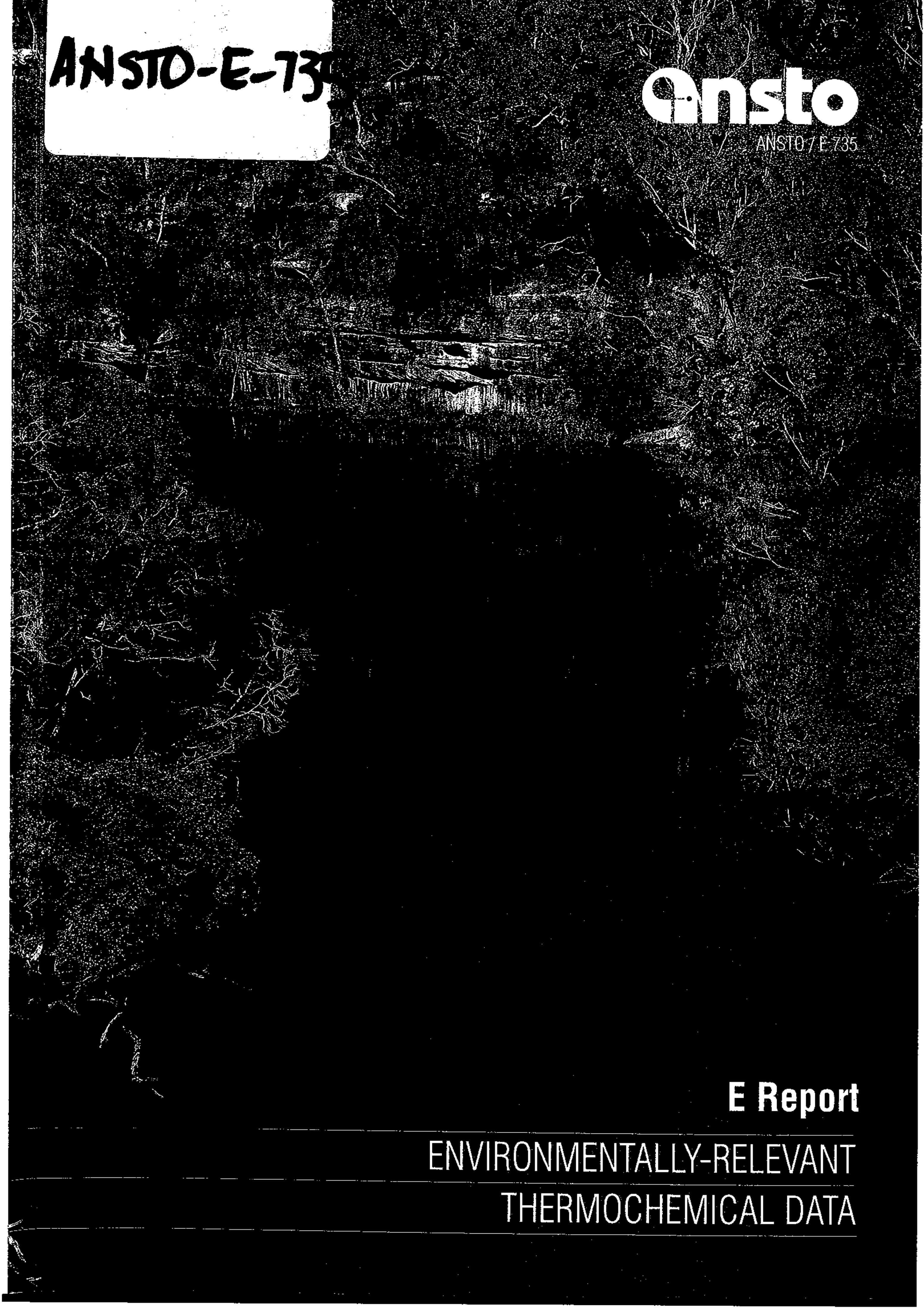

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E Report

ENVIRONMENTALLY-RELEVANT THERMOCHEMICAL DATA

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E Report

ENVIRONMENTALLY-RELEVANT THERMOCHEMICAL DATA

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THERMOCHEMICAL DATA (log K) FOR ENVIRONMENTALLY-RELEVANT ELEMENTS.

1. H, Na, K, Ca, Mg, Fe, Mn, U, Al, Pb, Zn, Cu and Cd with Model Fulvic Acid (Aspartate, Citrate, Malonate, Salicylate and Tricarballyate)

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ABSTRACT

This study provides an extensive stability constant (log K) database suitable for calculating the speciation of selected environmentally-relevant elements (H, Na, K, Ca, Mg, Fe, Mn, U, Al, Pb, Zn, Cu and Cd) in an aqueous system, where a model fulvic acid (comprising aspartic, citric, malonic, salicylic and tricarballylic acids) is used to simulate metal binding by dissolved organic material. Stability constants for inorganic metal complexes and minerals were selected primarily from critical literature compilations and/or reviews. In contrast, few critically evaluated data were available for metal complexes with aspartic, citric, malonic, salicylic and tricarballylic acids. Consequently, data from original research articles were carefully evaluated and compiled as part of the study, following defined selection criteria. To meet the objective of compiling a comprehensive and reliable database of stability constants, all relevant equilibria and species, ranging from simple binary metal complexes to more complex ternary, and even quaternary, metal complexes were included where possible. In addition to the selection of stability constants from empirical sources, estimates of stability constants were performed when this could be done reliably, based on the unified theory of metal ion complexation and/or linear free energy relationships. The stability constants are given as common logarithms ($\log_{10}$) in the form required by the HARPHRQ geochemical code and refer to the standard state, i.e. 298.15 K (25°C), 10^5 Pa (1 atm) and, for all species, infinite dilution (ionic strength = 0 mol L^{-1}). In addition to the compilation of stability constant data, an overview is given of geochemical speciation modelling in aqueous systems and available conceptual models of metal binding by humic substances.

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LIST OF ABBREVIATIONS

ANSTO	Australian Nuclear Science and Technology Organisation
Asp	Aspartic Acid
atm	Atmosphere
°C	Degrees Celsius/Centigrade
Cit	Citric Acid
COOH	Carboxylic Acid
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
FA	Fulvic Acid
HA	Humic Acid
HS	Humic Substances
I	Ionic Strength
K	Kelvin
LFER	Linear Free Energy Relationship(s)
log K	Logarithm of the Stability Constant
[M]	Free Metal Ion Activity
Mal	Malonic Acid
ML	Metal Complex
NEA	Nuclear Energy Agency
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
pe	Measure of Redox Potential (at 25°C, pe = $E_H/59$)
pK_a	Acid Dissociation Constant
Sal	Salicylic Acid
TDE	Truncated Davies Equation
Tri	Tricarballylic Acid
UTMIC	Unified Theory of Metal Ion Complexation

1 Introduction

Metals in aquatic systems exist in a variety of physicochemical forms, including the free metal ion (M^{z+}) and metal complexes with organic and inorganic ligands in dissolved, colloidal and/or particulate forms (**Table 1**). It is well established that the distribution of a metal amongst its various physicochemical forms (metal speciation) is paramount to understanding the geochemical and biological reactivity of metals in aquatic systems (Campbell 1995; Sigg 1998).

Table 1. Approximate size of the physicochemical forms of metals in aquatic systems. Adapted from Pickering (1995)

Physicochemical form	Examples	Approximate diameter (nm)
Dissolved		*< 5*
Simple hydrated metal ion	$Cu(H_2O)_6^{2+}$	0.8
Simple inorganic complexes	$Mn(H_2O)_3Cl^+$	1–2
Stable inorganic complexes	$ZnCO_3$, PbS	1–2
Simple organic complexes	Cu-glycinate	1–2
Stable organic complexes	Cu-fulvate	2–4
Colloidal		*10–450*
Adsorbed on inorganic colloids	Cu^{2+}, Fe_2O_3; Cd^{2+}, MnO_2	
Adsorbed on organic colloids	Cu^{2+}, humic acid	
Adsorbed on mixed (inorganic/organic) colloids	UO_2^{2+}, Fe_2O_3/humic acid	
Particulate		*> 450*
Precipitates, co-precipitates	$PbCO_3$	
Mineral particles	PbS	
Metals adsorbed on solids	Zn^{2+}, CuS, $PbCO_3$ on clay minerals, Mn(IV) oxides	
Metals incorporated with organic material	Metals in algae	

The reactivity of a metal on the surfaces of cells or particles can be related directly with metal speciation, often through the activity (or concentration) of the free metal ion (M^{z+}). Investigations of metal reactivity, therefore, require techniques for determining the activities (or concentrations) of free metal ions and/or other reactive metal species. These metal species can rarely be measured directly, particularly at trace concentrations (Nordstrom 1996). In the majority of cases, the required activity (or concentration) of a metal species must be calculated, using geochemical speciation modelling, from a knowledge of the total concentration of the metal and the chemical composition of the aquatic medium. Thus, geochemical speciation modelling usually plays a central role in interpreting the results of experimental studies on metal-organism or metal-particle interactions, in addition to providing the means to predict metal speciation and to identify non-equilibrium conditions (Nordstrom 1996).

