14.8000	14.8000	0.0000	0.0000	NIST46.2
309673	AlH[Citrate]	12.8500	12.8500	0.0000	0.0000	NIST46.2
8709671	Tl[Citrate]	1.6100	1.4800	0.0000	0.0000	NIST46.2
9509671	Zn[Citrate]	6.1000	6.2100	0.0000	0.0000	NIST46.2
9509672	Zn[Citrate]2	6.7000	7.4000	0.0000	0.0000	NIST46.2
9509673	ZnH[Citrate]	3.7800	10.2000	0.0000	0.0000	NIST46.2
9509674	ZnH2[Citrate]	1.6800	12.8400	0.0000	0.0000	SCD2.62
1609671	Cd[Citrate]	5.3000	4.9800	0.0000	0.0000	NIST46.2
1609672	CdH[Citrate]	3.3700	9.4400	0.0000	0.0000	NIST46.2
1609673	CdH2[Citrate]	2.0500	12.9000	0.0000	0.0000	NIST46.2
1609674	Cd[Citrate]2	5.3400	5.9000	0.0000	0.0000	NIST46.2
3619671	Hg[Citrate]	18.3000	18.3000	0.0000	0.0000	NIST46.2
2319671	Cu[Citrate]	7.2600	7.5700	0.0000	0.0000	SCD2.62
2319672	Cu[Citrate]2	8.7200	8.9000	0.0000	0.0000	SCD2.62
2319673	CuH[Citrate]	4.2700	10.8700	0.0000	0.0000	NIST46.2
2319674	CuH2[Citrate]	2.2000	13.2300	0.0000	0.0000	SCD2.62
2319675	Cu2[Citrate]2	16.9000	16.9000	41.8400	0.0000	NIST46.2
5409671	Ni[Citrate]	6.6200	6.5900	0.0000	0.0000	NIST46.2
5409672	NiH[Citrate]	4.0900	10.5000	0.0000	0.0000	NIST46.2
5409673	NiH2[Citrate]	2.1300	13.3000	0.0000	0.0000	NIST46.2
5409674	Ni[Citrate]2	8.7700	8.7700	12.5520	0.0000	NIST46.2
5409675	NiH[Citrate]2	14.9000	14.9000	32.6352	0.0000	NIST46.2
2009671	Co[Citrate]		6.1867		0.0000	NIST46.4
2009672	CoHCitrate]		10.4438		0.0000	NIST46.4
2009673	CoH2Citrate]		12.7859		0.0000	NIST46.4
2809671	Fe[Citrate]	5.7000	6.1000	0.0000	0.0000	NIST46.2
2809672	FeH[Citrate]	3.5000	10.2000	0.0000	0.0000	NIST46.2
2819671	Fe[Citrate]	12.5500	13.1000	0.0000	0.0000	NIST46.2
2819672	FeH[Citrate]	19.8000	14.4000	0.0000	0.0000	NIST46.2
4709671	Mn[Citrate]	5.2800	4.2800	0.0000	0.0000	SCD2.62
4709672	MnH[Citrate]	3.0200	9.6000	0.0000	0.0000	NIST46.2
1109671	Be[Citrate]		5.5340		0.0000	NIST46.4
1109672	BeH[Citrate]		9.4420		0.0000	NIST46.4
1509671	Ca[Citrate]	4.7300	4.8700	0.0000	0.0000	NIST46.2
1509672	CaH[Citrate]	3.0200	9.2600	0.0000	0.0000	NIST46.2
1509673	CaH2[Citrate]	1.2900	12.2570	0.0000	0.0000	SCD2.62
4609671	Mg[Citrate]	3.3700	4.8900	0.0000	0.0000	NIST46.2
4609672	MgH[Citrate]	8.1700	8.9100	0.0000	0.0000	NIST46.2
4609673	MgH2[Citrate]	11.5900	12.2000	0.0000	0.0000	SCD2.62
8009671	Sr[Citrate]		4.3367		0.0000	NIST46.4
8009672	SrH[Citrate]		8.9738		0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
8009673	SrH2[Citrate]		12.4859		0.0000	NIST46.4
1009671	Ba[Citrate]	4.0600	4.1000	0.0000	0.0000	NIST46.2
1009672	BaH[Citrate]	2.7000	8.7400	0.0000	0.0000	NIST46.2
1009673	BaH2[Citrate]	1.2700	12.3000	0.0000	0.0000	NIST46.2
5009671	Na[Citrate]	1.0300	1.0300	-2.8033	0.0000	SCD2.62
5009672	Na2[Citrate]	1.5000	1.5000	-5.1045	0.0000	SCD2.62
5009673	NaH[Citrate]	6.4500	6.4500	-3.5982	0.0000	SCD2.62
4109671	K[Citrate]	1.1000	1.1000	5.4392	0.0000	NIST46.2
3309681	H[NTA]	10.3340	10.2780	0.0000	0.0000	NIST46.2
3309682	H2[NTA]	13.2700	13.2200	0.0000	0.0000	NIST46.2
3309683	H3[NTA]	14.1200	15.2200	0.0000	0.0000	NIST46.2
3309684	H4[NTA]	16.2240	16.2200	0.0000	0.0000	NIST46.2
6009681	Pb[NTA]	11.6233	12.7000	0.0000	0.0000	NIST46.2
6009682	PbH[NTA]	3.7950	15.3000	0.0000	0.0000	NIST46.2
309681	Al[NTA]	13.3000	13.3000	0.0000	0.0000	NIST46.2
309682	AlH[NTA]	15.2000	15.2000	0.0000	0.0000	NIST46.2
309683	AlOH[NTA]	8.0000	8.0000	0.0000	0.0000	NIST46.2
8709681	Tl[NTA]	4.7100	5.3900	0.0000	0.0000	NIST46.2
9509681	Zn[NTA]	11.9500	11.9500	-3.7656	0.0000	NIST46.2
9509682	Zn[NTA]2	14.8800	14.8800	-15.0624	0.0000	NIST46.2
9509683	ZnOH[NTA]	1.4600	1.4600	46.4424	0.0000	NIST46.2
1609681	Cd[NTA]	9.4000	11.0700	0.0000	0.0000	NIST46.2
1609682	Cd[NTA]2	14.3000	15.0300	0.0000	0.0000	NIST46.2
1609683	CdOH[NTA]	-0.6100	-0.6100	29.2880	0.0000	NIST46.2
3619681	Hg[NTA]	21.7000	21.7000	0.0000	0.0000	NIST46.2
2319681	Cu[NTA]	13.1000	14.4000	0.0000	0.0000	NIST46.2
2319682	Cu[NTA]2	17.5000	18.1000	0.0000	0.0000	NIST46.2
2319683	CuH[NTA]	16.2000	16.2000	0.0000	0.0000	NIST46.2
2319684	CuOH[NTA]	4.8000	4.8000	25.5224	0.0000	NIST46.2
209681	Ag[NTA]	5.3600	6.0000	0.0000	0.0000	NIST46.2
5409681	Ni[NTA]	12.7900	12.7900	-10.0416	0.0000	NIST46.2
5409682	Ni[NTA]2	16.9600	16.9600	-32.6352	0.0000	NIST46.2
5409683	NiOH[NTA]	1.5000	1.5000	15.0624	0.0000	NIST46.2
2009681	Co[NTA]		11.6667		0.0000	NIST46.4
2009682	Co[NTA]2		14.9734		0.0000	NIST46.4
2009683	CoOH[NTA]		0.4378		0.0000	NIST46.4
2809681	Fe[NTA]	10.1900	10.1900	0.0000	0.0000	NIST46.2
2809682	Fe[NTA]2	12.6200	12.6200	0.0000	0.0000	NIST46.2
2809683	FeH[NTA]	12.2900	12.2900	0.0000	0.0000	NIST46.2
2809684	FeOH[NTA]	-1.0600	-1.0600	0.0000	0.0000	NIST46.2
2819681	Fe[NTA]	17.8000	17.8000	13.3888	0.0000	NIST46.2
2819682	Fe[NTA]2	25.9000	25.9000	0.0000	0.0000	NIST46.2
2819683	FeOH[NTA]	13.2300	13.2300	0.0000	0.0000	NIST46.2
4709681	Mn[NTA]	8.5730	8.5730	5.8576	0.0000	NIST46.2
4709682	Mn[NTA]2	11.5800	11.5800	-17.1544	0.0000	NIST46.2
2119681	Cr[NTA]	21.2000	21.2000	0.0000	0.0000	SCD2.62
2119682	Cr[NTA]2	29.5000	29.5000	0.0000	0.0000	SCD2.62
4809681	MoO3[NTA]		19.5434		0.0000	NIST46.4
4809682	MoO3H[NTA]		23.3954		0.0000	NIST46.4
4809683	MoO3H2[NTA]		25.3534		0.0000	NIST46.4
1109681	Be[NTA]		9.0767		0.0000	NIST46.4
4609681	Mg[NTA]	6.5000	6.5000	17.9912	0.0000	NIST46.2
1509681	Ca[NTA]	7.6080	7.6080	-5.6902	0.0000	NIST46.2
1509682	Ca[NTA]2	8.8100	8.8100	-32.6352	0.0000	NIST46.2
8009681	Sr[NTA]	0.0000	6.2767	0.0000	0.0000	NIST46.4
1009681	Ba[NTA]	5.8750	5.8750	-6.0250	0.0000	NIST46.2
3309691	H[EDTA]	9.9600	10.9480	0.0000	0.0000	NIST46.2
3309692	H2[EDTA]	16.2100	17.2210	0.0000	0.0000	NIST46.2
3309693	H3[EDTA]	18.8600	20.3400	0.0000	0.0000	NIST46.2
3309694	H4[EDTA]	20.9300	22.5000	0.0000	0.0000	NIST46.2
3309695	H5[EDTA]	23.4640	24.0000	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
7909691	Sn[EDTA]		27.0260		0.0000	NIST46.4
7909692	SnH[EDTA]		29.9340		0.0000	NIST46.4
7909693	SnH2[EDTA]		31.6380		0.0000	NIST46.4
6009691	Pb[EDTA]	17.8800	19.8000	0.0000	0.0000	NIST46.2
6009692	PbH[EDTA]	9.6800	23.0000	0.0000	0.0000	NIST46.2
6009693	PbH2[EDTA]	6.2200	24.9000	0.0000	0.0000	NIST46.2
309690	Al[EDTA]	18.9000	19.1000	0.0000	0.0000	NIST46.2
309691	AlH[EDTA]	21.6000	21.8000	0.0000	0.0000	NIST46.2
309692	AlOH[EDTA]	12.8000	12.8000	73.6384	0.0000	NIST46.2
8709691	Tl[EDTA]	6.4100	7.2700	0.0000	0.0000	NIST46.2
8709692	TlH[EDTA]	13.6800	13.6800	0.0000	0.0000	NIST46.2
9509691	Zn[EDTA]	16.4400	18.0000	0.0000	0.0000	NIST46.2
9509692	ZnH[EDTA]	9.0000	21.4000	0.0000	0.0000	NIST46.2
9509693	ZnOH[EDTA]	5.8000	5.8000	0.0000	0.0000	NIST46.2
1609691	Cd[EDTA]	16.2750	18.2000	0.0000	0.0000	NIST46.2
1609692	CdH[EDTA]	2.9000	21.5000	0.0000	0.0000	NIST46.2
3619691	Hg[EDTA]	29.3000	29.3000	-125.1016	0.0000	NIST46.2
3619692	HgH[EDTA]	32.9000	32.9000	-128.4488	0.0000	NIST46.2
2319691	Cu[EDTA]	18.7850	20.5000	0.0000	0.0000	NIST46.2
2319692	CuH[EDTA]	11.1950	24.0000	0.0000	0.0000	NIST46.2
2319693	CuH2[EDTA]	26.2000	26.2000	0.0000	0.0000	NIST46.2
2319694	CuOH[EDTA]	8.5000	8.5000	0.0000	0.0000	NIST46.2
209691	Ag[EDTA]	7.3550	8.0800	0.0000	0.0000	NIST46.2
209693	AgH[EDTA]	3.3600	15.2100	0.0000	0.0000	SCD2.62
5409691	Ni[EDTA]	20.3300	20.1000	0.0000	0.0000	NIST46.2
5409692	NiH[EDTA]	11.5600	23.6000	0.0000	0.0000	NIST46.2
5409693	NiOH[EDTA]	7.6000	7.6000	0.0000	0.0000	NIST46.2
2009691	Co[EDTA]		18.1657		0.0000	NIST46.4
2009692	CoH[EDTA]		21.5946		0.0000	NIST46.4
2009693	CoH2[EDTA]		23.4986		0.0000	NIST46.4
2019691	Co[EDTA]		43.9735		0.0000	NIST46.4
2019692	CoH[EDTA]		47.1680		0.0000	NIST46.4
2809690	Fe[EDTA]	16.1000	16.0000	0.0000	0.0000	NIST46.2
2809691	FeH[EDTA]	19.3000	19.0600	0.0000	0.0000	NIST46.2
2809692	FeOH[EDTA]	6.4000	6.5000	0.0000	0.0000	SCD2.62
2809693	Fe(OH)2[EDTA]	-4.3000	-4.0000	0.0000	0.0000	SCD2.62
2819690	Fe[EDTA]	27.7000	27.7000	0.0000	0.0000	NIST46.2
2819691	FeH[EDTA]	29.2000	29.2000	0.0000	0.0000	NIST46.2
2819692	FeOH[EDTA]	19.8000	19.9000	0.0000	0.0000	NIST46.2
2819693	Fe(OH)2[EDTA]	9.7000	9.8500	0.0000	0.0000	SCD2.62
4709691	Mn[EDTA]	15.6000	15.6000	-19.2464	0.0000	NIST46.2
4709692	MnH[EDTA]	19.1000	19.1000	-24.2672	0.0000	NIST46.2
2109691	Cr[EDTA]	13.6100	15.3000	0.0000	0.0000	NIST46.2
2109692	CrH[EDTA]	6.1000	19.1000	0.0000	0.0000	SCD2.62
2119691	Cr[EDTA]	35.5000	35.5000	0.0000	0.0000	NIST46.2
2119692	CrH[EDTA]	37.4000	37.4000	0.0000	0.0000	NIST46.2
2119693	CrOH[EDTA]	27.7000	27.7000	0.0000	0.0000	NIST46.2
1109691	Be[EDTA]	0.0000	11.4157	0.0000	0.0000	NIST46.4
4609690	Mg[EDTA]	10.6000	10.5700	0.0000	0.0000	NIST46.2
4609691	MgH[EDTA]	15.1000	14.9700	0.0000	0.0000	NIST46.2
1509690	Ca[EDTA]	12.4000	12.4200	0.0000	0.0000	NIST46.2
1509691	CaH[EDTA]	16.0000	15.9000	0.0000	0.0000	NIST46.2
8009691	Sr[EDTA]		10.4357		0.0000	NIST46.4
8009692	SrH[EDTA]		14.7946		0.0000	NIST46.4
1009691	Ba[EDTA]	8.0000	7.7200	0.0000	0.0000	SCD2.62
5009690	Na[EDTA]	2.5000	2.7000	0.0000	0.0000	NIST46.2
4109690	K[EDTA]	1.7000	1.7000	0.0000	0.0000	NIST46.2
3309711	H[Propionate]	4.8740	4.8740	0.0000	0.0000	NIST46.4
6009711	Pb[Propionate]	2.6400	2.6400	0.0000	0.0000	NIST46.4
6009712	Pb[Propionate]2	4.1500	3.1765	0.0000	0.0000	NIST46.4
9509711	Zn[Propionate]	0.7200	1.4389	0.0000	0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
9509712	Zn[Propionate]2	1.2300	1.8420	0.0000	0.0000	NIST46.4
1609711	Cd[Propionate]	1.1900	1.5980	0.0000	0.0000	NIST46.4
1609712	Cd[Propionate]2	1.8600	2.4720	0.0000	0.0000	NIST46.4
3619711	Hg[Propionate]	9.4170	10.5940	0.0000	0.0000	NIST46.4
2319711	Cu[Propionate]	2.2200	2.2200	0.0000	0.0000	NIST46.4
2319712	Cu[Propionate]2	2.6200	3.5000	0.0000	0.0000	NIST46.4
5409711	Ni[Propionate]	0.7300	0.9080	0.0000	0.0000	NIST46.4
2009711	Co[Propionate]		0.6710		0.0000	NIST46.4
2009712	Co[Propionate]2		0.5565		0.0000	NIST46.4
2819711	Fe[Propionate]	3.4000	4.0120	0.0000	0.0000	NIST46.4
2119711	Cr[Propionate]	14.3200	15.0773	0.0000	0.0000	NIST46.4
2119712	Cr[Propionate]2	16.6600	17.9563	0.0000	0.0000	NIST46.4
2119713	Cr[Propionate]3	19.3200	20.8858	0.0000	0.0000	NIST46.4
4609710	Mg[Propionate]	0.5400	0.9689	0.0000	0.0000	NIST46.4
1509710	Ca[Propionate]	0.5000	0.9289	0.0000	0.0000	NIST46.4
8009711	Sr[Propionate]	0.0000	0.8589	0.0000	0.0000	NIST46.4
1009711	Ba[Propionate]	0.3400	0.7689	0.0000	0.0000	NIST46.4
1009712	Ba[Propionate]2	1.1900	0.9834	0.0000	0.0000	NIST46.4
3309721	H[Butyrate]	4.7300	4.8190	0.0000	0.0000	NIST46.4
6009721	Pb[Butyrate]	2.1250	2.1010	0.0000	0.0000	NIST46.4
9509721	Zn[Butyrate]	0.9830	1.4289	0.0000	0.0000	NIST46.4
3619721	Hg[Butyrate]	10.0970	10.3529	0.0000	0.0000	NIST46.4
2319721	Cu[Butyrate]	2.1400	2.1400	0.0000	0.0000	NIST46.4
5409721	Ni[Butyrate]	0.7700	0.6910	0.0000	0.0000	NIST46.4
2009721	Co[Butyrate]		0.5910		0.0000	NIST46.4
2009722	Co[Butyrate]2		0.7765		0.0000	NIST46.4
4609720	Mg[Butyrate]	0.5300	0.9589	0.0000	0.0000	NIST46.4
1509720	Ca[Butyrate]	0.5100	0.9389	0.0000	0.0000	NIST46.4
8009721	Sr[Butyrate]		0.7889		0.0000	NIST46.4
1009721	Ba[Butyrate]	0.9400	0.7389	0.0000	0.0000	NIST46.4
1009722	Ba[Butyrate]2	0.8800	0.8800	0.0000	0.0000	SCD2.62
3309731	H[Isobutyrate]	4.8490	4.8490	0.0000	0.0000	NIST46.2
9509731	Zn[Isobutyrate]	1.4400	1.4400	0.0000	0.0000	NIST46.2
2319731	Cu[Isobutyrate]	2.1700	2.1700	0.0000	0.0000	NIST46.2
2319732	Cu[Isobutyrate]2	2.7000	3.3000	0.0000	0.0000	NIST46.2
2819731	Fe[Isobutyrate]	3.6000	4.2000	0.0000	0.0000	NIST46.2
1509731	Ca[Isobutyrate]	0.5100	0.5100	0.0000	0.0000	SCD2.62
3309801	H[2-Picoline]	5.9500	5.9500	0.0000	0.0000	NIST46.2
2319801	Cu[2-Picoline]	1.3000	1.3000	0.0000	0.0000	NIST46.2
2319802	Cu[2-Picoline]2	2.8000	2.8000	0.0000	0.0000	NIST46.2
2309801	Cu[2-Picoline]	5.4000	5.4000	0.0000	0.0000	NIST46.2
2309802	Cu[2-Picoline]2	7.6500	7.6500	0.0000	0.0000	NIST46.2
2309803	Cu[2-Picoline]3	8.5000	8.5000	0.0000	0.0000	NIST46.2
209801	Ag[2-Picoline]	2.3200	2.3200	0.0000	0.0000	NIST46.2
209802	Ag[2-Picoline]2	4.6800	4.6800	0.0000	0.0000	NIST46.2
5409801	Ni[2-Picoline]	0.4000	0.4000	0.0000	0.0000	NIST46.2
3309811	H[3-Picoline]	5.7000	5.7000	0.0000	0.0000	NIST46.2
9509811	Zn[3-Picoline]	1.0000	1.0000	0.0000	0.0000	NIST46.2
9509812	Zn[3-Picoline]2	2.1000	2.1000	0.0000	0.0000	NIST46.2
9509813	Zn[3-Picoline]3	2.6000	2.6000	0.0000	0.0000	NIST46.2
9509814	Zn[3-Picoline]4	3.7000	3.7000	0.0000	0.0000	NIST46.2
1609811	Cd[3-Picoline]	1.6200	1.4200	0.0000	0.0000	SCD2.62
1609812	Cd[3-Picoline]2	2.8000	2.2700	0.0000	0.0000	SCD2.62
1609813	Cd[3-Picoline]3	3.6000	3.6000	0.0000	0.0000	NIST46.2
1609814	Cd[3-Picoline]4	4.0000	4.0000	0.0000	0.0000	NIST46.2
2309811	Cu[3-Picoline]	5.6000	5.6000	0.0000	0.0000	NIST46.2
2309812	Cu[3-Picoline]2	7.7800	7.7800	0.0000	0.0000	NIST46.2
2309813	Cu[3-Picoline]3	8.6000	8.6000	0.0000	0.0000	NIST46.2
2309814	Cu[3-Picoline]4	9.0000	9.0000	0.0000	0.0000	NIST46.2
2319811	Cu[3-Picoline]	2.7400	2.7700	0.0000	0.0000	NIST46.2
2319812	Cu[3-Picoline]2	4.8000	4.8000	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
2319813	Cu[3-Picoline]3	6.3000	6.3000	0.0000	0.0000	NIST46.2
2319814	Cu[3-Picoline]4	7.2000	7.2000	0.0000	0.0000	NIST46.2
209811	Ag[3-Picoline]	2.2000	2.2000	0.0000	0.0000	NIST46.2
209812	Ag[3-Picoline]2	4.4600	4.4600	0.0000	0.0000	NIST46.2
5409811	Ni[3-Picoline]	2.0200	1.8700	0.0000	0.0000	NIST46.2
5409812	Ni[3-Picoline]2	3.3000	3.3000	0.0000	0.0000	NIST46.2
5409813	Ni[3-Picoline]3	4.1000	4.1000	0.0000	0.0000	NIST46.2
5409814	Ni[3-Picoline]4	4.6000	4.6000	0.0000	0.0000	NIST46.2
2009811	Co[3-Picoline]		1.4000		0.0000	NIST46.4
2009812	Co[3-Picoline]2		2.2000		0.0000	NIST46.4
2009813	Co[3-Picoline]3		2.5000		0.0000	NIST46.4
3309821	H[4-Picoline]	6.0000	6.0300	0.0000	0.0000	NIST46.2
9509821	Zn[4-Picoline]	1.4000	1.4000	0.0000	0.0000	NIST46.2
9509822	Zn[4-Picoline]2	2.1100	2.1100	0.0000	0.0000	NIST46.2
9509823	Zn[4-Picoline]3	2.8500	2.8500	0.0000	0.0000	NIST46.2
1609821	Cd[4-Picoline]	1.5100	1.5900	0.0000	0.0000	SCD2.62
1609822	Cd[4-Picoline]2	2.5000	2.4000	0.0000	0.0000	SCD2.62
1609823	Cd[4-Picoline]3	2.9000	3.1800	0.0000	0.0000	SCD2.62
1609824	Cd[4-Picoline]4	4.0000	4.0000	0.0000	0.0000	NIST46.2
2309821	Cu[4-Picoline]	5.6500	5.6500	0.0000	0.0000	NIST46.2
2309822	Cu[4-Picoline]2	8.2000	8.2000	0.0000	0.0000	NIST46.2
2309823	Cu[4-Picoline]3	8.8000	8.8000	0.0000	0.0000	NIST46.2
2309824	Cu[4-Picoline]4	9.2000	9.2000	0.0000	0.0000	NIST46.2
2319821	Cu[4-Picoline]	2.8800	2.8800	0.0000	0.0000	NIST46.2
2319822	Cu[4-Picoline]2	5.1600	5.1600	0.0000	0.0000	NIST46.2
2319823	Cu[4-Picoline]3	6.7700	6.7700	0.0000	0.0000	NIST46.2
2319824	Cu[4-Picoline]4	8.0800	8.0800	0.0000	0.0000	NIST46.2
2319825	Cu[4-Picoline]5	8.3000	8.3000	0.0000	0.0000	NIST46.2
209821	Ag[4-Picoline]	2.2100	2.0300	0.0000	0.0000	NIST46.2
209822	Ag[4-Picoline]2	4.6700	4.3900	0.0000	0.0000	NIST46.2
5409821	Ni[4-Picoline]	2.1100	2.1100	0.0000	0.0000	NIST46.2
5409822	Ni[4-Picoline]2	3.5900	3.5900	0.0000	0.0000	NIST46.2
5409823	Ni[4-Picoline]3	4.3400	4.3400	0.0000	0.0000	NIST46.2
5409824	Ni[4-Picoline]4	4.7000	4.7000	0.0000	0.0000	NIST46.2
2009821	Co[4-Picoline]		1.5600		0.0000	NIST46.4
2009822	Co[4-Picoline]2		2.5100		0.0000	NIST46.4
2009823	Co[4-Picoline]3		2.9400		0.0000	NIST46.4
2009824	Co[4-Picoline]4		3.1700		0.0000	NIST46.4
3309831	H[Formate]	3.7450	3.7450	0.0000	0.0000	NIST46.2
6009831	Pb[Formate]	2.2000	2.2000	0.0000	0.0000	SCD2.62
9509831	Zn[Formate]	1.4400	1.4400	0.0000	0.0000	NIST46.2
1609831	Cd[Formate]	1.7000	1.7000	0.0000	0.0000	SCD2.62
3619831	Hg[Formate]	9.6000	9.6000	0.0000	0.0000	NIST46.2
2319831	Cu[Formate]	2.0000	2.0000	0.0000	0.0000	NIST46.2
5409831	Ni[Formate]	1.2200	1.2200	0.0000	0.0000	SCD2.62
2009831	Co[Formate]		1.2090		0.0000	NIST46.4
2009832	Co[Formate]2		1.1365		0.0000	NIST46.4
2109831	Cr[Formate]	1.0700	1.0700	0.0000	0.0000	NIST46.2
4609831	Mg[Formate]	1.4300	1.4300	0.0000	0.0000	NIST46.2
1509831	Ca[Formate]	1.4300	1.4300	4.1840	0.0000	NIST46.2
8009831	Sr[Formate]		1.3900		0.0000	NIST46.4
1009831	Ba[Formate]	1.3800	1.3800	0.0000	0.0000	NIST46.2
3309841	H[Isovalerate]	4.7810	4.7810	0.0000	0.0000	NIST46.2
9509841	Zn[Isovalerate]	1.3900	1.3900	0.0000	0.0000	NIST46.2
2319841	Cu[Isovalerate]	2.0800	2.0800	0.0000	0.0000	NIST46.2
1509841	Ca[Isovalerate]	0.2000	0.2000	0.0000	0.0000	SCD2.62
3309851	H[Valerate]	4.8430	4.8430	0.0000	0.0000	NIST46.2
2319851	Cu[Valerate]	2.1200	2.1200	0.0000	0.0000	NIST46.2
1509851	Ca[Valerate]	0.3000	0.3000	0.0000	0.0000	SCD2.62
1009851	Ba[Valerate]	0.6600	-0.2000	0.0000	0.0000	SCD2.62
3309921	H[Acetate]	4.7600	4.7570	0.0000	0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
7909921	Sn[Acetate]		10.0213		0.0000	NIST46.4
7909922	Sn[Acetate]2		12.3200		0.0000	NIST46.4
7909923	Sn[Acetate]3		13.5500		0.0000	NIST46.4
6009921	Pb[Acetate]	2.8700	2.6800	0.0000	0.0000	NIST46.4
6009922	Pb[Acetate]2	4.0800	4.0800	0.0000	0.0000	NIST46.4
8709921	Tl[Acetate]	-0.1100	-0.1100	0.0000	0.0000	NIST46.4
9509921	Zn[Acetate]	1.5700	1.5800	0.0000	0.0000	NIST46.4
9509922	Zn[Acetate]2	1.9000	2.6434	0.0000	0.0000	NIST46.4
1609921	Cd[Acetate]	1.9300	1.9300	0.0000	0.0000	NIST46.4
1609922	Cd[Acetate]2	3.1500	2.8600	0.0000	0.0000	NIST46.4
3619920	Hg[Acetate]	9.4170	10.4940	0.0000	0.0000	NIST46.4
3619921	Hg[Acetate]2	13.1100	13.8300	0.0000	0.0000	NIST46.4
2319921	Cu[Acetate]	2.2200	2.2100	0.0000	0.0000	NIST46.4
2319922	Cu[Acetate]2	3.6300	3.4000	0.0000	0.0000	NIST46.4
2319923	Cu[Acetate]3	3.1000	3.9434	0.0000	0.0000	NIST46.4
209921	Ag[Acetate]	0.7300	0.7300	0.0000	0.0000	NIST46.4
209922	Ag[Acetate]2	0.6400	0.6400	0.0000	0.0000	NIST46.4
5409921	Ni[Acetate]	1.4300	1.3700	0.0000	0.0000	NIST46.4
5409922	Ni[Acetate]2	2.1000	2.1000	10.4600	0.0000	NIST46.4
2009921	Co[Acetate]		1.3800		0.0000	NIST46.4
2009922	Co[Acetate]2		0.7565		0.0000	NIST46.4
2809920	Fe[Acetate]	1.4000	1.4000	0.0000	0.0000	NIST46.4
2819920	Fe[Acetate]	3.2100	4.0234	0.0000	0.0000	NIST46.4
2819921	Fe[Acetate]2	6.5000	7.5723	0.0000	0.0000	NIST46.4
2819922	Fe[Acetate]3	8.3000	9.5867	0.0000	0.0000	NIST46.4
4709920	Mn[Acetate]	1.4000	1.4000	0.0000	0.0000	NIST46.4
2109921	Cr[Acetate]	1.8000	1.8000	0.0000	0.0000	NIST46.4
2109922	Cr[Acetate]2	2.9200	2.9200	0.0000	0.0000	NIST46.4
2119921	Cr[Acetate]	14.2500	15.0073	0.0000	0.0000	NIST46.4
2119922	Cr[Acetate]2	16.6800	17.9963	0.0000	0.0000	NIST46.4
2119923	Cr[Acetate]3	19.2000	20.7858	0.0000	0.0000	NIST46.4
1109921	Be[Acetate]		2.0489		0.0000	NIST46.4
1109922	Be[Acetate]2		3.0034		0.0000	NIST46.4
4609920	Mg[Acetate]	1.2700	1.2700	0.0000	0.0000	NIST46.4
1509920	Ca[Acetate]	1.1800	1.1800	0.0000	0.0000	NIST46.4
8009921	Sr[Acetate]		1.1400		0.0000	NIST46.4
1009921	Ba[Acetate]	1.0700	1.0700	0.0000	0.0000	NIST46.4
5009920	Na[Acetate]	-0.1800	-0.1800	0.0000	0.0000	NIST46.4
4109921	K[Acetate]	-0.2000	-0.1955	4.1840	0.0000	NIST46.4
3309931	H[Tartrate]	4.1600	4.3660	0.0000	0.0000	NIST46.2
3309932	H2[Tartrate]	6.6700	7.4020	0.0000	0.0000	NIST46.2
7909931	Sn[Tartrate]		13.1518		0.0000	NIST46.4
6009931	Pb[Tartrate]	3.7800	3.9800	0.0000	0.0000	NIST46.2
309931	Al[Tartrate]2	9.3700	9.3700	0.0000	0.0000	NIST46.2
8709931	Tl[Tartrate]	1.4000	1.4000	0.0000	0.0000	NIST46.2
8709932	TlH[Tartrate]	4.8000	4.8000	0.0000	0.0000	NIST46.2
9509931	Zn[Tartrate]	3.4300	3.4300	0.0000	0.0000	NIST46.2
9509932	Zn[Tartrate]2	5.5000	5.5000	0.0000	0.0000	NIST46.2
9509933	ZnH[Tartrate]	5.9000	5.9000	0.0000	0.0000	NIST46.2
1609931	Cd[Tartrate]	3.9000	2.7000	0.0000	0.0000	NIST46.2
1609932	Cd[Tartrate]2	4.1000	4.1000	0.0000	0.0000	NIST46.2
3619931	Hg[Tartrate]	14.0000	14.0000	0.0000	0.0000	NIST46.2
2319931	Cu[Tartrate]	3.9700	3.9700	0.0000	0.0000	NIST46.2
2319932	CuH[Tartrate]	6.7000	6.7000	0.0000	0.0000	NIST46.2
5409931	Ni[Tartrate]	3.4600	3.4600	0.0000	0.0000	NIST46.2
5409932	NiH[Tartrate]	5.8900	5.8900	0.0000	0.0000	NIST46.2
2009931	Co[Tartrate]		3.0500		0.0000	NIST46.4
2009932	Co[Tartrate]2		4.0000		0.0000	NIST46.4
2009933	CoH[Tartrate]		5.7540		0.0000	NIST46.4
2809931	Fe[Tartrate]	3.1000	3.1000	0.0000	0.0000	NIST46.2
2819931	Fe[Tartrate]	7.7800	7.7800	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
4709931	Mn[Tartrate]	3.3800	3.3800	0.0000	0.0000	NIST46.2
4709932	MnH[Tartrate]	6.0000	6.0000	0.0000	0.0000	NIST46.2
4609931	Mg[Tartrate]	2.3000	2.3000	0.0000	0.0000	NIST46.2
4609932	MgH[Tartrate]	5.7500	5.7500	0.0000	0.0000	NIST46.2
1109931	Be[Tartrate]		2.7680		0.0000	NIST46.4
1109932	Be[Tartrate]2		4.0080		0.0000	NIST46.4
1509931	Ca[Tartrate]	2.8000	2.8000	-8.3680	0.0000	NIST46.2
1509932	CaH[Tartrate]	5.8600	5.8600	-9.1211	0.0000	NIST46.2
8009931	Sr[Tartrate]		2.5500		0.0000	NIST46.4
8009932	SrH[Tartrate]		5.8949		0.0000	NIST46.4
1009931	Ba[Tartrate]	2.5400	2.5400	0.0000	0.0000	NIST46.2
1009932	BaH[Tartrate]	5.7700	5.7700	0.0000	0.0000	NIST46.2
5009931	Na[Tartrate]	0.9000	0.9000	-0.8368	0.0000	NIST46.2
5009932	NaH[Tartrate]	4.5800	4.5800	-2.8451	0.0000	NIST46.2
4109931	K[Tartrate]	0.8000	0.8000	0.0000	0.0000	NIST46.2
3309941	H[Glycine]	9.7800	9.7780	0.0000	0.0000	NIST46.2
3309942	H2[Glycine]	12.1200	12.1280	0.0000	0.0000	NIST46.2
6009941	Pb[Glycine]	5.4700	5.4700	0.0000	0.0000	NIST46.2
6009942	Pb[Glycine]2	8.3200	8.8600	0.0000	0.0000	SCD2.62
8709941	Tl[Glycine]	1.7200	1.7200	0.0000	0.0000	NIST46.2
9509941	Zn[Glycine]	5.3800	5.3800	0.0000	0.0000	NIST46.2
9509942	Zn[Glycine]2	9.8100	9.8100	0.0000	0.0000	NIST46.2
9509943	Zn[Glycine]3	12.3000	12.3000	0.0000	0.0000	NIST46.2
1609941	Cd[Glycine]	4.8000	4.6900	0.0000	0.0000	NIST46.2
1609942	Cd[Glycine]2	8.4000	8.4000	0.0000	0.0000	NIST46.2
1609943	Cd[Glycine]3	10.7000	10.7000	0.0000	0.0000	NIST46.2
3619941	Hg[Glycine]	17.0000	17.0000	0.0000	0.0000	SCD2.62
3619942	Hg[Glycine]2	25.8000	25.8000	0.0000	0.0000	SCD2.62
2309941	Cu[Glycine]2	10.3000	10.3000	0.0000	0.0000	NIST46.2
2319941	Cu[Glycine]	8.6200	8.5700	0.0000	0.0000	NIST46.2
2319942	Cu[Glycine]2	15.6400	15.7000	0.0000	0.0000	NIST46.2
209941	Ag[Glycine]	3.5100	3.5100	0.0000	0.0000	NIST46.2
209942	Ag[Glycine]2	3.3800	6.8900	0.0000	0.0000	NIST46.2
5409941	Ni[Glycine]	6.1800	6.1500	0.0000	0.0000	NIST46.2
5409942	Ni[Glycine]2	11.1300	11.1200	0.0000	0.0000	NIST46.2
5409943	Ni[Glycine]3	14.2000	14.6300	0.0000	0.0000	SCD2.62
2009941	Co[Glycine]		5.0700		0.0000	NIST46.4
2009942	Co[Glycine]2		9.0700		0.0000	NIST46.4
2009943	Co[Glycine]3		11.6000		0.0000	NIST46.4
2009944	CoOH[Glycine]		-5.0200		0.0000	NIST46.4
2809941	Fe[Glycine]	4.3100	4.3100	-15.0624	0.0000	NIST46.2
2809942	Fe[Glycine]2	8.2900	8.2900	0.0000	0.0000	NIST46.2
2819941	Fe[Glycine]	9.3800	9.3800	0.0000	0.0000	NIST46.2
2819942	FeH[Glycine]	11.5500	11.5500	0.0000	0.0000	NIST46.2
4709941	Mn[Glycine]	3.1900	3.1900	-1.2552	0.0000	NIST46.2
4709942	Mn[Glycine]2	5.4000	5.4000	0.0000	0.0000	NIST46.2
2119941	Cr[Glycine]	8.4000	18.7000	0.0000	0.0000	SCD2.62
2119942	Cr[Glycine]2	6.4000	25.6000	0.0000	0.0000	SCD2.62
2119943	Cr[Glycine]3	5.7000	31.6000	0.0000	0.0000	SCD2.62
4609941	Mg[Glycine]	2.0800	2.0800	4.1840	0.0000	NIST46.2
1509941	Ca[Glycine]	1.3900	1.3900	-4.1840	0.0000	NIST46.2
1509942	CaH[Glycine]	10.1000	10.1000	-35.9824	0.0000	NIST46.2
8009941	Sr[Glycine]		0.9100		0.0000	NIST46.4
1009941	Ba[Glycine]	0.7700	0.7700	0.0000	0.0000	NIST46.2
3309951	H[Salicylate]	13.4000	13.7000	0.0000	0.0000	NIST46.2
3309952	H2[Salicylate]	16.4000	16.8000	0.0000	0.0000	NIST46.2
9509951	Zn[Salicylate]	7.7100	7.7100	0.0000	0.0000	SCD2.62
9509952	ZnH[Salicylate]	15.5000	15.5000	0.0000	0.0000	NIST46.2
1609951	Cd[Salicylate]	6.2000	6.2000	0.0000	0.0000	NIST46.2
1609952	CdH[Salicylate]	16.0000	16.0000	0.0000	0.0000	NIST46.2
2319951	Cu[Salicylate]	10.6400	11.3000	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
2319952	Cu[Salicylate]2	16.9400	19.3000	0.0000	0.0000	NIST46.2
2319953	CuH[Salicylate]	14.8000	14.8000	0.0000	0.0000	NIST46.2
5409951	Ni[Salicylate]	6.9500	8.2000	0.0000	0.0000	NIST46.2
5409952	Ni[Salicylate]2	11.7500	12.6400	0.0000	0.0000	SCD2.62
2009951	Co[Salicylate]		7.4289		0.0000	NIST46.4
2009952	Co[Salicylate]2		11.8000		0.0000	NIST46.4
2809951	Fe[Salicylate]	7.2000	7.2000	0.0000	0.0000	NIST46.2
2809952	Fe[Salicylate]2	11.6000	11.6000	0.0000	0.0000	NIST46.2
2819951	Fe[Salicylate]	17.6000	17.6000	0.0000	0.0000	NIST46.2
2819952	Fe[Salicylate]2	29.3000	29.3000	0.0000	0.0000	NIST46.2
4709951	Mn[Salicylate]	6.5000	6.5000	0.0000	0.0000	NIST46.2
4709952	Mn[Salicylate]2	10.1000	10.1000	0.0000	0.0000	NIST46.2
1109951	Be[Salicylate]		13.3889		0.0000	NIST46.4
1109952	Be[Salicylate]2		23.2500		0.0000	NIST46.4
4609951	Mg[Salicylate]	5.7600	5.7600	0.0000	0.0000	NIST46.2
4609952	MgH[Salicylate]	15.3000	15.3000	0.0000	0.0000	SCD2.62
1509951	Ca[Salicylate]	4.0500	4.0500	0.0000	0.0000	NIST46.2
1509952	CaH[Salicylate]	14.3000	14.3000	0.0000	0.0000	NIST46.2
1009951	BaH[Salicylate]	0.2100	13.9000	0.0000	0.0000	SCD2.62
3309961	H[Glutamate]	9.9500	9.9600	0.0000	0.0000	NIST46.2
3309962	H2[Glutamate]	14.3700	14.2600	0.0000	0.0000	NIST46.2
3309963	H3[Glutamate]	16.6000	16.4200	0.0000	0.0000	NIST46.2
6009961	Pb[Glutamate]	4.7000	6.4300	0.0000	0.0000	SCD2.62
6009962	Pb[Glutamate]2	7.5500	8.6100	0.0000	0.0000	SCD2.62
6009963	PbH[Glutamate]	14.0800	14.0800	0.0000	0.0000	SCD2.62
309961	AlH[Glutamate]	13.0700	13.0700	0.0000	0.0000	NIST46.2
9509961	Zn[Glutamate]	3.7900	6.2000	0.0000	0.0000	SCD2.62
9509962	Zn[Glutamate]2	8.2500	9.1300	0.0000	0.0000	SCD2.62
9509963	Zn[Glutamate]3	9.8000	9.8000	0.0000	0.0000	SCD2.62
1609961	Cd[Glutamate]	4.7800	4.7000	0.0000	0.0000	NIST46.2
1609962	Cd[Glutamate]2	2.7800	7.5900	0.0000	0.0000	NIST46.2
3619961	Hg[Glutamate]	19.8000	19.8000	0.0000	0.0000	SCD2.62
3619962	Hg[Glutamate]2	26.2000	26.2000	0.0000	0.0000	SCD2.62
2319961	Cu[Glutamate]	8.3300	9.1700	0.0000	0.0000	NIST46.2
2319962	Cu[Glutamate]2	14.8400	15.7800	0.0000	0.0000	NIST46.2
2319963	CuH[Glutamate]	13.3000	13.3000	-28.0328	0.0000	NIST46.2
209961	Ag[Glutamate]	3.7900	4.2200	0.0000	0.0000	NIST46.2
209962	Ag[Glutamate]2	6.5500	7.3600	0.0000	0.0000	SCD2.62
209963	Ag2[Glutamate]	3.4000	3.4000	0.0000	0.0000	NIST46.2
5409961	Ni[Glutamate]	5.9000	6.4700	0.0000	0.0000	NIST46.2
5409962	Ni[Glutamate]2	10.7000	10.7000	-30.9616	0.0000	NIST46.2
2009961	Co[Glutamate]		5.4178		0.0000	NIST46.4
2009962	Co[Glutamate]2		8.7178		0.0000	NIST46.4
4709961	Mn[Glutamate]	4.9500	4.9500	0.0000	0.0000	SCD2.62
4709962	Mn[Glutamate]2	8.4800	8.4800	0.0000	0.0000	SCD2.62
2119961	Cr[Glutamate]	22.6000	22.6000	0.0000	0.0000	SCD2.62
2119962	Cr[Glutamate]2	30.7000	30.7000	0.0000	0.0000	SCD2.62
2119963	CrH[Glutamate]	25.2000	25.2000	0.0000	0.0000	SCD2.62
4609961	Mg[Glutamate]	2.8000	2.8000	0.0000	0.0000	NIST46.2
1509961	Ca[Glutamate]	2.0600	2.0600	0.0000	0.0000	NIST46.2
1509962	CaH[Glutamate]	11.1300	11.1300	0.0000	0.0000	NIST46.2
8009961	Sr[Glutamate]		2.2278		0.0000	NIST46.4
1009961	Ba[Glutamate]	1.2800	2.1400	0.0000	0.0000	NIST46.2
3309971	H[Phthalate]	5.4000	5.4080	0.0000	0.0000	NIST46.2
3309972	H2[Phthalate]	8.3500	8.3580	0.0000	0.0000	NIST46.2
6009971	Pb[Phthalate]	2.7800	4.2600	0.0000	0.0000	SCD2.62
6009972	Pb[Phthalate]2	4.0100	4.8300	0.0000	0.0000	NIST46.2
6009973	PbH[Phthalate]	6.5600	6.9800	0.0000	0.0000	NIST46.2
309971	Al[Phthalate]	4.5600	4.5600	0.0000	0.0000	NIST46.2
309972	Al[Phthalate]2	7.2000	7.2000	0.0000	0.0000	NIST46.2
9509971	Zn[Phthalate]	2.9100	2.9100	0.0000	0.0000	NIST46.2

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
9509972	Zn[Phthalate]2	4.2000	4.2000	0.0000	0.0000	NIST46.2
1609971	Cd[Phthalate]	2.5000	3.4300	0.0000	0.0000	NIST46.2
1609973	CdH[Phthalate]	5.8800	6.3000	0.0000	0.0000	NIST46.2
1609972	Cd[Phthalate]2	2.8800	3.7000	0.0000	0.0000	NIST46.2
2319971	Cu[Phthalate]	4.0400	4.0200	0.0000	0.0000	NIST46.2
2319970	CuH[Phthalate]	6.7400	7.1000	0.0000	0.0000	NIST46.2
2319972	Cu[Phthalate]2	5.3000	5.3000	0.0000	0.0000	NIST46.2
5409971	Ni[Phthalate]	2.9500	2.9500	0.0000	0.0000	NIST46.2
5409972	NiH[Phthalate]	6.1000	6.6000	0.0000	0.0000	NIST46.2
2009971	Co[Phthalate]		2.8300		0.0000	NIST46.4
2009972	CoH[Phthalate]		7.2270		0.0000	NIST46.4
4709971	Mn[Phthalate]	2.7400	2.7400	10.0416	0.0000	NIST46.2
2119971	Cr[Phthalate]	15.1400	16.3000	0.0000	0.0000	SCD2.62
2119972	Cr[Phthalate]2	19.6200	21.2000	0.0000	0.0000	SCD2.62
2119973	Cr[Phthalate]3	22.1000	23.3000	0.0000	0.0000	SCD2.62
1109971	Be[Phthalate]		4.8278		0.0000	NIST46.4
1109972	Be[Phthalate]2		6.5478		0.0000	NIST46.4
4609971	Mg[Phthalate]	2.4900	2.4900	0.0000	0.0000	SCD2.62
1509970	Ca[Phthalate]	2.4200	2.4500	0.0000	0.0000	NIST46.2
1509971	CaH[Phthalate]	6.4300	6.4300	0.0000	0.0000	NIST46.2
1009971	Ba[Phthalate]	2.3300	2.3300	0.0000	0.0000	NIST46.2
5009970	Na[Phthalate]	0.7000	0.8000	0.0000	0.0000	NIST46.2
4109971	K[Phthalate]	0.7000	0.7000	3.7656	0.0000	NIST46.2
73100	Sulfur	2.1100	2.1449	17.5728	16.3000	CODATA89
76000	Se metal (hex,blk)	7.6963	7.7084	-15.8992	-15.9000	NIST2.1.1
76001	Se metal (am)	7.1099	7.1099	-10.8784	-10.8784	MTQ3.11
74001	Sb metal	11.7058	11.6889	-83.8683	-83.8900	NIST2.1.1
79000	Sn metal (wht)		2.3266		0.0000	CODATA89
60000	Pb metal	-4.2700	-4.2462	-1.6736	-0.9200	CODATA89
87000	Tl metal	-5.6733	-5.6762	-5.3555	-5.3600	NIST2.1.1
95000	Zn metal	-25.7570	-25.7886	153.8875	153.3900	CODATA89
16000	Cd metal (alpha)	-13.4900	-13.5147	75.3120	75.3300	NIST2.1.1
16001	Cd metal (gamma)	-13.5900	-13.6180	75.8978	75.9200	NIST2.1.1
36000	Hg metal (l)	13.4552	13.4517	-83.4080	-83.4350	CODATA89
23000	Cu metal	8.7600	8.7560	-71.6719	-71.6700	CODATA89
2000	Ag metal	13.5100	13.5065	-105.5791	-105.7900	CODATA89
21000	Cr metal	-32.2440	-30.4831	143.5112	172.0000	NIST13.1
90000	V metal	-42.3500	-44.0253	263.1736	259.0000	NIST13.1
1074000	STIBNITE	60.1560	50.4600	-289.9094	-293.7800	NIST46.4
1006000	ORPIMENT	60.9710	61.0663	-346.8118	-350.6799	NIST2.1.1
1006001	REALGAR	19.7470	19.7470	-127.8003	-127.8003	MTQ3.11
1079001	SnS		19.1140		0.0000	NIST46.4
1079101	SnS2		57.4538		0.0000	Bard85
1060001	GALENA	15.1320	13.9700	-81.1696	-80.0000	DKa1990
1087000	Tl2S	7.1832	7.1900	-90.2070	-91.5200	NIST46.4
1095000	ZnS (am)	9.0520	9.0520	-15.3553	-15.3553	MTQ3.11
1095001	SPHALERITE	11.6180	11.4500	-34.5180	-30.0000	DHa1993
1095002	WURTZITE	9.6820	8.9500	-21.1710	-21.1710	DKa1990
1016000	GREENOCKITE	15.9300	14.3600	-68.4502	-55.0000	DHa1992
1036000	Hg2S	11.6765	11.6765	-69.7473	-69.7473	MTQ3.11
1036100	CINNABAR	45.1885	45.6940	-252.8391	-253.7600	DKa1990
1036101	METACINNABAR	44.8220	45.0940	-249.0735	-253.7200	Dka1990
1023000	CHALCOCITE	34.6190	34.9200	-206.4804	-168.0000	NIST46.4
1023001	DJURLEITE	33.9200	33.9200	-200.3341	-200.3341	MTQ3.11
1023002	ANILITE	31.8780	31.8780	-182.1504	-182.1504	MTQ3.11
1023003	BLAUBLEI II	27.2790	27.2790	0.0000	0.0000	MTQ3.11
1023100	BLAUBLEI I	24.1620	24.1620	0.0000	0.0000	MTQ3.11
1023101	COVELLITE	23.0380	22.3000	-100.4578	-97.0000	DKa1990
1023102	CHALCOPYRITE	35.2700	35.2700	-148.4483	-148.4483	MTQ3.11
1002000	ACANTHITE	36.0500	36.2200	-223.0072	-227.0000	NIST46.4
1054001	NiS (alpha)		5.6000		0.0000	DKa1990