From both a geochemical and biological perspective, the most important speciation parameter is probably the degree of metal complexation:

$$\Delta pM = \frac{[M]_T}{[M]} \qquad [1]$$

where ΔpM is the degree of metal complexation, $[M]_T$ is the total dissolved metal concentration and [M] is the concentration of the free metal ion (Stumm and Morgan 1996).

Key factors that influence the degree of metal complexation in natural waters include:
(i) the total dissolved metal concentration (M_T);
(ii) the nature and concentration of competing ligands (e.g. CO_3^{2-}, fulvic acid);
(iii) the concentrations of competing cations, including H^+, Ca^{2+} and/or Mg^{2+};
(iv) the stability of the various ML forms;
(v) redox potential;
(vi) temperature; and
(vii) the degree to which chemical equilibrium is attained (reaction kinetics).

The speciation and bioavailability of a dissolved metal are governed by key water chemistry parameters including pH (H^+), redox potential (e^-), hardness (Ca^{2+} and/or Mg^{2+}), inorganic ligands (e.g. CO_3^{2} or SO_4^{2-}) and organic agents (e.g. fulvic and humic acids, generally known as humic substances). Fulvic and humic acids are important organic macromolecules that govern the transport and bioavailability of trace metals in aquatic systems (Buffle 1988). Fulvic acid is the major component (*ca.* 90%) of dissolved humic substances (Aiken *et al.* 1985) and has been shown to serve as a useful analogue of dissolved organic matter (DOM) in aqueous systems (McKnight *et al.* 1983; Cabaniss and Shuman 1988; Breault *et al.* 1996).

The purpose of this study is to provide an extensive stability constant (log K) database suitable for calculating the speciation of selected environmentally-relevant elements (H, Na, K, Ca, Mg, Fe, Mn, U, Al, Pb, Zn, Cu and Cd) in an aqueous system, where a model fulvic acid (comprising aspartic, citric, malonic, salicylic and tricarballylic acids) (Gregor *et al.* 1989a) is used to simulate metal-DOM binding.

2 Use of Geochemical Speciation Modelling to Predict Metal Speciation in Aquatic Systems

2.1 Methods, assumptions and limitations

A geochemical speciation model is a mathematical statement (system of equations) of the methods and assumptions used to describe some aspects of 'reality' (metal-ligand equilibria) (Guerin *et al.* 1997). Two distinct, but thermodynamically related, methods are used by geochemical speciation models to calculate metal-ligand equilibria in aqueous systems: the *equilibrium constant* method and the *Gibbs free-energy* method (Nordstrom and Ball 1984). Both methods are subject to the conditions of mass balance and chemical equilibrium. The mass balance condition requires that the calculated sum of the free and derived species be equal to the given total concentration. Chemical equilibrium requires that the most stable arrangement for a given system be found, as defined by the stability constants for all mass action expressions of the system, or through the use of Gibbs free-energy values for all components and derived species. In the equilibrium constant method, the mass action expressions are substituted into the mass balance conditions, resulting in a set of non-linear equations that must be solved simultaneously. The Gibbs free-energy method is simply a transformation of variables through the thermodynamic relation, which allows a different numerical approach (Nordstrom and Munoz 1994).

A geochemical speciation code (e.g. MINTEQA2, PHREEQE or MINEQL) is the practical realisation of the solution to a geochemical speciation model (it executes calculations based on a model), typically written in a 'high-level' computer language (Guerin *et al.* 1997). Most codes employ the equilibrium constant method, which uses measured stability constants for all mass action expressions of the system. The Gibbs free-energy method requires Gibbs free-energy values and employs minimisation techniques to obtain a minimum in the free-energy of the system modelled. In both cases, the most stable condition is sought, and a solution to a set of non-linear equations is required. The Gibbs free-energy method is primarily useful for simple systems because of the limited availability of free-energy values. The equilibrium constant method has the advantage of a larger and more reliable database and is, therefore, generally preferable (Nordstrom and Ball 1984). The model inputs required for both methods include pH, pe, temperature and total metal and ligand concentrations. As output, each method calculates the percentage formation of relevant species, such as the free metal ion and metal complexes (Mattigod 1995). The extent of adsorption, cation exchange and precipitation may also be indicated if simulated in a particular geochemical speciation code. Both methods are considered to be functionally equivalent (van Zeggeren and Storey 1970), and the selection of one method over the other is usually arbitrary.

The historical evolution of geochemical speciation codes has not been documented. However, several publications are available that describe the variety of codes which may be used in aquatic systems (Jenne 1981; Nordstrom and Ball 1984; Bassett and Melchior 1990; Nordstrom and Munoz 1994). A decade ago, Nordstrom and Ball (1984) listed 57 different codes. One distinct trend over the last decade has been the cessation of the rapid increase in the number of new codes being developed. This has been replaced with a more focussed effort to improve and qualify existing codes. Several codes (e.g. MINTEQA2, PHREEQE or MINEQL) have become the mainstay for geochemical applications (Nordstrom and Munoz 1994; OECD 1996).

Although a variety of geochemical speciation codes are now widely available, all have significant limitations, and these are discussed in detail by Nordstrom and Ball (1984), Campbell and Tessier (1987) and Nordstrom and Munoz (1994). One limitation is that most geochemical speciation codes assume *equilibrium conditions*; i.e. the kinetics of precipitation, oxidation-reduction and adsorption are generally ignored. This may not be a valid assumption in some cases, because of kinetically unfavourable chemical processes, biological transformation and physical transport. However, it provides a good approximation for many aqueous systems, where chemical reactions occur very rapidly (Nordstrom and Ball 1984).

For all geochemical speciation codes, there can be large variation in the stability constants used for the same reaction (see reviews by Turner (1995) and Nordstrom (1996)). This problem is particularly obvious for trace metals, for which published stability constants of a given metal complex may differ by one or more orders of magnitude (see Campbell and Tessier (1987) for an overview of copper hydroxide). Serkiz *et al.* (1996) reported a substantial number of errors in the stability constant database used in the popular MINTEQA2 geochemical speciation code. Errors in stability constant databases result primarily because of differences in the:
(i) selection of stability constants from the literature; and/or
(ii) methods used to correct stability constants to the appropriate ionic strength (usually infinite dilution; $I = 0$).

The output from a geochemical speciation model is only as reliable as the input data. There is a clear requirement for a reliable and internally consistent database of stability constants to model chemical equilibria. The types of stability constant (and kinetic) databases that may be used with geochemical speciation models have recently been surveyed by the OECD (1996). Until a central coordination centre for chemical modelling databases is established, errors in the predictions of chemical equilibria are not expected to improve. However, some progress has been made through the CHEMVAL initiative (Bennett *et al.* 1995; Falck 1996).

The modelling of adsorption is not well developed, owing to a general lack of understanding of the phenomenon (Nordstrom 1996). However, knowledge in this area is improving. In addition, surface modifications may cause solids in natural systems to behave quite differently from pure phases (Turner 1995). Modelling of adsorption processes can be accomplished using stability constants, which are frequently estimated in the laboratory and later adjusted in field applications.

There is no general-purpose geochemical speciation code that can be used for all applications. While there are several limitations in using geochemical speciation codes, the general consensus is that they can provide useful results if applied correctly and with an understanding of the differences between simulated and real systems (Nordstrom 1996). The capability of predicting the species distribution of a metal is potentially most satisfactory in an aqueous system (e.g. experimental water) where the physicochemical parameters (e.g. pH, total metal and ligand concentrations) are well defined (Campbell and Tessier 1987; Turner 1995). Several studies have shown close agreement between measured (analytical) and predicted (modelled) trace metal speciation in both experimental and natural waters (McGrath *et al.* 1986; Hirsch and Banin 1990; Breault *et al.* 1996; Markich 1998). Geochemical speciation modelling should be used to complement analytical speciation techniques (e.g. ion-selective electrode potentiometry, anodic stripping voltammetry) whenever possible (Campbell and Tessier 1987; Nordstrom 1996).

In natural waters, however, metal binding by DOM is not accounted for by many geochemical speciation models (Campbell and Tessier 1987). Natural DOM may account for a significant portion of the metal binding capacity of surface waters, and hence, markedly influences the speciation, transport and bioavailability of many trace metals (Livens 1991; Campbell 1995; Buckau 1999). Therefore, metal-DOM binding may not be considered, or greatly underestimated, in surface waters by many geochemical speciation models. As a result, such models may markedly overestimate the formation of inorganic trace metal species, and hence, overestimate trace metal bioavailability. The development of realistic models of trace metal speciation and bioavailability in natural waters requires an understanding of the nature of metal-DOM interactions and quantitative measures of such interactions.

2.2 Metal-DOM interactions

Humic substances (HS) are a major component (55–80%) of natural DOM in aquatic systems (Vaughan *et al.* 1993); concentrations usually range from 20 µg L^{-1} in groundwaters to 30 mg L^{-1} in organic-rich surface waters (Thurman and Malcolm 1981). They comprise a physically and chemically heterogeneous mixture of relatively high molecular weight, yellow-black organic compounds of aliphatic and aromatic nature, formed by secondary synthesis reactions (humification) during the decay process and transformation of biomolecules that originate from dead organisms and microbial activity (Senesi 1993). According to their solubility in water at different pH values, HS are divided into three main fractions:

(i) fulvic acid (FA), the portion that is soluble at any pH;
(ii) humic acid (HA), the portion that is fully soluble only at pH > 9.5; and
(iii) humin, the portion that is insoluble at any pH (Aiken *et al.* 1985).

Fulvic acid is the major component (*ca.* 90%) of dissolved HS (HA *ca.* 10%) (Aiken *et al.* 1985) and has been shown to serve as a useful analogue of DOM in fresh surface waters (McKnight *et al.* 1983; Cabaniss and Shuman 1988; Breault *et al.* 1996).

Humic and fulvic acids cannot be defined as single chemical entities or described by unique, chemically-defined, molecular structures. Instead, they are defined by a model structure based on available compositional, structural, functional and behavioural data, and contain the same basic structural units and the same type of reactive functional groups (Buffle 1988; Senesi 1993). Humic and fulvic acids are homologous complexants with three unique properties, namely

(i) polyelectrolyte (oligoelectrolyte) macromolecules (develop a pH dependent surface charge);
(ii) polyfunctional (possess a variety of dissociable functional groups (e.g. COOH and OH) on the same molecule); and
(iii) can undergo conformational changes resulting from electrostatic interactions among the various functional groups on a single molecule, which may make the coordination properties of the molecule highly dependent on the extent of cation binding and on the ionic strength of the solution (Buffle 1988; Ephraim and Allard 1997).

As a result, fulvic and humic acids are capable of forming many types of potential metal binding sites. Additionally, the heterogeneous nature of fulvic and humic acids makes it impossible to assign a molecular weight to these compounds (e.g. 500–2000 daltons for aquatic FA and 2000–5000 daltons for aquatic HA) (Aiken *et al.* 1985).

Fulvic and humic acids contain a variety of dissociable functional groups that can form inner-sphere complexes (strong covalent interactions) with metals, the predominant ones being the oxygen containing carboxylic (-COOH) and phenolic (-OH) groups (Aiken *et al.* 1985; Ephraim and Allard 1997). Due to the high proportion of these oxygen-containing groups, particularly in FA, they usually dominate metal binding in natural waters, even though nitrogen and sulfur containing functional groups have a high affinity for metals such as Cd or Cu (Buffle 1988). Most of the functional groups are acidic in nature (Aiken *et al.* 1985; Senesi 1993) and tend to dissociate protons with increasing pH, thus developing a negative charge on the surface of the molecule. The development of a negative surface charge allows, in addition to the covalently bonded inner-sphere metal complexes, the retention of exchangeable outer-sphere complexes (weak electrostatic interactions) on the same molecule. As the concentration of complexing ligands cannot be expressed readily in molar concentrations for fulvic and humic acids, the value of the titratable acidity is often used to estimate the binding capacity of natural DOM. The pK_a values of acidic functional groups on fulvic and humic acids are discussed by Aiken *et al.* (1985).

Due to the complex nature of HS, attempts to describe metal binding, particularly in terms of the number of binding sites (stoichiometry) and binding strength (stability constants), have often yielded contradictory results (see reviews by Turner (1995) and Wood (1996)). Although metal binding by HS has been extensively studied (Turner 1995; Wood 1996; Ephraim and Allard 1997; Tipping 1998), the extent of any given metal-binding reaction cannot be predicted with confidence. Predictions are typically based on stability constants, and for any given system the available constants are likely to vary. The differences can generally be attributed to a number of phenomena (Warwick *et al.* 1996) including:

(i) variable fulvic and humic acid properties arising from local and seasonal differences;
(ii) variable extraction procedures used to isolate fulvic and humic acids and consequent differences in their purity;
(iii) the absence of specific analytical techniques suitable only for fulvic and humic acids;
(iv) variable experimental techniques and the interpretive models used to derive stability constants; and
(v) the conditional nature of the derived stability constants. Generally, the values reported are dependent on factors such as pH, ionic strength and the presence of competing ions.

From a geochemical speciation modelling perspective, simple ligands of known molecular structure have reactions of well-defined stoichiometry at a discrete binding site and can be dealt with using the mass action/mass balance method described in Section 2.1. In contrast, HS are polyelectrolyte macromolecules of unknown molecular structure and are heterogeneous in nature, so they represent a wide spectrum of molecular sizes and potentially many different types of binding sites. As a result, it is difficult to define discrete stability constants for each binding reaction. In addition, any such stability constant defined will seem to differ with factors such as the electrostatic charge related to the degree of dissociation of the molecule and interferences between sites. Consequently, the incorporation of metal-DOM binding into geochemical speciation codes has been problematic (Turner 1995; Hummel 1997).

2.3 Conceptual models of metal binding by humic substances

A number of conceptual models have been developed to describe some of the observed behaviour of HS in an attempt to predict their metal-binding using geochemical speciation codes. These models are discussed in detail by Wood (1996), Ephraim and Allard (1997) and Hummel (1997) and will be only briefly summarised here. The conceptual models fall broadly into three main categories:

(i) those assuming that metal binding by HS can be represented by one or more binding sites of different, but constant, strength (*discrete ligand model* – type I);
(ii) those assuming that a spectrum of sites exist which grade from very strong to very weak without any sharp dividing line among them (*continuous distribution model* – type II); and
(iii) those based on the equating of binding sites on HS with simple organic analogue moieties (*analogue-based model* – type III).

All three models have been employed with and without provision for the electrostatic effects associated with the build-up of charge on a polyelectrolyte as a function of increasing pH and changes in surface potential owing to variations in ionic strength. Type I and II models are typically (semi-) empirical in that, to obtain stability constants for metal interaction with each binding site, the model must be fitted to experimental data and the constants adjusted until a best fit is obtained. Type III models are ideally *a priori*, in the sense that published stability constants for complexes formed between the metal of interest and simple analogue moieties are used. In theory, there is no requirement to perform any experimental measurements on the metal-HS system itself to apply type III models, although in practice, some parameter adjustment has been required to obtain a best fit.

Non-electrostatic type I models attempt to approximate the large humic molecule into a number of sites and site types, each of which can be defined in terms of a binding reaction. They are easily incorporated into geochemical speciation codes which, perhaps, accounts for their comparative widespread use to fit experimental data. However, non-electrostatic type I models are not particularly representative of reality (Wood 1996). A fundamental problem with the use of such models is that the stability constants defined for each reaction are highly conditional, rather than true thermodynamic values, because they neglect effects resulting from variations in parameters such as pH and ionic strength, and do not take into account binding resulting from electrostatic forces in a diffuse layer (non-specific binding) around the humic molecule (Hummel 1997). Examples of non-electrostatic type I models are given by Sposito *et al.* (1979), Giesy *et al.* (1986), Turner *et al.* (1986) and Holm and Curtis (1990). The model developed by Sposito *et al.* (1979) has been incorporated into the geochemical code GEOCHEM (Mattigod and Sposito 1979).

Electrostatic type I models differ in that they treat the binding constant as being comprised of an intrinsic component related to the thermodynamics of the reaction and an electrostatic component which accounts for variable solution conditions (e.g. pH and ionic strength) and the charge on the humic molecule. Since specific reactions are defined, such an approach is compatible with geochemical speciation codes, and because intrinsic thermodynamic values are being considered, these models are less conditional than the non-electrostatic models. Examples of electrostatic type I models are given by Bartschat *et al.* (1992), Tipping and Hurley (1992), de Wit *et al.* (1993), Benedetti *et al.* (1996) and Tipping (1998). The model developed by Tipping and Hurley (1992) (i.e. Humic Ion-Binding Model V) has been incorporated into the PHREEQE geochemical code, to yield the code PHREEQEV (Crawford 1996).

Type II models consider experimental data for humic binding in terms of a statistical distribution function. The probability of locating a binding site with a particular stability constant within the overall range can then be defined. This approach attempts to address the heterogeneity of acid functional groups and the numerical spread of their concomitant acid dissociation constants. However, the processes of binding are not modelled explicitly and because stability constants are not provided for defined sites, it is more difficult to incorporate into geochemical speciation codes than the type I models. As a result, the type II models described are not always satisfactory and are often restricted to the ionic strengths at which the modelling parameters were determined, since they generally do not consider electrostatic effects resulting from the polyelectrolyte behaviour. Nevertheless, where electrostatic effects have been considered, the models are considerably improved. Examples of type II models are given by Perdue and Lytle (1983), Gamble and Langford (1988), Dobbs *et al.* (1989) and Marinsky *et al.* (1995). The model developed by Dobbs *et al.* (1989) has been incorporated into the MINTEQA2 geochemical code (Allison and Brown 1995). The MINTEQA2 database of metal-DOM binding constants is based on a study of metal interactions with Suwannee River FA using lanthanide ion probe spectroscopy (Susetyo *et al.* 1991).

Type III models are a relatively new development in predicting metal binding by HS. In this approach, a mixture of organic acids are used, whose reactions with metal cations and protons are well characterised, as simple analogues of the functional groups, or metal binding sites, of fulvic and humic acids. The distribution of the organic acids may be adjusted to simulate the acid-base or metal binding behaviour of the fulvic and/or humic acid. Such models have the advantage of:
(i) being generally applicable over a range of pH values and ionic strengths;
(ii) being easy to incorporate into geochemical speciation codes; and
(iii) not requiring the modeller to measure stability constants for metal complexes with HS to apply them.
Type III models, however, do not account for electrostatic or conformational effects; such effects are characteristic of HS, but are absent in a mixture of organic acids.