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
1054002	NiS (beta)		11.1000		0.0000	DKa1990
1054003	NiS (gamma)		12.8000		0.0000	DKa1990
1020001	CoS (alpha)		7.4400		0.0000	DKa1990
1020002	CoS (beta)		11.0700		0.0000	DKa1990
1028000	FeS (ppt)	3.9150	2.9500	0.0000	11.0000	Da1991
1028001	GREIGITE	45.0350	45.0350	0.0000	0.0000	MTQ3.11
1028002	MACKINAWITE	4.6480	3.6000	0.0000	0.0000	Da1991
1028003	PYRITE	18.4790	18.5082	-47.2792	-49.8440	NIST13.1
1047000	MnS (grn)	-3.8000	-0.1700	24.2254	32.0000	DKa1990
1047001	MnS (pnk)		-3.3400		0.0000	DKa1990
1048001	MoS2		70.2596		-389.0199	Bard85
1011001	BeS		-19.3800		0.0000	NIST46.4
1010001	BaS		-16.1800		0.0000	NIST46.4
1136001	Hg2(CN)2		39.3000		0.0000	NIST46.4
1123001	CuCN	19.4974	19.5000	-126.3568	19.0000	NIST46.4
1102002	AgCN	16.2180	15.7400	-110.3948	-110.3948	NIST46.4
1102004	Ag2(CN)2		11.3289		0.0000	NIST46.4
1150001	NaCN (cubic)	-2.2869	-1.6012	2.1757	-0.9690	NIST13.1
1141002	KCN (cubic)	-1.4403	-1.4188	-11.4642	-11.9300	NIST13.1
1160002	Pb2Fe(CN)6	27.5895	53.4200	0.0000	0.0000	NIST46.4
1195002	Zn2Fe(CN)6	29.9263	51.0800	0.0000	0.0000	NIST46.4
1116002	Cd2Fe(CN)6	28.2243	52.7800	0.0000	0.0000	NIST46.4
1102003	Ag4Fe(CN)6	193.9140	79.4700	-1091.6475	0.0000	NIST46.4
1102005	Ag3Fe(CN)6		72.7867		0.0000	NIST46.4
1147001	Mn3[Fe(CN)6]2		105.4000		0.0000	NIST46.4
1274000	Sb2Se3	67.7571	67.7571	-343.0461	-343.0461	PNL89
1279001	SnSe		30.4940		0.0000	NIST46.4
1279101	SnSe2		65.1189		0.0000	Bard85
1260000	CLAUSTHALITE	21.2162	27.1000	-117.1520	-119.7200	NIST46.4
1287000	Tl2Se	6.6848	18.1000	-85.1862	-85.6200	NIST46.4
1295000	ZnSe	11.3642	14.4000	-26.9408	-25.5100	NIST46.4
1216000	CdSe	18.0739	20.2000	-75.9814	-75.9814	NIST46.4
1236101	HgSe		55.6940		0.0000	NIST46.4
1223000	Cu2Se (alpha)	36.0922	45.8000	-214.2626	-214.2626	NIST46.4
1223001	Cu3Se2	63.4911	63.4911	-340.3265	-340.3265	MTQ3.11
1223100	CuSe	26.5121	33.1000	-121.1268	-121.1268	NIST46.4
1223101	CuSe2	33.3655	33.3655	-140.5824	-140.5824	MTQ3.11
1202000	Ag2Se	43.6448	48.7000	-271.7508	-265.4800	NIST46.4
1254000	NiSe	17.7382	17.7000	0.0000	0.0000	NIST46.4
1220000	CoSe	16.2723	16.2000	0.0000	0.0000	NIST46.4
1228000	FeSe	7.1466	11.0000	-2.0920	-2.0920	NIST46.4
1228001	FERROSELITE	18.5959	18.5959	-47.2792	-47.2792	MTQ3.11
1247000	MnSe	-5.3508	-3.5000	56.3166	98.1500	NIST46.4
1474003	AlSb	-65.6241	-65.6241	0.0000	0.0000	PNL89
1474002	ZnSb	-11.0138	-11.0138	54.8773	54.8773	PNL89
1474004	CdSb	0.3943	0.3501	-22.3635	-22.3600	NIST2.1.1
1474012	Cu2Sb:3H2O	34.8827	34.8827	-233.2371	-233.2371	PNL89
1474014	Cu3Sb	42.5937	42.5937	-308.1307	-308.1307	PNL89
1474006	Ag4Sb	56.1818	56.1818	0.0000	0.0000	PNL89
1474001	BREITHAUPTITE	18.5225	18.5225	-96.0019	-96.0019	PNL89
1474013	MnSb	2.9099	2.9099	-21.1083	-21.1083	PNL89
1474009	Mn2Sb	-61.0796	-61.0796	0.0000	0.0000	PNL89
1474011	USb2	-29.5246	-29.5771	103.2611	103.5601	NIST2.1.1
1474015	U3Sb4	-152.3288	-152.3834	986.2525	986.0400	NIST2.1.1
1474005	Mg2Sb3	-74.6838	-74.6838	0.0000	0.0000	PNL89
1474010	Ca3Sb2	-142.9738	-142.9738	732.7440	732.7440	PNL89
1474008	NaSb	-23.1770	-23.1658	93.6588	93.4500	NIST2.1.1
1474007	Na3Sb	-94.4084	-94.4517	431.9771	432.1300	NIST2.1.1
2076100	SeO2	-0.1246	-0.1246	-1.4016	-1.4016	MTQ3.11
2076200	SeO3	-21.0440	-21.0440	146.3772	146.3772	MTQ3.11
2074100	Sb2O5	12.4827	9.6674	0.0000	0.0000	NIST2.1.1