Examples of type III models are given by Murray and Linder (1983, 1984), Gregor *et al.* (1989a, 1989b), Mountney and Williams (1992) and Town and Powell (1993). The RANDOM model developed by Murray and Linder (1983, 1984), and extended by Woolard and Linder (1999), generates random molecular structures that are consistent with input values of elemental composition (%C, %N, %S and %O), functional group concentration, percentage aromaticity and the molecular mass of the HS. RANDOM then searches for, and counts, the number of different types of binding sites based on a limited number of simple organic acid analogues. Mountney and Williams (1992) used 13 simple organic acids to demonstrate a relatively good agreement between the results of their model calculations and published experimental data on the binding of Co, Cu, Ni or U with fulvic and humic acids at low concentrations of total metal. The model developed by Mountney and Williams (1992) has been incorporated into the PHREEQE geochemical speciation code (Parkhurst *et al.* 1980).

Using a rather different approach, Gregor *et al.* (1989a, 1989b) and Town and Powell (1993) matched experimental Cu(II) binding curves (i.e. % Cu^{2+} vs pH at fixed Cu: ligand ratios and % Cu^{2+} vs total Cu at a fixed ligand concentration and pH) for HS with those measured or calculated for finite mixtures of organic acids. This approach allows for variation in coordination mode with a change in pH. The fits obtained indicate a great potential for this type of model (see Section 2.4).

Few tests of the predictive capabilities of the conceptual models, outside the conditions of experimental measurements, have been performed. Warwick *et al.* (1996) compared the real predictive capabilities of three conceptual models that have been incorporated into geochemical speciation codes; a non-electrostatic discrete ligand (type I) model (GEOCHEM), an electrostatic discrete ligand (type I) model (PHREEQEV) and a continuous distribution (type II) model (MINTEQA2). Each model was applied to three unrelated test problems: Ni interactions with FA, Eu interactions with FA and HA and actinide speciation in ground water. The model predictions were compared with experimental data. Overall, it was concluded that of the three models tested, the electrostatic discrete ligand (type I) model offered the most advantages for predictive modelling. The non-electrostatic discrete ligand (type I) model had a severely limited application due to the absence of necessary stability constants. The continuous distribution (type II) model had a wider applicability, but lacked stability constants for the actinides (e.g. U).

Christensen *et al.* (1999) compared the predictive capabilities of an electrostatic discrete ligand (type I) model (WHAM) and a continuous distribution (type II) model (MINTEQA2) with measured data for the binding of Cu and Pb with DOC in two polluted groundwater samples. The MINTEQA2 model and its default database gave the best estimates of Cu and Pb complexation for both samples. The deviation of free ion activity between MINTEQA2 model predictions and experimental results was within a factor of two, which is considered to be good. The WHAM model overestimated the Cu and Pb complexation in both groundwater samples, particularly at high DOC (40 mg L^{-1}), where the deviation of free ion activity was close to an order of magnitude. However, when the binding parameters for Cu and Pb with FA were adjusted, the WHAM model provided close agreement with the experimental results.

Benedetti *et al.* (1996) compared the predictive capability of an electrostatic discrete ligand (type I) model with measured data for the binding of Cd or Cu by DOM from three field systems: a mountain lake and two sandy soils. The predictions closely matched the experimental data. Markich (1998) compared the predictive capability of an analogue-based (type III), model, as developed by Gregor *et al.* (1989a), with measured data for the binding of Cu by FA isolated from two freshwater streams. The predictions closely matched the measured experimental data (see Section 2.4).

The success of a particular model in describing metal-DOM binding does not provide any evidence for the correctness of the model at the molecular level. In terms of the best representation of the molecular reality of metal binding by DOM, the electrostatic models are generally considered to be the most suitable at the present time (Ephraim and Allard 1997; Hummel 1997). The choice of the 'best' model ultimately depends on the intention of the modeller and the purpose of the model. It should be remembered that "models are, for the most part, caricatures of reality, but if they are good, then like good caricatures, they portray, though perhaps in a distorted manner, some of the features of the real world" (Kac 1973).

2.4 An analogue-based (type III) model of metal binding with fulvic acid

The FA model selected in this study was developed by Gregor *et al.* (1989a) and consists of a mixture of five simple organic acids—aspartic (Asp), citric (Cit), malonic (Mal), salicylic (Sal) and tricarballylic (Tri) acids—representing a mixture of ligand moieties. The ligand moiety composition used accounts for the observed percentage N (with *ca.* 50% as amino acids) and with the proportions of carboxyl groups in tetraprotic moieties (*ca.* 36%, range 24–40%), triprotic (*ca.* 6%, 3–18%) and mono- plus diprotic acid moieties (*ca.* 56%) determined from protonation-constant studies (Gregor and Powell 1988). Curves calculated on the basis of these criteria were compared with those for FA. Fulvic acid models were derived by matching experimental Cu binding curves (% Cu^{2+} vs pH at two fixed Cu(II):ligand ratios; Gregor *et al.* 1989a) for FA with those measured or calculated for finite mixtures of organic acids.

The FA model described by Gregor *et al.* (1989a) does not calculate conditional stability constants for metal-fulvic acid complexes. This decision recognises the proliferation of stability constants and equilibrium models that can be made to 'fit' a single complex formation curve for a simple metal-ligand system (e.g. Al-citrate). Further, the model recognises that even in simple metal-ligand systems, several complex species may contribute simultaneously to solution stoichiometry for a given pH and total concentration of metal and ligand. This allows for variation in coordination mode with a change in pH. Thus, a single conditional stability constant may not indicate the number and stoichiometry of complexes in solution.

Markich (1998) identified a small error with the FA model described by Gregor *et al.* (1989a). One of the organic acid components of the FA model, tricarballylic acid, was assigned a COOH number of four by the authors (Dr Kip Powell, personal communication), instead of three, which would result in a slightly lower concentration than required.

The measured Cu binding properties of natural FA from the fresh surface waters of Magela Creek (tropical northern Australia) and the Hawkesbury-Nepean River (temperate eastern Australia) were used by Markich (1998) to derive FA models. This procedure required the isolation, purification and chemical characterisation of natural FA from both freshwater systems (Markich 1998). As an alternative strategy, Markich (1998) compared the Cu binding properties of natural FA with filtered water from each system. The FA models derived by Markich (1998) for Magela Creek and the Hawkesbury-Nepean River are shown in **Tables 2 and 3**, respectively. A comparison of the Cu binding properties of natural FA, model FA and filtered surface water are given in **Figs 1 and 2** for Magela Creek and the Hawkesbury-Nepean River, respectively.

The chemical characterisation of natural FA, coupled with a knowledge of the chemistry of a surface-, ground- or soil-water, permits the formulation of a model FA that could be readily incorporated into a geochemical speciation code for predicting metal speciation. This, in turn, will assist in providing an understanding of trace metal-DOM interactions. Selected stability constants for metal complexes with aspartic, citric, malonic, salicylic and tricarballylic acids are given in Section 3.

The FA model used to represent FA isolated from the surface waters of Magela Creek (**Table 2**) during low flow conditions, was derived as follows:

(i) the mean DOC concentration in Magela Creek water during low-median flow conditions in the main Wet season is 3.70 mg L^{-1};
(ii) 44.0% of DOC is FA (i.e. 0.440 x 3.70 mg L^{-1} FA = 1.63 mg C L^{-1} as FA);
(iii) FA consists of 51.7% C (i.e. 1.63/0.517 = 3.15 mg L^{-1} as FA);
(iv) FA has a COOH concentration of 4.94 µmol mg^{-1} (i.e. 3.15 x 4.94 = 15.6 µmol L^{-1} as COOH); and

(v) based on the COOH concentration of natural FA, a model FA (equivalent in COOH concentration to natural FA), comprising a mixture of organic acids (**Table 2**), was selected that best described the Cu binding properties of natural FA, over a pH range of 3.0–6.0 (i.e. FA model B in Fig. 4 of Gregor *et al.* (1989a)).

Table 2. Composition of the FA models used to simulate natural FA in Magela Creek water during low and high flow conditions

Organic acid	Concentration (COOH) (μmol L^{-1})	
	Low flow[A]	High flow[B]
Aspartic acid	1.78 (3.56)	4.29 (8.58)
Citric acid	0.31 (0.93)	0.76 (2.28)
Malonic acid	1.82 (3.64)	4.38 (8.76)
Salicylic acid	1.82 (1.82)	4.38 (4.38)
Tricarballylic acid	1.87 (5.61)	4.50 (13.5)

A Equivalent to a nominal COOH concentration of 15.6 μmol L^{-1}
B Equivalent to a nominal COOH concentration of 37.5 μmol L^{-1}

Copper(II) binding by model FA was determined by titrating Cu(II) (0.78 and 3.12 µmol L^{-1}) – COOH (14.7 ± 0.7 µmol L^{-1}; mean ± 95% CL (n = 3)) (i.e. 1:20 and 1:5, Cu(II):COOH) solutions over the pH range 3.0–7.0, as described by Markich (1998). The resulting Cu binding curves were not significantly ($P > 0.05$) different (generalised *F* test) to those determined for natural FA (15.1 ± 0.6 µmol L^{-1} COOH) and filtered water (16.0 ± 0.6 µmol L^{-1} COOH) from Magela Creek, indicating that the selected FA model was a suitable analogue of the Cu binding properties of natural FA and filtered water samples. **Figure 1a** shows, as an example, the mean Cu binding curve at 0.78 µmol L^{-1} Cu(II):15.6 ± 0.7 µmol L^{-1} COOH (i.e. 1:20, Cu(II):COOH) relative to natural FA and filtered water from Magela Creek under low flow conditions. The Cu(II) binding curves for model FA, natural FA and filtered creek water at the higher Cu(II) concentration (3.12 µmol L^{-1} Cu(II); 1:5, Cu(II):COOH) were displaced to a higher pH (by 0.20 log units at 50% Cu^{2+} ('d_{50}') and 0.30 at d_{10}) (weaker Cu binding) relative to those shown in **Fig. 1a** for the lower Cu(II) concentration (0.78 µmol L^{-1} Cu(II), 1:20, Cu(II):COOH). The displacement of the Cu binding curves at the higher Cu(II) concentration indicates the heterogeneity of available chelation sites (Town and Powell 1993).