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
2074102	SbO2	27.8241	27.8241	0.0000	0.0000	PNL89
2074001	Sb2O4	-3.4597	-3.4021	68.0737	68.0400	NIST2.1.1
2074002	Sb4O6 (cubic)	19.6586	18.2612	-61.0864	-61.1801	NIST46.4
2074003	Sb4O6 (orth)	17.0346	17.9012	-37.6142	-37.6801	NIST46.4
2074004	Sb(OH)3	7.1099	7.1099	-30.1248	-30.1248	PNL89
2074006	SENARMONTITE	12.3654	12.3654	-30.6478	-30.6478	PNL89
2074007	VALENTINITE	8.4806	8.4806	-19.0163	-19.0163	PNL89
2077000	CHALCEDONY	3.5230	3.5500	-19.3092	-19.7000	Nord90
2077001	CRISTOBALITE	3.5870	3.3500	-23.0120	-20.0060	NIST46.4
2077002	QUARTZ	4.0060	4.0000	-26.0245	-22.3600	NIST46.4
2077003	SiO2 (am,gel)	3.0180	2.7100	-18.5770	-14.0000	Nord90
2077004	SiO2 (am,ppt)	2.7100	2.7400	-16.3594	-15.1500	NIST46.4
2079001	SnO		4.9141		0.0000	CODATA89
2079101	SnO2		28.9749		0.0000	CODATA89
2079002	Sn(OH)2		5.4309		0.0000	Bard85
2079102	Sn(OH)4		22.2808		0.0000	Bard85
2079103	H2Sn(OH)6		23.5281		0.0000	Bard85
2060000	MASSICOT	-12.9100	-12.8940	70.2075	66.8480	NIST46.4
2060001	LITHARGE	-12.7200	-12.6940	68.5339	65.5010	NIST46.4
2060002	PbO:0.3H2O	-12.9800	-12.9800	0.0000	0.0000	MTQ3.11
2060003	PLATTNERITE	-49.3000	-49.6001	295.9343	296.2700	NIST13.1
2060004	Pb(OH)2	-8.1500	-8.1500	58.5342	58.5342	MTQ3.11
2060005	Pb2O(OH)2	-26.2000	-26.1880	0.0000	0.0000	NIST46.4
2003000	Al(OH)3 (am)	-10.3800	-10.8000	113.1563	111.0000	Nord90
2003001	BOEHMITE	-8.5780	-8.5780	117.6959	117.6959	MTQ3.11
2003002	DIASPORE	-6.8730	-6.8730	103.0519	103.0519	MTQ3.11
2003003	GIBBSITE	-8.7700	-8.2910	95.3952	95.3952	NIST46.4
2087000	Tl2O	-27.0984	-27.0915	96.4621	96.4100	NIST2.1.1
2087001	TlOH	-12.9225	-12.9186	41.5680	41.5700	NIST2.1.1
2087100	AVICENNITE	16.3236	13.0000	0.0000	0.0000	NIST46.4
2087101	Tl(OH)3	6.4503	5.4410	0.0000	0.0000	SCD3.02
2095000	Zn(OH)2 (am)	-12.4500	-12.4740	0.0000	80.6200	NIST46.4
2095001	Zn(OH)2	-12.2000	-12.2000	0.0000	0.0000	MTQ3.11
2095002	Zn(OH)2 (beta)	-11.7500	-11.7540	0.0000	83.1400	NIST46.4
2095003	Zn(OH)2 (gamma)	-11.7100	-11.7340	0.0000	0.0000	NIST46.4
2095004	Zn(OH)2 (epsilon)	-11.5000	-11.5340	0.0000	81.8000	NIST46.4
2095005	ZnO (active)	-11.3100	-11.1884	0.0000	88.7600	CODATA89
2095006	ZINCITE	-11.1400	-11.3340	91.4622	89.6200	NIST46.4
2016000	Cd(OH)2 (am)	-13.7300	-13.7300	86.9017	86.9017	MTQ3.11
2016001	Cd(OH)2	-13.6500	-13.6440	0.0000	94.6200	NIST46.4
2016002	MONTEPONITE	-15.1200	-15.1034	103.5958	103.4000	CODATA89
2036000	Hg2(OH)2	-5.2603	-5.2603	0.0000	0.0000	MTQ3.11
2036100	MONTROYDITE	3.6503	3.6400	-21.4012	38.9000	NIST46.4
2036101	Hg(OH)2	3.4963	3.4963	0.0000	0.0000	MTQ3.11
2023000	CUPRITE	1.5500	1.4060	-26.1291	124.0200	NIST46.4
2023100	Cu(OH)2	-8.6400	-8.6740	63.8060	56.4200	NIST46.4
2023101	TENORITE	-7.6200	-7.6440	63.7642	64.8670	NIST46.4
2002000	Ag2O	-12.5800	-12.5740	43.6391	45.6200	NIST46.4
2054000	Ni(OH)2	-10.8000	-12.7940	-127.4028	95.9600	NIST46.4
2054001	BUNSENITE	-12.4500	-12.4456	100.0813	100.1300	NIST2.1.1
2020001	CoO	-13.5500	-13.5864	106.1062	106.2950	NIST13.1
2020002	Co(OH)2	-13.7660	-13.0940	0.0000	0.0000	NIST46.4
2020101	Co(OH)3		2.3090		92.4300	NIST46.4
2028000	WUSTITE	-11.6870	-11.6879	103.9557	103.9377	NIST13.1
2028001	Fe(OH)2		-13.5640		0.0000	NIST46.4
2028100	FERRIHYDRITE	-4.8910	-3.1910	0.0000	73.3740	NIST46.4
2028101	Fe3(OH)8	-20.2220	-20.2220	0.0000	0.0000	MTQ3.11
2028102	GOETHITE	-0.5000	-0.4910	60.5843	60.5843	NIST46.4
2047000	PYROLUSITE	-15.8610	-41.3800	122.0891	272.0000	Nord90
2047001	BIRNESSITE	-18.0910	-18.0910	0.0000	0.0000	MTQ3.11
2047002	NSUTITE	-17.5040	-17.5040	0.0000	0.0000	MTQ3.11