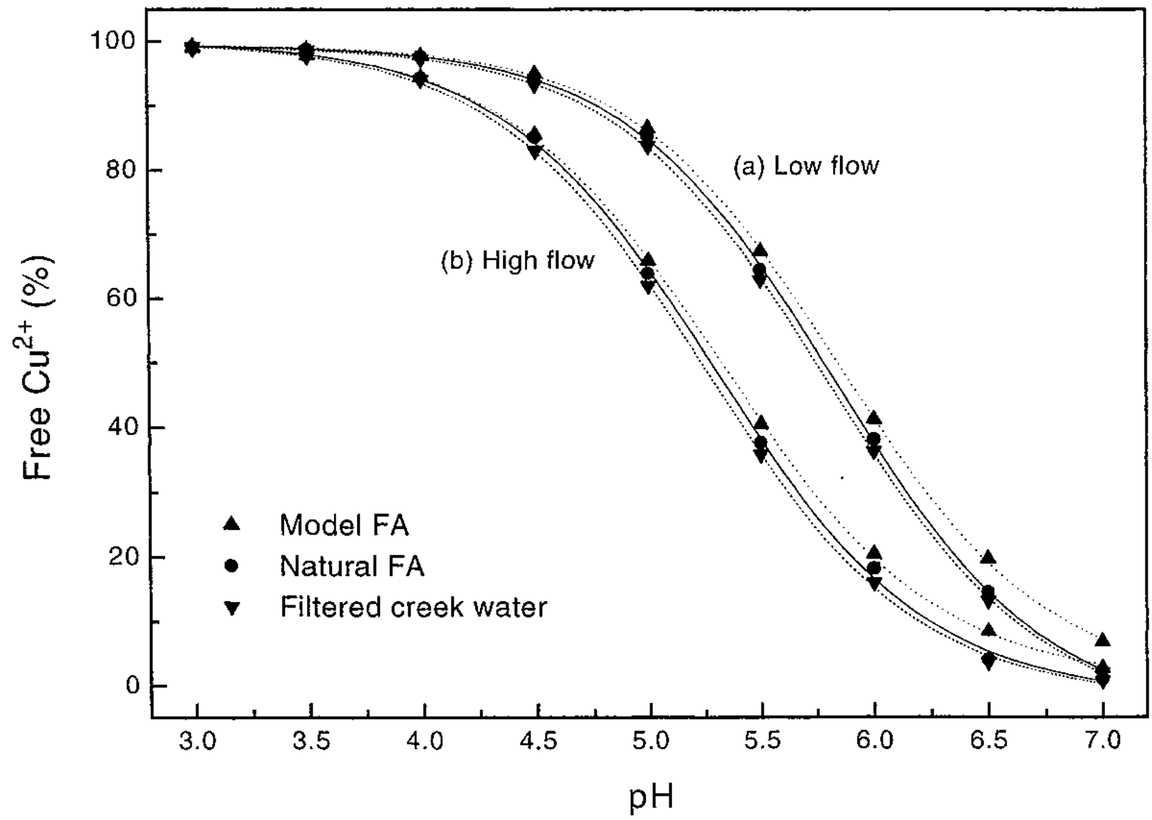

Figure 1. Copper(II) binding curves for model FA, natural FA and filtered water typical of (a) low and (b) high flow conditions in Magela Creek during the wet season. For all Cu(II) binding curves representative of low flow conditions, Cu(II) = 0.78 μmol L^{-1} and COOH = 15.6 ± 0.7 μmol L^{-1} (model FA), 15.6 ± 0.6 μmol L^{-1} (natural FA) and 16.0 ± 0.6 μmol L^{-1} (filtered creek water). For all Cu(II) binding curves representative of high flow conditions, Cu(II) = 1.88 μmol L^{-1} and COOH = 37.5 ± 1.5 μmol L^{-1} (model FA), 37.5 ± 1.2 μmol L^{-1} (natural FA) and 39.2 ± 1.2 μmol L^{-1} (filtered creek water). The mean values of duplicate titrations are shown. Standard errors (excluded for clarity) ranged from 3% (high Cu^{2+} concentrations) to 90% (very low Cu^{2+} concentration) of the mean values, but averaged 14%.

The FA model used to represent natural FA isolated from surface waters of the Magela Creek during high flow conditions (**Table 2**) was derived in the same manner as described above for low flow conditions. Copper(II) binding by model FA was determined by titrating Cu(II) (1.88 and 7.50 μmol L^{-1}) – COOH (37.5 ± 1.5 μmol L^{-1}; mean ± 95% CL (n = 3)) (i.e. 1:20 and 1:5, Cu(II):COOH) solutions over the pH range 3.0–7.0. The resulting Cu binding curves were not significantly ($P > 0.05$) different (generalised *F* test) to those determined for natural FA (37.5 ± 1.2 μmol L^{-1} COOH) and filtered water (39.2 ± 1.2 μmol L^{-1} COOH) from Magela Creek. **Figure 1b** shows, as an example, the mean Cu binding curve at 1.88 μmol L^{-1} Cu(II):37.5 ± 1.5 μmol L^{-1} COOH (1:20, Cu(II):COOH) relative to natural FA and filtered water from Magela Creek under high flow conditions. The Cu binding curves for model FA, natural FA and filtered creek water at the higher Cu(II) concentration (7.50 μmol L^{-1} Cu(II); 1:5, Cu(II):COOH) were displaced to a higher pH (by 0.24 pH units at 50% Cu^{2+} ('d_{50}') and 0.44 at d_{10}) (weaker Cu binding) relative to those in **Fig. 1b** for the lower Cu(II) concentration (1.88 μmol L^{-1} Cu(II), 1:20, Cu(II):COOH).

The FA model used to represent FA isolated from the fresh surface waters of the Hawkesbury-Nepean River (**Table 3**) during low flow conditions, was derived as follows:

(i) the mean DOC concentration in Hawkesbury-Nepean River water during low flow conditions is 4.5 mg L^{-1};

(ii) 48.1% of DOC is FA (i.e. 0.480 x 4.5 mg L^{-1} FA = 2.16 mg C L^{-1} as FA);
(iii) FA consists of 51.2% C (i.e. 2.16/0.514 = 4.20 mg L^{-1} as FA);
(iv) FA has a COOH concentration of 5.21 µmol mg^{-1} (i.e. 4.20 x 5.21 = 21.9 µmol L^{-1} as COOH); and
(v) based on the COOH concentration of natural FA, a model FA (equivalent in COOH concentration to natural FA), comprising a mixture of organic acids (**Table 3**), was selected that best described the Cu binding properties of natural FA, over a pH range of 6.0–7.0 (i.e. FA model C in Fig. 4 of Gregor *et al.* (1989a)).

Table 3. Composition of the FA models used to simulate natural FA in Hawkesbury-Nepean River water during low and high flow conditions

Organic acid	Concentration (COOH) (µmol L^{-1})	
	Low flow^A	High flow^B
Aspartic acid	2.61 (5.22)	7.13 (14.3)
Citric acid	1.14 (3.42)	3.13 (9.4)
Malonic acid	2.61 (5.22)	7.13 (14.3)
Tricarballylic acid	2.67 (8.01)	7.47 (22.4)

A Equivalent to a nominal COOH concentration of 21.9 µmol L^{-1}
B Equivalent to a nominal COOH concentration of 60.4 µmol L^{-1}

The composition of the FA model used to simulate natural FA in the fresh surface waters of the Hawkesbury-Nepean River (**Table 3**) differed slightly from that used for Magela Creek (**Table 2**). Salicylic acid (Sal) was omitted, and the concentration of citric acid (Cit) increased (by a factor of 2.5), in the FA model used in the Hawkesbury-Nepean River study. This was necessary to accurately describe the Cu binding capacity of natural FA at a slightly higher pH; i.e. pH 6.5–7.5 in the Hawkesbury-Nepean River compared with pH 5.0–6.0 in Magela Creek. Gregor *et al.* (1989a) showed that Cu binding by Sal was negligible at neutral pH (6.5–7.5), hence its omission from the Hawkesbury-Nepean FA model. Conversely, Cu binds strongly to Cit in the same pH region, hence its increased concentration in the same FA model.

The paradox exists, that although a number of studies (e.g. Schnitzer and Khan 1972; Murray and Linder 1983) have shown that Sal is a numerically dominant functional group of FA, it makes a negligible contribution to Cu binding at pH 6.5–7.5. In macromolecules like FA, where several ligands with different functional groups effectively compete for the available metal ions, coordination will not necessarily involve the numerically dominant functional groups (Gregor *et al.* 1989a). Consequently, no single organic ligand adequately describes metal-FA binding over the entire pH range (Gregor *et al.* 1989a, 1989b; Town and Powell 1993).

Copper(II) binding by model FA, representative of low flow conditions, was determined by titrating Cu(II) (1.11 and 4.44 µmol L^{-1}) – COOH (21.9 ± 1.1 µmol L^{-1}; mean ± 95% CL (n = 3)) (i.e. 1:20 and 1:5, Cu(II):COOH) solutions over the pH range 3.0–7.0 (Markich 1998). The resulting Cu binding curves were not significantly ($P > 0.05$) different (generalised *F* test) to those determined for natural FA (21.9 ± 1.0 µmol L^{-1} COOH) and filtered water (23.2 ± 0.9 µmol L^{-1}

COOH) from the Hawkesbury-Nepean River (generalised *F* test). **Figure 2a** shows, as an example, the mean Cu binding curve at 1.11 µmol L^{-1} Cu(II):21.9 ± 1.1 µmol L^{-1} (i.e. 1:20, Cu(II):COOH) relative to natural FA and filtered freshwater from the Hawkesbury-Nepean River under low flow conditions. The Cu binding curves for model FA, natural FA and filtered river water at the higher Cu(II) concentration (4.44 µmol L^{-1} Cu(II); 1:5, Cu(II):COOH) were displaced to a higher pH (by 0.21 pH units at 50% Cu^{2+} ('d_{50}') and 0.31 at d_{10}) (weaker Cu binding) relative to those shown in **Fig. 2a** for the lower Cu(II) concentration (1.11 µmol L^{-1} Cu(II), 1:20, Cu(II):COOH).

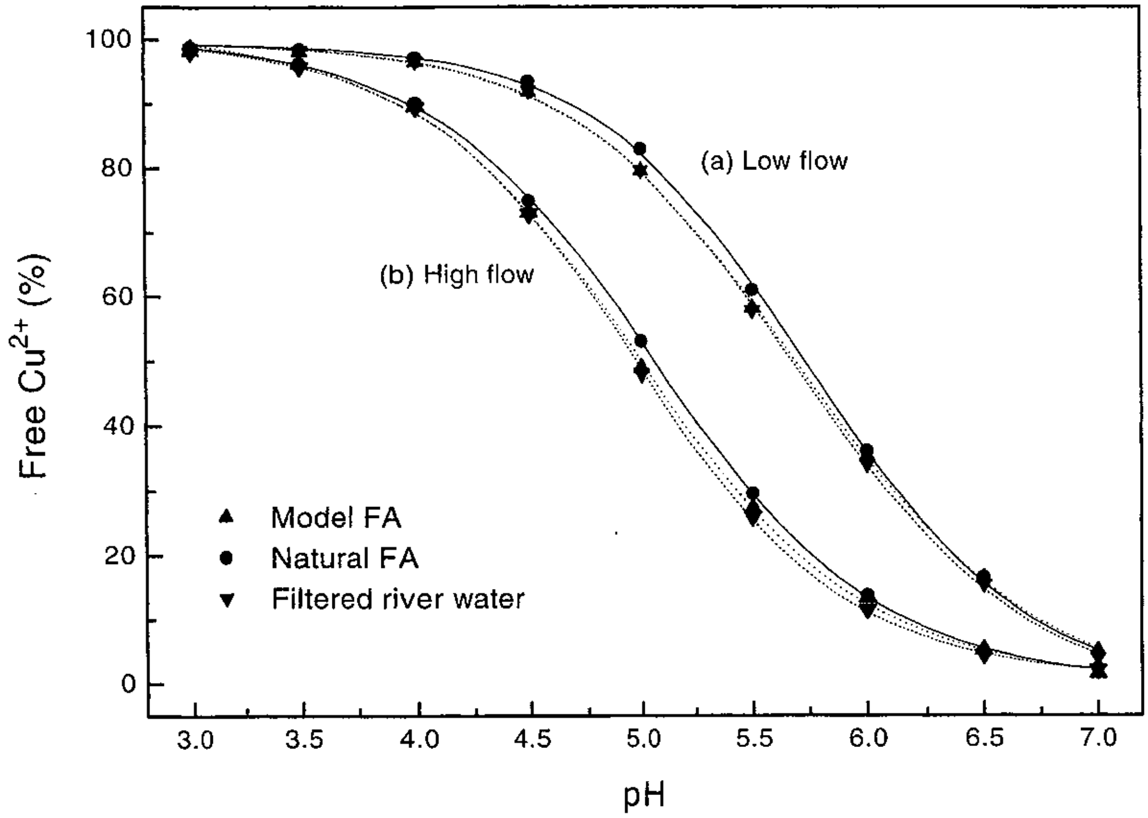

Figure 2. Copper(II) binding curves for model FA, natural FA and filtered river water typical of (a) low and (b) high flow conditions in the Hawkesbury-Nepean River. For all Cu(II) binding curves representative of low flow conditions, Cu(II) = 1.11 µmol L^{-1} and COOH = 21.9 ± 1.1 µmol L^{-1} (model FA), 21.9 ± 1.0 µmol L^{-1} (natural FA) and 23.2 ± 0.9 µmol L^{-1} (filtered river water). For all Cu(II) binding curves representative of high flow conditions, Cu(II) = 3.02 µmol L^{-1} and COOH = 60.4 ± 2.9 µmol L^{-1} (model FA), 60.4 ± 2.7 µmol L^{-1} (natural FA) and 63.2 ± 2.8 µmol L^{-1} (filtered water). The mean values of duplicate titrations are shown. Standard errors (excluded for clarity) ranged from 3% (high Cu^{2+} concentrations) to 95% (very low Cu^{2+} concentration) of the mean values, but averaged 15%.

Copper(II) binding by model FA was determined by titrating Cu(II) (Cu, 3.02 and 12.08 µmol L^{-1}) – COOH (60.4 ± 2.9 µmol L^{-1}; mean ± 95% CL (n = 3)) (i.e. 1:20 and 1:5, Cu(II):COOH) solutions over the pH range 3.0–7.0. The resulting Cu binding curves were not significantly ($P > 0.05$) different (generalised *F* test) to those determined for natural FA (60.4 ± 2.7 µmol L^{-1} COOH) and filtered water (63.2 ± 2.8 µmol L^{-1} COOH) from the Hawkesbury-Nepean River, indicating that the selected FA model was a suitable analogue of the Cu binding properties of natural FA and filtered water samples. **Figure 2b** shows, as an example, the mean Cu binding curve at 3.02 µmol L^{-1} Cu(II):60.4 ± 2.7 µmol L^{-1} COOH (1:20, Cu(II):COOH) relative to natural FA and filtered water from the Hawkesbury-Nepean River under high flow conditions. The Cu binding curves for model

FA, natural FA and filtered river water at the higher Cu(II) concentration (12.08 µmol L^{-1} Cu(II); 1:5, Cu(II):COOH) were displaced to a higher pH (by 0.24 pH units at 50% Cu^{2+} ('d_{50}') and 0.45 at d_{10}) (weaker Cu binding) relative to those shown in **Fig. 2b** for the lower Cu(II) concentration (3.02 µmol L^{-1} Cu(II), 1:20, Cu(II):COOH).

From a practical perspective, given that model FA was found by Markich (1998) to be a suitable analogue of the Cu-binding capacity of natural FA and filtered surface water from two freshwater systems, the measurement of total COOH concentration in a filtered water sample could be used to directly prepare a model FA. This approach would certainly reduce the time and cost of isolating and characterising natural FA. It should be acknowledged that fulvic and humic acids do more than bind metals and protons in solution, as modelled in the work by Markich (1998) and others. The amphiphilic character of these macromolecules confers surfactant properties, which favours their aggregation in solution and accumulation at abiotic (e.g. iron oxides) and biotic (e.g. cell membrane) interfaces (Waite *et al.* 1994; Campbell *et al.* 1997).

3 Stability Constants

3.1 Introduction

Selected stability constants for H, Na, Ca, Mg, Mn, Fe, Al, U, Pb, Zn, Cu and Cd complexes with inorganic and organic ligands and minerals, are given in Section 3.6 (due to the overall size of the database). Metal complexes with aspartic, citric, malonic, salicylic and tricarballylic acids were used to simulate metal binding by FA (see Section 2.4). The stability constants are given as common logarithms ($\log_{10}$) in the form required by the HARPHRQ geochemical code (Brown *et al.* 1991).

3.2 Selection of stability constants

Inorganic metal complexes and minerals were selected primarily from critical literature compilations and/or reviews (e.g. Nordstrom *et al.* 1990; Parkhurst *et al.* 1990; Falck 1992; Grenthe *et al.* 1992, 1995; Smith *et al.* 1998). Data were also selected from original research articles, often accompanied by a literature review of previous data (e.g. Palmer and Nguyen-Trung 1995; Brendler *et al.* 1996, Ridley *et al.* 1999). Stability constants for the inorganic metal complexes and minerals showed reasonable agreement between several independent and critically reviewed sources (see references listed above). Data selected from original research articles were critically evaluated according to the selection criteria outlined by Wanner (1991), Fuger *et al.* (1992) and Smith and Martell (1995).