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
2047003	PYROCHROITE	-15.0880	-15.1940	94.5166	97.0099	NIST46.4
2047100	MANGANITE	0.2380	-25.3400	0.0000	0.0000	Nord90
2021100	Cr(OH)2	-10.8189	-10.8189	35.6058	35.6058	MTQ3.11
2021102	Cr(OH)3 (am)	0.7500	0.7500	0.0000	0.0000	MTQ3.11
2021101	Cr(OH)3	-1.7005	-1.3355	29.7692	29.7692	NIST46.4
2021200	CrO3	3.2105	3.2105	5.2091	5.2091	MTQ3.11
2048001	MoO3		8.0000		0.0000	NIST46.4
2090000	VO	-13.0800	-14.7563	117.2357	113.0410	NIST13.1
2090100	V(OH)3	-7.6500	-7.5910	0.0000	0.0000	NIST46.4
2090200	VO(OH)2	-5.8500	-5.1506	0.0000	0.0000	NIST46.4
2089100	URANINITE	4.7000	4.6693	77.9479	77.8600	CODATA89
2089101	UO2 (am)	-0.9340	-0.9340	109.7463	109.7463	MTQ3.11
2089300	UO3	-7.7190	-7.7000	80.8140	81.0299	CODATA89
2089301	GUMMITE	-10.4030	-7.6718	96.2948	81.0299	NIST2.1.1
2089302	UO2(OH)2 (beta)	-5.5440	-5.6116	57.4463	56.7599	NIST2.1.1
2089303	SCHOEPITE	-5.4040	-5.9940	50.3963	49.7900	NIST46.4
2011001	Be(OH)2 (am)		-7.1940		0.0000	NIST46.4
2011002	Be(OH)2 (alpha)		-6.8940		0.0000	NIST46.4
2011003	Be(OH)2 (beta)		-6.4940		0.0000	NIST46.4
2046000	BRUCITE	-16.7920	-16.8440	108.1146	113.9959	NIST46.4
2046001	PERICLASE	-21.5100	-21.5841	151.1888	151.2300	CODATA89
2046002	Mg(OH)2 (active)		-18.7940		0.0000	NIST46.4
2015000	LIME	-32.7970	-32.6993	193.5728	193.9100	CODATA89
2015001	PORTLANDITE	-22.6750	-22.8040	128.4070	128.6200	NIST46.4
2010001	Ba(OH)2:8H2O		-24.3940		54.3200	NIST46.4
2074005	Cu(SbO3)2	-45.2105	-45.2105	0.0000	0.0000	PNL89
3006000	ARSENOLITE	2.8010	2.7600	-59.9567	-59.9567	NIST46.4
3006001	CLAUDETITE	3.0650	3.0650	-55.6054	-55.6054	MTQ3.11
3006100	As2O5	-6.6990	-6.7061	22.6145	22.6400	NIST2.1.1
3060000	Pb2O3	-61.0400	-61.0400	0.0000	0.0000	MTQ3.11
3060001	MINIUM	-73.6900	-73.5219	429.9478	421.8740	NIST13.1
3003000	Al2O3	-22.9800	-19.6524	0.0000	258.5901	CODATA89
3020001	Co3O4		10.4956		107.4999	NIST13.1
3020002	CoFe2O4		3.5281		158.8199	NIST2.1.1
3028000	MAGNETITE	-3.7370	-3.4028	211.1246	208.5259	NIST13.1
3028001	HERCYNITE	-27.1620	-22.8930	327.8582	313.9199	NIST2.1.1
3028100	HEMATITE	4.0080	1.4180	129.0555	128.9870	NIST46.4
3028101	MAGHEMITE	-6.3860	-6.3860	0.0000	0.0000	MTQ3.11
3028102	LEPIDOCROCITE	-1.3710	-1.3710	0.0000	0.0000	MTQ3.11
3047000	HAUSMANNITE	-61.5400	-61.0300	335.3058	421.0000	Nord90
3047100	BIXBYITE	0.6110	0.6445	63.7851	124.4900	NIST2.1.1
3021102	Cr2O3	3.3937	2.3576	50.7310	50.7310	SCD3.02
3090100	V2O3	-4.9000	-4.9000	82.5085	82.5085	MTQ3.11
3090101	V3O5	-1.8700	-1.8361	98.4495	98.4600	NIST2.1.1
3090200	V2O4	-4.2700	-4.2700	58.8689	58.8689	MTQ3.11
3090201	V4O7	-7.1400	-7.1865	163.8036	163.8901	NIST2.1.1
3090202	V6O13	60.8600	60.8600	-271.4998	-271.4998	MTQ3.11
3090300	V2O5	0.7200	1.3600	17.4054	-34.0000	NIST46.4
3089100	U4O9	3.3840	3.0198	423.5672	426.8701	NIST2.1.1
3089101	U3O8	-21.1070	-21.0834	485.4277	485.4399	CODATA89
3046000	SPINEL	-36.3330	-36.8476	372.7484	388.0122	NIST13.1
3046001	MAGNESIOFERRITE	-16.7650	-16.8597	278.8176	278.9199	NIST2.1.1
3050000	NATRON	1.3110	1.3110	-65.8771	-65.8771	MTQ3.11
3023000	CUPROUS FERRITE	8.9200	8.9171	15.8992	15.8900	NIST2.1.1
3023100	CUPRIC FERRITE	-5.8800	-5.9882	161.8790	210.2099	NIST2.1.1
3021100	FeCr2O4	0.9016	-7.2003	104.0142	140.4000	NIST2.1.1
3021101	MgCr2O4	-12.0796	-16.2007	166.7742	179.4000	NIST2.1.1
4274000	SbF3	10.2251	10.2251	6.7279	6.7279	PNL89
4260000	PbF2	7.4400	7.4400	2.9288	-20.0000	NIST46.4
4295000	ZnF2	1.5200	0.5343	54.7267	59.6900	NIST2.1.1
4216000	CdF2	2.9800	1.2124	40.6685	46.2200	NIST2.1.1