In contrast to the inorganic metal complexes and minerals, few data were available (e.g. Smith *et al.* 1998) for metal complexes with aspartic, citric, malonic, salicylic and tricarballylic acids that comprised the FA models. Consequently, data from original research articles were critically evaluated, according to the selection criteria outlined by Wanner (1991), Fuger *et al.* (1992) and Smith and Martell (1995), as part of this study (Section 5; **Tables A1–A5**). The stability constant database used in this study was considered to be the most reliable at the time, but may change for particular metal complexes (e.g. aluminium aspartate and uranyl tricarballyate complexes) as additional data becomes available. To meet the objective of compiling a comprehensive and reliable database of stability constants, all relevant equilibria and species, ranging from simple binary metal complexes to more complex ternary, and even quaternary, metal complexes were included where possible.

Where possible, stability constants measured by different investigators were recalculated using the dissociation constants (e.g. HCO_3^-, $HCit^{2-}$) selected in this study (Section 3.6). Such recalculations consistently resulted in better agreement between stability constants. In addition to the selection of stability constants from empirical sources, estimates of stability constants were performed, when this could be done reliably, based on:
(i) the unified theory of metal ion complexation (UTMIC) (see Section 3.5);
(ii) inter-relationships between analogous systems; e.g. linear free energy relationships (LFER) (see Section 3.5); and
(iii) other less theoretical procedures (see May *et al.* (1977), for example).

No attempt has been made to critically discuss the stability constants provided in Section 3.6. Similarly, enthalpy and entropy data have not been provided; these are available elsewhere (e.g. Cox *et al.* 1989; Pearson *et al.* 1992; Grenthe *et al.* 1992, 1995; Smith *et al.* 1998).

The uncertainty (error) in each stability constant has not been given, but can usually be derived from the relevant reference source (inorganic complexes and minerals) or calculated from the raw data (organic complexes). However, in some instances, a quantitative value of uncertainty (±) cannot be assigned to a stability constant due to a lack of data (only one value); therefore the evaluation has a subjective component. Unless noted otherwise, all data refer to the standard state, i.e. 298.15 K (25°C), 10^5 Pa (1 atm) and, for all species, infinite dilution (ionic strength (I) = 0 mol L^{-1}).

3.3 Correction of stability constants for differences in ionic strength

Most published stability constants have been experimentally measured in concentrated solutions (I = 0.1–1.0 mol L^{-1}). However, stability constants typically need to be corrected to infinite dilution, using an appropriate extrapolation method, prior to use in geochemical speciation codes. As recommended by Chandratillake and Robinson (1990), published stability constants derived from solutions with $I \leq 0.3$ mol L^{-1} were corrected to infinite dilution in this study using the following extended form of the Debye-Hückel equation, as proposed by Davies (1962):

$$\log K(I) = \log K_0 + A\Delta z^2 \left[\left(\frac{\sqrt{I}}{1+\sqrt{I}} \right) - 0.3I \right] \qquad [2]$$

where:
- I is the ionic strength;
- K(I) is the stability constant at ionic strength I, $0 < I < 0.3$ mol L^{-1};
- K_0 is the stability constant at $I = 0$ mol L^{-1};
- A is the Debye-Hückel limiting constant, which is temperature dependent (at 298.15 K and 10^5 Pa, A = 0.5091) (see Grenthe *et al.* 1992); and
- Δz^2 is the sum of squares of charges of products minus the sum of squares of charges of reactants.

A fundamental property of any stability constant database is that all entries in the database should be derived from original source measurements using the same method (Chandratillake and Robinson 1990). Owing to the scarcity of published information relating to activity coefficient (γ) correction methods in saline solutions, and an inherent inability to estimate relevant parameters where data are lacking, a decision was made to base corrections to infinite dilution on the Davies Equation. To minimise gross errors in more saline waters, activity coefficients (γ) were assumed to remain constant at ionic strengths above 0.3 mol L^{-1}. Hence, all relevant data measured at $I > 0.3$ mol L^{-1} were corrected to infinite dilution using the Truncated Davies

Equation (TDE) (Chandratillake and Robinson 1990; Bruno *et al.* 1993).

The TDE minimises errors introduced by employing the standard Davies Equation at $I > 0.3$ mol L^{-1}. In fact, the TDE (equation 3) comprises the standard Davies Equation for $I < 0.3$ mol L^{-1} and a linear expression for $I > 0.3$ mol L^{-1}:

$$\log \gamma = -A(0.3539\Delta z^2 - 0.09) \qquad [3]$$

where:

- γ is the activity coefficient; and
- A and Δz^2 are as in equation 2.

The TDE has a number of operational advantages over more complex methods such as Pitzer equations (Pitzer 1973) and the specific ion interaction theory (Grenthe *et al.* 1992). These are discussed at length by Chandratillake and Robinson (1990) and Bruno *et al.* (1993). The TDE appears to work well for all common ions in dilute solutions (Chandratillake and Robinson 1990) but, more importantly, may be applied in a consistent manner for all species in the database. This approach has also been adopted for other database compilations (e.g. CHEMVAL; Falck *et al.* 1996). The uncertainty (error) introduced by correcting data from an ionic strength of 0.1–0.3 mol L^{-1} to infinite dilution by the standard Davies Equation (Davies 1962), or assuming that activity coefficients (γ) remain constant above $I = 0.3$ mol L^{-1} (the TDE approach), is often minimal in comparison to the uncertainty associated with the mean value of a particular stability constant. The TDE was considered a pragmatic approach for a relatively short-term study such as this.

Notwithstanding the above discussion, there is little theoretical justification for the TDE (Chandratillake and Robinson 1990). More rigorous methods that can be consistently implemented are currently being sought. From a theoretical standpoint, the preferred method would be the development of Pitzer equations (Elizalde and Aparicio 1995; Millero and Pierrot 1998). However, the body of data available for the necessary interaction parameters is limited (Anderegg and Kholeif 1994), but is steadily improving (Millero and Pierrot 1998). Extrapolation techniques for correcting stability constants to infinite dilution have been reviewed by Anderegg and Kholeif (1994), Daniele *et al.* (1997) and Grenthe and Plyasunov (1997).

3.4 Equilibrium reactions

The forms of the various chemical reactions, as required by the HARPHRQ geochemical speciation code, are detailed below. Other geochemical codes (e.g. MINTEQA2) do not necessarily use this form.

3.4.1 Stability constants

Stability constants are based on the general equilibrium (charges are omitted for brevity):

$$_{p}M + {}_{(q-t)}H + {}_{r}L1 + {}_{s}L2 + {}_{t}H_2O \Leftrightarrow M_pH_qL1_rL2_s\,(OH)_t\,(aq) \qquad [4]$$

where:

- M is the cation in the complex;
- H is the proton;
- L1 and L2 are the first and second ligands, respectively, in the complex;
- H_2O is water;
- p, q, r, s and t are stoichiometric coefficients;
- three, at most, of the stoichiometric coefficients may simultaneously be zero; and

- q and t cannot simultaneously be non-zero.

The corresponding stability constant is defined as:

$$K = \frac{[M_wH_qL1_rL2_s(OH)_t(aq)]}{[M]^p[H]^{q-t}[L1]^r[L2]^s} \qquad [5]$$

3.4.2 Redox constants

Redox constants are based on the general equilibrium:

(i) Acid media:

$$v[OxH_tO_s]^{y+} + [2(vs-uz) + (uw-vt)]H^+ + [(vy-ux) + 2(vs-uz) + (uw-vt)]e^-$$
$$\Leftrightarrow u[RedH_wO_z]^{x+} + (vs-uz)H_2O \qquad [6]$$

(ii) Alkaline media:

$$v[OxH_tO_s]^{y+} + [(vs-uz) + (uw-vt)]H_2O + [(vy-ux) + 2(vs-uz) + (uw-vt)]e^-$$
$$\Leftrightarrow u[RedH_wO_z]^{x+} + [2(vs-uz) + (uw-vt)]OH^- \qquad [7]$$

where:

- Red is the reduced element;
- Ox is the oxidised element;
- H is hydrogen;
- H^+ is the proton;
- H_2O is water;
- O is oxygen;
- OH^- is hydroxide;
- e^- is the electron;
- s, t, u, v, w and z are stoichiometric coefficients;
- four, at most, of the stoichiometric coefficients may simultaneously be zero; and
- x and y are the charge of the reduced and oxidised species, respectively ($x \geq 1$ and $y \geq 1$; only cationic species have two oxidation states in the database under consideration).

The corresponding redox constant is defined as:

(i) Acid media:

$$K = \frac{[\{RedH_wO_z\}^{x+}]^u}{[\{OxH_tO_s]^{y+}]^v[H^+]^{\{2(vs-uz) + (uw-vt)\}}} \qquad [8]$$

(ii) Alkaline media:

$$K = \frac{[\{RedH_wO_z\}^{x+}]^u[OH^-]^{\{2(vs-uz) + (uw-vt)\}}}{[\{OxH_tO_s\}^{y+}]^v} \qquad [9]$$

The stability constant of an oxidised species may also be obtained by combining the general equilibrium form given in Section 3.4.1 with one of (i) or (ii) given in Section 3.4.2. For example, $Fe^{3+} + H_2O \Leftrightarrow Fe(OH)_2^{2+} + H^+$ can be combined with $Fe^{2+} \Leftrightarrow Fe^{3+} + e^-$ to form the overall equation $Fe^{2+} + H_2O \Leftrightarrow Fe(OH)_2^{2+} + H^+ + e^-$.