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
4236000	Hg2F2	3.0811	10.3623	18.5435	18.4860	NIST13.1
4223000	CuF	-7.0800	4.9056	51.7561	-16.6480	NIST13.1
4223100	CuF2	0.6200	-1.1150	55.7309	66.9010	NIST13.1
4223101	CuF2:2H2O	4.5500	4.5500	15.2716	15.2716	MTQ3.11
4202000	AgF:4H2O	-0.5500	-1.0491	-17.8657	-15.4202	NIST2.1.1
4220000	CoF2	5.1500	1.5969	36.8610	57.3680	NIST13.1
4220101	CoF3		1.4581		123.6921	NIST13.1
4221100	CrF3	13.2597	11.3367	18.2548	23.3901	NIST2.1.1
4290200	VF4	-14.9300	-14.9300	199.1166	199.1166	MTQ3.11
4289100	UF4	18.6060	29.5371	79.0776	79.0776	SCD3.02
4289101	UF4:2.5H2O	27.5700	32.7179	2.4602	-24.3250	NIST2.1.1
4246001	MgF2		8.1300		8.0000	NIST46.4
4215000	FLUORITE	10.9600	10.5000	-19.7066	-8.0000	NIST46.4
4280000	SrF2	8.5400	8.5800	-5.2300	-4.0000	NIST46.4
4210000	BaF2	5.7600	5.8200	-4.1840	-4.0000	NIST46.4
4250000	CRYOLITE	31.4900	33.8400	-45.6223	-38.0000	Nord90
4174000	SbCl3	-0.5915	-0.5719	35.2042	35.1800	NIST2.1.1
4179001	SnCl2		9.2752		0.0000	Bard85
4160000	COTUNNITE	4.7700	4.7800	-23.4304	-26.1660	NIST46.4
4160001	MATLOCKITE	9.4300	8.9733	-33.2628	-33.1900	NIST2.1.1
4160002	PHOSGENITE	19.8100	19.8100	0.0000	0.0000	MTQ3.11
4160003	LAURIONITE	-0.6230	-0.6230	0.0000	0.0000	MTQ3.11
4160004	Pb2(OH)3Cl	-8.7930	-8.7930	0.0000	0.0000	MTQ3.11
4187000	TlCl	3.7243	3.7400	-42.4132	-41.0000	NIST46.4
4195000	ZnCl2	-7.0300	-7.0500	73.1363	72.5000	NIST2.1.1
4195001	Zn2(OH)3Cl	-15.2000	-15.1910	0.0000	0.0000	NIST46.4
4195002	Zn5(OH)8Cl2	-38.5000	-38.5000	0.0000	0.0000	MTQ3.11
4116000	CdCl2	0.6800	0.6588	18.7025	18.5800	NIST2.1.1
4116001	CdCl2:1H2O	1.7100	1.6932	7.6149	7.4700	NIST2.1.1
4116002	CdCl2:2.5H2O	1.9400	1.9130	-7.1546	-7.2849	NIST2.1.1
4116003	CdOHCl	-3.5200	-3.5373	30.9909	30.9300	NIST2.1.1
4136000	CALOMEL	17.8427	17.9100	-98.0897	-92.0000	NIST46.4
4136100	HgCl2	21.7858	21.2621	-114.0726	-107.8200	NIST13.1
4123000	NANTOKITE	6.7600	6.7300	-41.7563	-42.6620	NIST46.4
4123100	MELANOTHALLITE	-3.7300	-6.2572	51.5469	63.4070	NIST13.1
4123101	ATACAMITE	-7.3400	-7.3910	78.1990	93.4300	NIST46.4
4102000	CERARGYRITE	9.7500	9.7500	-65.4880	-65.2000	NIST46.4
4120000	CoCl2	-8.2500	-8.2672	79.8307	79.8150	NIST13.1
4120003	CoCl2:6H2O	-2.5600	-2.5365	-8.0751	-8.0598	NIST2.1.1
4120101	[Co(NH3)6]Cl3		-20.0317		33.1000	Bard85
4120102	[Co(NH3)5OH2]Cl3		-11.7351		25.3700	Bard85
4120103	[Co(NH3)5Cl]Cl2		-4.5102		10.7400	Bard85
4128100	Fe(OH)2.7Cl.3	3.0400	3.0400	0.0000	0.0000	MTQ3.11
4147000	MnCl2:4H2O	-2.7100	-2.7151	-72.7179	10.8300	NIST2.1.1
4121000	CrCl2	-15.8676	-14.0917	82.2825	110.7600	NIST2.1.1
4121100	CrCl3	-13.5067	-15.1145	115.0977	121.0800	NIST2.1.1
4190000	VCl2	-17.9700	-18.8744	149.7872	141.1600	NIST2.1.1
4190100	VCl3	-21.7300	-23.4326	183.9286	179.5400	NIST2.1.1
4190101	VOCl	-9.4100	-11.1524	109.4953	104.9100	NIST2.1.1
4190200	VOCl2	-12.7900	-12.7603	117.9888	117.7600	NIST2.1.1
4190300	VO2Cl	-2.8100	-2.8413	40.3756	40.2800	NIST2.1.1
4150000	HALITE	-1.5820	-1.6025	-3.8409	-3.7000	NIST13.1
4074000	SbBr3	-1.0562	-0.9689	21.2212	20.9400	NIST2.1.1
4079001	SnBr2		9.5443		0.0000	Bard85
4079101	SnBr4		28.8468		0.0000	Bard85
4060000	PbBr2	5.1800	5.3000	-33.8904	-35.4990	NIST46.4
4060001	PbBrF	8.4900	8.4900	0.0000	0.0000	MTQ3.11
4087000	TlBr	5.4190	5.4400	-57.0739	-54.0000	NIST46.4
4095000	ZnBr2:2H2O	-5.2100	-5.2005	31.4218	30.6700	NIST2.1.1
4016000	CdBr2:4H2O	2.4200	2.4250	-30.2503	-30.5001	NIST2.1.1
4036000	Hg2Br2	22.2091	22.2500	-130.7584	-133.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
4036100	HgBr2	25.3730	25.2734	-144.1472	-138.4920	NIST13.1
4023000	CuBr	8.2100	8.3000	-54.7267	-54.8600	NIST46.4
4023101	Cu2(OH)3Br		-7.9085		93.4300	NIST46.4
4002000	BROMYRITE	12.2700	12.3000	-84.3913	-84.5000	NIST46.4
4020101	[Co(NH3)6]Br3		-18.3142		21.1899	Bard85
4020102	[Co(NH3)5Cl]Br2		-5.0295		6.4000	Bard85
4021100	CrBr3	-19.9086	-19.9086	141.3230	141.3230	MTQ3.11
4306000	AsI3	-4.1550	-4.2307	-7.8450	-3.1500	NIST2.1.1
4374000	SbI3	0.5380	0.5380	-13.5896	-13.5896	PNL89
4360000	PbI2	8.0700	8.1000	-63.4294	-62.0000	NIST46.4
4387000	TlI	7.1964	7.2300	-72.3037	-75.0000	NIST46.4
4395000	ZnI2	-7.2300	-7.3055	56.2330	58.9200	NIST2.1.1
4316000	CdI2	3.6100	3.5389	-17.0707	-13.8200	NIST2.1.1
4336000	Hg2I2	28.2782	28.3400	0.0000	-163.0000	NIST46.4
4336100	COCCINITE	34.6599	34.9525	-208.0787	-210.7200	NIST46.4
4336102	HgI2:2NH3	16.1066	16.2293	-136.5323	-132.1800	NIST2.1.1
4336103	HgI2:6NH3	-33.8566	-33.7335	86.0565	90.3599	NIST2.1.1
4323000	CuI	11.8900	12.0000	-84.2658	-82.6900	NIST46.4
4302000	IODYRITE	16.0700	16.0800	-112.2149	-110.0000	NIST46.4
4320101	[Co(NH3)6]I3		-16.5831		9.6999	Bard85
4320102	[Co(NH3)5Cl]I2		-5.5981		-0.6600	Bard85
4321100	CrI3	-20.4767	-20.4767	134.4194	134.4194	MTQ3.11
5060000	CERRUSITE	13.1300	13.1300	-20.3342	-24.7900	NIST46.4
5060001	Pb2OCO3	0.5000	0.5578	47.9486	40.8199	NIST2.1.1
5060002	Pb3O2CO3	-11.0200	-11.0200	110.5831	110.5831	MTQ3.11
5060003	HYDROCERRUSITE	17.4600	18.7705	0.0000	0.0000	NIST46.4
5060004	Pb10(OH)6O(CO3)6		8.7600		0.0000	NIST46.4
5087000	Tl2CO3	3.8482	3.8367	-33.5557	-35.4900	NIST2.1.1
5095000	SMITHSONITE	10.0000	10.0000	18.2422	15.8400	NIST46.4
5095001	ZnCO3:1H2O	10.2600	10.2600	0.0000	0.0000	MTQ3.11
5016000	OTAVITE	13.7400	12.0000	2.4267	0.5500	NIST46.4
5036000	Hg2CO3	13.9586	16.0500	0.0000	-45.1400	NIST46.4
5036101	Hg3O2CO3		29.6820		0.0000	NIST46.4
5023100	CuCO3	9.6300	11.5000	0.0000	0.0000	NIST46.4
5023101	MALACHITE	5.1800	5.3060	65.3122	-76.3800	NIST46.4
5023102	AZURITE	16.9200	16.9060	99.4537	95.2200	NIST46.4
5002000	Ag2CO3	11.0700	11.0900	-39.8735	-42.1500	NIST46.4
5054000	NiCO3	6.8400	6.8700	41.5890	41.5890	NIST46.4
5020000	CoCO3	9.9800	9.9800	12.7612	12.7612	NIST46.4
5028000	SIDERITE	10.5500	10.2400	22.2924	16.0000	NIST46.4
5047000	RHODOCHROSITE	10.4100	10.5800	8.6985	1.8800	NIST46.4
5089300	RUTHERFORDINE	14.4390	14.5000	6.0250	3.0300	NIST46.4
5046000	ARTINITE	-9.6000	-9.6000	120.2565	120.2565	MTQ3.11
5046001	HYDROMAGNESITE	8.7660	8.7660	218.4466	218.4466	MTQ3.11
5046002	MAGNESITE	8.0290	7.4600	25.8111	-20.0000	NIST46.4
5046003	NESQUEHONITE	5.6210	4.6700	24.2212	24.2212	NIST46.4
5015000	ARAGONITE	8.3600	8.3000	10.9412	12.0000	NIST46.4
5015001	CALCITE	8.4750	8.4800	10.8156	8.0000	NIST46.4
5015002	DOLOMITE (ordered)	17.0000	17.0900	34.6854	39.5000	Nord90
5015004	DOLOMITE (disordered		16.5400		46.4000	Nord90
5015003	HUNTITE	29.9680	29.9680	107.7798	107.7798	MTQ3.11
5080000	STRONTIANITE	9.2500	9.2700	2.8870	0.0000	NIST46.4
5010000	WITHERITE	8.5850	8.5700	-1.5062	-4.0000	NIST46.4
5050001	THERMONATRITE	-0.1250	-0.6370	11.7236	10.4799	NIST2.1.1
5187000	TlNO3	1.5319	1.6127	-41.9237	-42.4400	NIST2.1.1
5195000	Zn(NO3)2:6H2O	-3.4400	-3.3153	-23.0538	-24.5698	NIST2.1.1
5123100	Cu2(OH)3NO3	-9.2400	-9.2510	72.5924	72.5924	NIST46.4
5120101	[Co(NH3)6](NO3)3		-17.9343		-1.5900	Bard85
5120102	[Co(NH3)5Cl](NO3)2		-6.2887		-6.4199	Bard85
5189300	UO2(NO3)2	-12.3690	-12.1476	84.2658	83.3999	NIST2.1.1
5189301	UO2(NO3)2:2H2O	-4.8510	-4.8510	25.3550	25.3550	MTQ3.11

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
5189302	UO2(NO3)2:3H2O	-3.6420	-3.3900	10.0625	9.1599	NIST2.1.1
5189303	UO2(NO3)2:6H2O	-2.3000	-2.0464	-19.9577	-20.8201	NIST2.1.1
5260000	Pb(BO2)2	-7.6100	-6.5192	24.2672	15.6119	NIST13.1
5295000	Zn(BO2)2	-8.2900	-8.2900	0.0000	0.0000	MTQ3.11
5216000	Cd(BO2)2	-9.8400	-9.8400	0.0000	0.0000	MTQ3.11
5220001	Co(BO2)2		-27.0703		0.0000	NIST2.1.1
6079001	SnSO4		56.9747		0.0000	Bard85
6079101	Sn(SO4)2		15.2123		0.0000	Bard85
6060000	LARNAKITE	0.2800	0.4344	26.9450	21.8300	NIST2.1.1
6060001	Pb3O2SO4	-10.4000	-10.6864	86.8180	79.1400	NIST2.1.1
6060002	Pb4O3SO4	-22.1000	-21.8772	146.7329	136.4501	NIST2.1.1
6060003	ANGLESITE	7.7900	7.7900	-8.9956	-12.0000	NIST46.4
6060004	Pb4(OH)6SO4	-21.1000	-21.1000	0.0000	0.0000	MTQ3.11
6003000	AlOHSO4	3.2300	3.2300	0.0000	0.0000	MTQ3.11
6003001	Al4(OH)10SO4	-22.7000	-22.7000	0.0000	0.0000	MTQ3.11
6087000	Tl2SO4	3.6942	3.7868	-33.2210	-33.1799	NIST2.1.1
6095000	Zn2(OH)2SO4	-7.5000	-7.5000	0.0000	0.0000	MTQ3.11
6095001	Zn4(OH)6SO4	-28.4000	-28.4000	0.0000	0.0000	MTQ3.11
6095002	Zn3O(SO4)2	-19.0200	-18.9135	259.4080	258.0801	NIST2.1.1
6095003	ZINCOSITE	-3.0100	-3.9297	80.3328	82.5860	NIST13.1
6095004	ZnSO4:1H2O	0.5700	0.6380	44.5178	44.0699	NIST2.1.1
6095005	BIANCHITE	1.7650	1.7650	0.6694	0.6694	MTQ3.11
6095006	GOSLARITE	1.9600	2.0112	-13.8072	-14.2100	NIST2.1.1
6016000	Cd3(OH)4SO4	-22.5600	-22.5600	0.0000	0.0000	MTQ3.11
6016001	Cd3OH2(SO4)2	-6.7100	-6.7100	0.0000	0.0000	MTQ3.11
6016002	Cd4(OH)6SO4	-28.4000	-28.4000	0.0000	0.0000	MTQ3.11
6016003	CdSO4	0.1000	0.1722	61.6722	51.9800	NIST2.1.1
6016004	CdSO4:1H2O	1.6570	1.7261	31.4637	31.5399	NIST2.1.1
6016005	CdSO4:2.67H2O	1.8730	1.8730	17.9912	17.9912	MTQ3.11
6036000	Hg2SO4	6.1593	6.1300	-0.9623	-5.4000	NIST46.4
6036100	HgSO4	9.4189	9.4189	-14.6858	-14.6858	MTQ3.11
6023000	Cu2SO4	1.9500	1.9500	19.0790	19.0790	MTQ3.11
6023100	ANTLERITE	-8.2900	-8.7880	0.0000	0.0000	SCD3.02
6023101	BROCHANTITE	-15.3400	-15.2220	0.0000	202.8600	NIST46.4
6023102	LANGITE	-16.7900	-17.4886	165.7282	165.5500	NIST2.1.1
6023103	CuOCuSO4	-11.5300	-10.3032	148.8458	137.7770	NIST13.1
6023104	CuSO4	-3.0100	-2.9395	75.8978	73.0400	CODATA89
6023105	CHALCANTHITE	2.6400	2.6400	-6.0250	-6.0250	MTQ3.11
6002000	Ag2SO4	4.9200	4.8200	-17.7820	-17.0000	NIST46.4
6054000	Ni4(OH)6SO4	-32.0000	-32.0000	0.0000	0.0000	MTQ3.11
6054001	RETGERSITE	2.0400	2.0400	-4.6024	-4.6024	MTQ3.11
6054002	MORENOSITE	2.3600	2.1449	-12.3010	-12.1802	NIST2.1.1
6020000	CoSO4	-2.9100	-2.8024	79.2031	79.2770	NIST13.1
6020002	CoSO4:6H2O	2.3800	2.4726	-1.1715	-1.0801	NIST2.1.1
6028000	MELANTERITE	2.4700	2.2090	-11.9662	-20.5000	Nord90
6028100	Fe2(SO4)3	-3.5800	3.7343	247.3581	242.0281	NIST13.1
6028101	H-JAROSITE	12.1000	12.1000	230.7476	230.7476	MTQ3.11
6050000	Na-JAROSITE	11.2000	11.2000	151.3771	151.3771	MTQ3.11
6041002	K-JAROSITE	14.8000	14.8000	130.8755	130.8755	MTQ3.11
6047000	MnSO4	-2.6690	-2.5831	64.7683	64.8401	NIST2.1.1
6047100	Mn2(SO4)3	5.7110	5.7110	163.4270	163.4270	MTQ3.11
6090200	VOSO4	-3.5700	-3.6097	86.6925	86.7401	NIST2.1.1
6046000	EPSOMITE	2.1400	2.1265	-11.7989	-11.5601	NIST2.1.1
6015000	ANHYDRITE	4.6370	4.3600	15.7695	7.2000	Nord90
6015001	GYPSUM	4.8480	4.6100	-1.0920	-1.0000	NIST46.4
6080000	CELESTITE	6.4650	6.6200	1.9665	-2.0000	NIST46.4
6010000	BARITE	9.9760	9.9800	-26.2755	-23.0000	NIST46.4
6050001	MIRABILITE	1.1140	1.1140	-79.4416	-79.4416	MTQ3.11
6050002	THENARDITE	0.1790	-0.3217	2.3932	9.1210	NIST13.1
6041000	K-ALUM	5.1700	5.1700	-30.2085	-30.2085	MTQ3.11
6041001	ALUNITE	1.3460	1.4000	-16.3929	210.0000	Nord90

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
3021209	(NH4)2CrO4	-0.4046	-0.4046	-9.1630	-9.1630	MTQ3.11
3021212	PbCrO4	13.6848	12.6000	-42.8023	-44.1800	NIST46.4
3087000	Tl2CrO4	12.0136	12.0100	-105.8970	-74.2700	NIST46.4
3036000	Hg2CrO4	8.7031	8.7000	0.0000	0.0000	NIST46.4
3021204	CuCrO4	5.4754	5.4400	0.0000	0.0000	NIST46.4
3021200	Ag2CrO4	11.5548	11.5900	-58.7434	-62.0000	NIST46.4
3021208	MgCrO4	-5.3801	-5.3801	88.9518	88.9518	MTQ3.11
3015000	CaCrO4	2.2657	2.2657	26.9450	26.9450	MTQ3.11
3021214	SrCrO4	4.8443	4.6500	10.1253	10.1253	SCD3.02
3021201	BaCrO4	9.6681	9.6700	-26.7358	-33.0000	NIST46.4
3021207	Li2CrO4	-4.8568	-4.8568	45.2792	45.2792	MTQ3.11
3021210	Na2CrO4	-3.2618	-2.9302	19.2882	19.6301	NIST2.1.1
3021211	Na2Cr2O7	9.8953	9.8953	-22.1961	-22.1961	MTQ3.11
3021205	K2CrO4	-0.0073	0.5134	-17.7820	-18.2699	NIST2.1.1
3021206	K2Cr2O7	15.6712	17.2424	-75.8350	-80.7499	NIST2.1.1
6136000	Hg2SeO3	4.6570	4.6570	0.0000	0.0000	MTQ3.11
6136100	HgSeO3	12.6953	12.4300	0.0000	0.0000	NIST46.4
6102000	Ag2SeO3	7.0700	7.1500	-39.6225	-39.6800	NIST46.4
6123100	CuSeO3:2H2O	-0.4838	-0.5116	36.8610	36.8610	NIST46.4
6154000	NiSeO3:2H2O	-2.8147	-2.8147	31.0034	31.0034	MTQ3.11
6120000	CoSeO3	-0.1906	-1.3200	0.0000	0.0000	NIST46.4
6128100	Fe2(SeO3)3:2H2O	20.6262	20.6262	0.0000	0.0000	MTQ3.11
6128101	Fe2(OH)4SeO3	-1.5539	-1.5539	0.0000	0.0000	MTQ3.11
6147000	MnSeO3	-1.2100	-1.1300	0.0000	0.0000	NIST46.4
6147001	MnSeO3:2H2O	-0.9822	-0.9822	-8.4935	-8.4935	MTQ3.11
6146000	MgSeO3:6H2O	-4.0314	-3.0554	-5.2300	-5.2300	NIST46.4
6115000	CaSeO3:2H2O	-2.8139	-2.8139	19.4556	19.4556	MTQ3.11
6180000	SrSeO3	-0.1034	-2.3000	0.0000	0.0000	NIST46.4
6110000	BaSeO3	-4.1634	-1.8300	26.2755	-11.9800	NIST46.4
6150001	Na2SeO3:5H2O		-10.3000		0.0000	NIST46.4
6160000	PbSeO4	6.8387	6.8400	-15.8992	-15.0000	NIST46.4
6187000	Tl2SeO4	4.0168	4.1000	-40.8358	-43.0000	NIST46.4
6195001	ZnSeO4:6H2O		1.5200		0.0000	NIST46.4
6116001	CdSeO4:2H2O		1.8500		0.0000	NIST46.4
6102001	Ag2SeO4	8.9014	8.9100	-43.7228	43.5000	NIST46.4
6123101	CuSeO4:5H2O		2.4400		0.0000	NIST46.4
6154001	NiSeO4:6H2O		1.5200		0.0000	NIST46.4
6120001	CoSeO4:6H2O		1.5300		0.0000	NIST46.4
6147002	MnSeO4:5H2O		2.0500		0.0000	NIST46.4
6189301	UO2SeO4:4H2O		2.2500		0.0000	NIST46.4
6146001	MgSeO4:6H2O		1.2000		0.0000	NIST46.4
6115001	CaSeO4:2H2O	2.9473	3.0200	-3.6819	8.3000	NIST46.4
6180001	SrSeO4	6.8747	4.4000	-11.2550	-0.4000	NIST46.4
6110001	BaSeO4	5.1895	7.4600	-8.3680	-22.0000	NIST46.4
6111001	BeSeO4:4H2O		2.9400		0.0000	NIST46.4
6150002	Na2SeO4		-1.2800		0.0000	NIST46.4
6141001	K2SeO4		0.7300		0.0000	NIST46.4
6149001	(NH4)2SeO4		-0.4500		0.0000	NIST46.4
6233001	H2MoO4		12.8765		-49.0000	Bard85
6260001	PbMoO4		15.6200		-53.9300	NIST46.4
6203001	Al2(MoO4)3		-2.3675		260.8000	Bard85
6287001	Tl2MoO4		7.9887		0.0000	Bard85
6295001	ZnMoO4		10.1254		10.6901	Bard85
6216001	CdMoO4		14.1497		-19.4800	Bard85
6223101	CuMoO4		13.0762		-12.2000	Bard85
6202001	Ag2MoO4		11.5500		-52.7000	NIST46.4
6254001	NiMoO4		11.1421		-1.3000	Bard85
6220001	CoMoO4		7.7609		23.3999	Bard85
6228001	FeMoO4		10.0910		11.1000	Bard85
6211001	BeMoO4		1.7817		56.4000	Bard85
6246001	MgMoO4		1.8500		0.0000	NIST46.4

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
6215001	CaMoO4		7.9500		2.0000	NIST46.4
6210001	BaMoO4		6.9603		-10.9600	Bard85
6244001	Li2MoO4		-2.4416		33.9399	Bard85
6250001	Na2MoO4		-1.4901		9.9800	Bard85
6250002	Na2MoO4:2H2O		-1.2240		0.0000	Bard85
6250003	Na2Mo2O7		16.5966		-56.2502	Bard85
6241001	K2MoO4		-3.2619		3.3800	Bard85
7060006	PbHPO4	23.9000	23.8050	0.0000	0.0000	NIST46.4
7060007	Pb3(PO4)2	44.5000	43.5300	0.0000	0.0000	NIST46.4
7060001	PYROMORPHITE	84.4300	84.4300	0.0000	0.0000	MTQ3.11
7060002	HYDROXYLPYROMORPHITE	62.7900	62.7900	0.0000	0.0000	MTQ3.11
7060003	PLUMBGUMMITE	32.7900	32.7900	0.0000	0.0000	MTQ3.11
7060004	HINSDALITE	2.5000	2.5000	0.0000	0.0000	MTQ3.11
7060005	TSUMEBITE	9.7900	9.7900	0.0000	0.0000	MTQ3.11
7095000	Zn3(PO4)2:4H2O	32.0400	35.4200	0.0000	0.0000	NIST46.4
7016000	Cd3(PO4)2	32.6000	32.6000	0.0000	0.0000	MTQ3.11
7036000	Hg2HPO4	25.9795	24.7750	0.0000	0.0000	NIST46.4
7023100	Cu3(PO4)2	36.8500	36.8500	0.0000	0.0000	MTQ3.11
7023101	Cu3(PO4)2:3H2O	35.1200	35.1200	0.0000	0.0000	MTQ3.11
7002000	Ag3PO4	17.5500	17.5900	0.0000	0.0000	NIST46.4
7054000	Ni3(PO4)2	31.3000	31.3000	0.0000	0.0000	MTQ3.11
7020000	CoHPO4	19.0600	19.0607	0.0000	0.0000	NIST2.1.1
7020001	Co3(PO4)2	34.6700	34.6877	0.0000	0.0000	NIST2.1.1
7028001	VIVIANITE	36.0000	36.0000	0.0000	0.0000	NIST46.4
7028100	STRENGITE	26.4000	26.4000	8.4935	9.3601	NIST46.4
7047000	Mn3(PO4)2	23.8270	23.8270	-8.8701	-8.8701	MTQ3.11
7047001	MnHPO4	25.4000	25.4000	0.0000	0.0000	MTQ3.11
7090200	(VO)3(PO4)2	8.3700	25.1000	0.0000	0.0000	NIST46.4
7046002	Mg3(PO4)2		23.2800		0.0000	NIST46.4
7046001	MgHPO4:3H2O		18.1750		0.0000	NIST46.4
7015002	FCO3APATITE	114.4000	114.4000	-164.8078	-164.8078	MTQ3.11
7015003	HYDROXYLAPATITE	44.1990	44.3330	0.0000	0.0000	NIST46.4
7015004	CaHPO4:2H2O		18.9950		-23.0000	NIST46.4
7015005	CaHPO4		19.2750		-31.0000	NIST46.4
7015006	Ca3(PO4)2 (beta)		28.9200		-54.0000	NIST46.4
7015007	Ca4H(PO4)3:3H2O		47.0800		0.0000	NIST46.4
7080001	SrHPO4		19.2950		0.0000	NIST46.4
7010001	BaHPO4		19.7750		0.0000	NIST46.4
7089100	U(HPO4)2:4H2O	51.5840	51.5840	-16.0666	-16.0666	MTQ3.11
7089300	(UO2)3(PO4)2	49.0370	49.4000	-397.0616	-397.0616	NIST46.4
7089302	UO2HPO4		24.2250		0.0000	NIST46.4
7049000	URAMPHITE	51.7490	51.7490	-40.5848	-40.5848	MTQ3.11
7060000	PRZHEVALSKITE	44.3650	44.3650	46.0240	46.0240	MTQ3.11
7023102	TORBERNITE	45.2790	45.2790	66.5256	66.5256	MTQ3.11
7028000	BASSETITE	44.4850	44.4850	83.2616	83.2616	MTQ3.11
7046000	SALEEITE	43.6460	43.6460	84.4331	84.4331	MTQ3.11
7015000	NINGYOITE	53.9060	53.9060	9.4977	9.4977	MTQ3.11
7089301	H-AUTUNITE	47.9310	47.9310	15.0624	15.0624	MTQ3.11
7015001	AUTUNITE	43.9270	43.9270	59.9986	59.9986	MTQ3.11
7080000	Sr-AUTUNITE	44.4570	44.4570	54.6012	54.6012	MTQ3.11
7050000	Na-AUTUNITE	47.4090	47.4090	1.9246	1.9246	MTQ3.11
7041000	K-AUTUNITE	48.2440	48.2440	-24.5182	-24.5182	MTQ3.11
7010000	URANOCIRCITE	44.6310	44.6310	42.2584	42.2584	MTQ3.11
7260000	Pb3(AsO4)2	-5.8000	-5.8000	0.0000	0.0000	MTQ3.11
7203000	AlAsO4:2H2O	-4.8000	-4.8000	0.0000	0.0000	MTQ3.11
7295000	Zn3AsO42:2.5H2O	-13.6500	-13.6500	0.0000	0.0000	MTQ3.11
7223100	Cu3(AsO4)2:2H2O	-6.1000	-6.1000	0.0000	0.0000	MTQ3.11
7202001	Ag3AsO3		-2.1573		0.0000	NIST46.4
7202002	Ag3AsO4		2.7867		0.0000	NIST46.4
7254000	Ni3(AsO4)2:8H2O	-15.7000	-15.7000	0.0000	0.0000	MTQ3.11
7220001	Co3(AsO4)2		-13.0341		0.0000	NIST2.1.1

ID No	NAME	Old Log K	New Log K	Old del H	New del H	Source
7228100	FeAsO4:2H2O	-0.4000	-0.4000	0.0000	0.0000	MTQ3.11
7247000	Mn3(AsO4)2:8H2O	-12.5000	-12.5000	0.0000	0.0000	MTQ3.11
7215000	Ca3(AsO4)2:4H2O	-22.3000	-22.3000	0.0000	0.0000	MTQ3.11
7210000	Ba3(AsO4)2	8.9100	8.9100	-11.0458	-11.0458	MTQ3.11
7349000	NH4VO3	-2.6900	-3.8000	15.7737	-30.0000	NIST46.4
7360000	Pb3(VO4)2	-6.1400	-6.1400	72.6342	72.6342	MTQ3.11
7360001	Pb2V2O7	1.9000	1.9000	26.9450	26.9450	MTQ3.11
7302000	AgVO3	-0.7700	-0.7700	0.0000	0.0000	MTQ3.11
7302001	Ag2HVO4	-1.4800	-1.4800	0.0000	0.0000	MTQ3.11
7302002	Ag3H2VO5	-5.1800	-5.1800	0.0000	0.0000	MTQ3.11
7328000	Fe(VO3)2	3.7200	3.7200	61.6722	61.6722	MTQ3.11
7347000	Mn(VO3)2	-4.9000	-4.9000	92.4664	92.4664	MTQ3.11
7346000	Mg(VO3)2	-11.2800	-11.2800	136.6494	136.6494	MTQ3.11
7346001	Mg2V2O7	-26.3600	-26.3600	255.2240	255.2240	MTQ3.11
7346002	CARNOTITE	-0.2300	-0.2300	36.4008	36.4008	MTQ3.11
7315000	TYUYAMUNITE	-4.0800	-4.0800	153.1344	153.1344	MTQ3.11
7315001	Ca(VO3)2	-5.6600	-5.6600	84.7678	84.7678	MTQ3.11
7315002	Ca3(VO4)2	-38.9600	-38.9600	293.4658	293.4658	MTQ3.11
7315003	Ca2V2O7	-17.5000	-17.5000	159.4941	159.4941	MTQ3.11
7315004	Ca3(VO4)2:4H2O		-39.8600		0.0000	NIST46.4
7315005	Ca2V2O7:2H2O		-21.5520		0.0000	NIST46.4
7310001	Ba3(VO4)2:4H2O		-32.9400		0.0000	NIST46.4
7310002	Ba2V2O7:2H2O		-15.8720		0.0000	NIST46.4
7350000	NaVO3	-3.7100	-3.8582	29.3298	30.1799	NIST2.1.1
7350001	Na3VO4	-36.9400	-36.6812	185.8533	184.6100	NIST2.1.1
7350002	Na4V2O7	-37.4000	-37.4000	201.0830	201.0830	MTQ3.11
8603000	HALLOYSITE	-8.9940	-9.5749	166.2303	181.4297	NIST2.1.1
8603001	KAOLINITE	-5.7260	-7.4350	147.6115	148.0000	Nord90
8628000	GREENALITE	-20.8100	-20.8100	0.0000	0.0000	MTQ3.11
8646000	CHRYSOTILE	-32.1880	-32.2000	219.5972	196.0000	Nord90
8646003	SEPIOLITE	-15.9130	-15.7600	114.0893	114.0893	Nord90
8646004	SEPIOLITE (A)	-18.7800	-18.7800	0.0000	0.0000	MTQ3.11
3300021	O2 (g)	-83.1200	-83.0894	559.9447	571.6600	CODATA89
3301404	CH4 (g)	40.1000	41.0452	-255.2240	-257.1330	NIST13.1
3301403	CO2 (g)	18.1600	18.1470	-2.2175	-4.0600	NIST46.4
3307302	H2S (g)		8.0100		0.0000	NIST46.4
3307602	H2Se (g)		4.9600		15.3000	NIST46.4
3600001	Hg (g)	7.8708	7.8733	-22.0288	-22.0550	CODATA89
3600002	Hg2 (g)	14.9630	14.9554	-58.0321	-58.0700	NIST2.1.1
3611400	Hg(CH3)2 (g)	73.7240	73.7066	-482.8336	-481.9899	NIST2.1.1
3602700	HgF (g)	-32.7200	-32.6756	254.8725	254.8440	NIST13.1
3612700	HgF2 (g)	-0.3800	-12.5652	0.0000	165.1860	NIST13.1
3601800	HgCl (g)	-20.5000	-19.4966	167.7700	162.0950	NIST13.1
3601300	HgBr (g)	-16.7900	-16.7566	142.2727	142.1570	NIST13.1
3611300	HgBr2 (g)	18.4700	18.3881	-60.0404	-54.4940	NIST13.1
3603800	HgI (g)	-11.1500	-11.3322	105.7046	106.8150	NIST13.1
3613800	HgI2 (g)	27.2800	27.2259	-119.7879	-114.4290	NIST13.1

APPENDIX B

FORMAT OF THE THERMODYNAMIC DATABASE V4.0

This listing specifies the format of entries in the ASCII text file that contains the main thermodynamic database for MINTEQA2 v4.0. The files containing solid phases, redox couples, and gas species are identical in format to that shown here. This information is useful for adding new reactions to any of these four database files. (The database files are referred to by their default names in the explanation that follows: THERMO.DBS, TYPE6.DBS, REDOX.DBS, and GASES.DBS, respectively.) Before attempting to add to or modify these files, note the following:

- Make backup copies first
- When editing the thermodynamic database, if the species to be added or modified is an aqueous species, the file THERMO.DBS is the only one that must be modified. If the species is a solid, redox couple, or gas species, the file TYPE6.DBS, REDOX.DBS, or GASES.DBS, respectively, must be modified in addition to THERMO.DBS.
- The main database file, THERMO.DBS, contains several delimiter lines with zeros and blank entries. These must not be deleted or altered.
- After all desired changes are made to THERMO.DBS, new versions of the corresponding files that are actually used by MINTEQA2 and PRODEFA2 must be created using the UNFRMT.EXE program included on the v4.0 diskettes.

Explanation of Entries in the Thermodynamic Database Files

The first line in the database is for general descriptive information (28 characters).

Each species occupies three lines if the number of components is five of fewer; otherwise, four lines.
FIRST line for an species entry:

Columns	Meaning
1 - 7	Species ID number.
8	blank
9 - 29	Species name.
30 - 39	Enthalpy of reaction (kJ/mol)
40 - 49	Log K for formation of the product from the components
50 - 57	Maximum reported log K (not used in calculations; may not be present)
58 - 65	Minimum reported log K (not used in calculations; may not be present)

Columns	Meaning
66 - 70	Charge of species reaction product
71 - 75	"a" parameter for “WATEQ” Debye-Huckel equations
76 - 80	"b" parameter for “WATEQ” Debye-Huckel equations

SECOND line for a species entry:

1 - 5	Carbonate alkalinity factor (Zero for species not containing carbonate)
6	blank
7	Number of components in the formation reaction
8 - 10	blank
11 - 17	Stoichiometry of the first component (Negative products)
18	blank
19 - 21	Component ID number of the first component
22 - ?	Additional stoichiometry/component ID # pairs with separating spaces so that the total number of pairs is equal to the number of components as specified in column 7. All are entered in the same manner as the first pair in columns 8 - 21. Species with more that five components continue on the next line.

THIRD (or fourth) line for a species entry:

1 - 9	Species gram formula weight (zero for redox couple)
10	blank
11 - 40	Source information for the log K value
41 - 70	Source information for the enthalpy of reaction
71 - 80	Ionic strength and temperature of the original (uncorrected) log K value as obtained from the source.