3.4.3 Solubility constants

Solubility constants are based on the general equilibrium (charges are omitted for brevity):

$$M1_pM2_qH_rL_sL2_t\,(OH)(s) + (u\text{-}r)H \Leftrightarrow pM1 + qM2 + sL1 + tL2 + uH_2O \qquad [10]$$

where:

- M1 and M2 are the first and second cations, respectively, in the solid;
- H is hydrogen;
- L1 and L2 are the first and second ligands, respectively, in the solid;
- OH is hydroxide;
- H_2O is water;
- p, q, r, s, t and u are stoichiometric coefficients;
- four, at most, of the stoichiometric coefficients may simultaneously be zero; and
- r and u cannot simultaneously be non-zero.

The corresponding solubility constant is defined as:

$$K = \frac{[M1]^p[M2]^q[L1]^s[L2]^t}{[M1_pM2_qH_rL1_sL2_t(OH)(s)][H]^{(u\text{-}r)}} \qquad [11]$$

Examples of this general equilibrium form include the dissolution of brushite ($CaHPO_4{\cdot}2H_2O \Leftrightarrow Ca^{2+} + HPO_4^{2-} + 2H_2O$) and dolomite ($CaMg(CO_3)_2 \Leftrightarrow Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$).

3.5 Estimation of stability constants

The compilation of selected stability constants given in Section 3.6 represent an effort to produce a consistent and critically reviewed database that is internationally acceptable and useful in the field of environmental science. However, an inherent problem with such compilations is that, in some areas, data are limited, uncertain, and non-existent, often due to difficulties and limitations in experimental techniques used to acquire stability constants. This situation could be rectified by further measurements of stability constants to fill data gaps, but this would be an onerous task for even the simplest experimental system. For this reason, accurate and reliable methods for estimating uncertain and unmeasured stability constants were required for several key metals of interest in environmental studies, with a variety of inorganic and organic ligands. A comprehensive review of historical and extant methods for estimating stability constants is provided by Dimmock *et al.* (1995) and Hancock (1997).

Two independent methods were used to estimate stability constants in this study, namely:

(i) UTMIC; and
(ii) LFER.

The theory and practical application of both methods are comprehensively described elsewhere (UTMIC: Brown and Sylva 1987; Brown and Wanner 1987; Brown 1989; LFER: Irving and Rossotti 1956; Nieboer and McBryde 1973; Marsicano and Hancock 1978; Hummel 1993; Dimmock *et al.* 1995). In summary, the UTMIC estimates a stability constant based on chemical and physical properties of the reacting metal ion and ligand. This approach introduces the principle of electronicity (the freeness of the valance electrons) (Brown and Sylva 1987), in developing the unified theory, which describes quantitatively the ability of a ligand to complex a metal ion. The UTMIC quantifies the earlier concepts of hard and soft acids and bases on one scale. The exploitation of the fundamental nature of the electronicity of metal ions and ligands requires the invocation of a remarkably small number of parameters (**Table 4**) considering the universal nature of its application. Brown and coworkers (Brown and Sylva 1987; Brown and Wanner 1987; Brown 1989) showed excellent agreement between measured and estimated stability constants for a wide range of metal complexes with inorganic ligands.

Table 4. Chemical and physical parameters† used to estimate stability constants using the unified theory of metal ion complexation (UTMIC)

Metal	z_M	r_M^A	$g(n)$	n	D	d	S	g_1	g_2	z_M/r_M^2	$g_1(z_M/r_M^2 + g_2)$
Mn	2	0.83	1	3	1	5	0	8	0	2.90	23.2
Pb	2	0.99	1	5	1	0	1	10.2	1	2.04	31
Zn	2	0.75	1	3	1	10	0	8	-1	3.56	20.5
Cu	2	0.62	1	3	1	9	0	8	-0.8	5.20	35.2
Co	2	0.75	1	3	1	7	0	8	-0.4	3.56	25.3
Ni	2	0.69	1	3	1	8	0	8	-0.6	4.2	28.8
La	3	1.18	1	5	1	0	0	10	2	2.15	41.5
Sm	3	1.09	1	5	1	0	0	10	2	2.52	45.2
Eu	3	1.07	1	5	1	0	0	10	2	2.62	46.2
Gd	3	1.06	1	5	1	0	0	10	2	2.67	46.7
Cd	2	0.97	1	4	1	10	0	8	0.5	2.13	21.0
Fe(II)	2	0.78	1	3	1	6	0	8	-0.2	3.29	24.7
Fe(III)	3	0.65	1	3	1	5	0	10	0	7.10	71.0
U(VI)	2	0.63^B	1	6	1	0	0	8	1	5.02	48.1

† The parameters are defined as follows:

- z_M is the charge of the metal ion;
- r_M is the ionic radius of the metal ion;
- $g(n)$ is the Slater function: $g(n) = 1$ if n, the principal quantum number is greater than unity, otherwise $g(n) = 0$;
- $D = 1$ if *d*-orbitals are available for bonding (otherwise $D = 0$);
- d is the number of *d*-electrons in the outermost shell of the ion;
- S depends on the absence ($S = 0$) or presence ($S = 1$) of *s*-electrons in the outermost shell of the metal ion (those ions possess the inert pair of electrons);
- $g_1 = (1 + \varepsilon_L^2 S + D)(z_M + 2)$, where ε_L is the electronicity of the ligand ($\varepsilon_L = 0.74$ for citric and tricarballylic acids);
- $g_2 = g(n)(z_M - 1) - 0.05d[(\gamma - 1)(\varepsilon_L^4 - 3) - 1][n - (3 + 2\gamma)]^2(1 - \gamma z_M)(1 - S)$ where γ is termed the ligand parameter and has a value of zero when the corresponding acids of the ligands are binary acids, and unity when they are oxy-acids.

A Ionic radii (r_M) were taken from Shannon (1976)

B Effective ionic radius of U(VI) when reacting with citric and tricarballylic acids (see Brown and Wanner 1987)

Alternatively, it has often been noted that the logarithms of the stability constants (log K) of complexes of similar structure can be related linearly, and such correlations are defined as LFER. The validity of such correlations has been examined both experimentally and theoretically and are well accepted (see reviews by Dimmock *et al.* (1995) and Hancock (1997)). Linear free energy relationships are very useful for interpolation and comparative evaluation; they aim to convert qualitative ideas to quantitative theories of reactivity. Irving and Rossotti (1956), in rationalising the LFER, concluded there were three types:

(i) where the stability constants of the complexes of one metal ion and those of the proton, with a series of ligands, are compared (log K_{ML} is compared to log K_{HL});

(ii) where the stability constants of the complexes of two metal ions with a series of ligands are compared (log K_{M1L} is compared to log K_{M2L}); and

(iii) where the stability constants of the complexes of two ligands with a series of metal ions are compared (log K_{ML1} as compared to log K_{ML2}).

All three types of LFER have received extensive experimental and theoretical verification (Irving and Rossotti 1956; Nieboer and McBryde 1973; Marsicano and Hancock 1978; Hummel 1993; Dimmock *et al.* 1995).

Stability constants were estimated for both inorganic and organic metal complexes using the UTMIC and LFER. Those estimated exclusively in this study are shown in **Table 5**. These estimates were based on the results of simple linear regression analyses, using both the UTMIC and LFER, and are shown in **Figs 3–10**. The general agreement between the two methods (when available) was very good (**Table 5**). Furthermore, this agreement enhances the veracity of stability constants that could only be estimated using LFER (**Table 5**). Stability constants used in the LFER were acquired from an internally consistent database (Smith *et al.* 1998). The results of the present study provide a sound rationale for the use of both methods in estimating uncertain or unmeasured stability constants.

Table 5. Stability constants estimated using the unified theory of metal ion complexation (UTMIC) and/or linear free energy relationships (LFER)

Metal species	Estimate of log K_o		
	UTMIC	LFER	Mean value (where relevant)
$UO_2(OH)Cit^{2-}$	4.73	4.76	**4.75**
$(UO_2)_2(OH)_2(Cit)_2{}^{4-}$		11.85	**11.85**
$Mn(OH)Mal^-$		-4.27	**-4.27**
$Cu(OH)Mal^-$		-0.34	**-0.34**
$Cd(OH)Mal^-$		-4.86	**-4.86**
MnHTri	8.88	8.73	**8.81**
$Mn(OH)Tri^{2-}$		-4.16	**-4.16**
UO_2Tri^-	6.29	6.35	**6.32**
UO_2HTri	10.73	10.74	**10.74**
$UO_2(OH)Tri^{2-}$		0.33	**0.33**
$CdTri^-$	3.37	3.51	**3.44**
CdHTri	8.71	8.73	**8.72**
$Cd(OH)Tri^{2-}$		-4.16	**-4.16**
$Cu(OH)Tri^{2-}$		-1.77	**-1.77**

A worked example of how stability constants were estimated using each method is described as follows. **Figure 9** provides an example of the UTMIC method, where a simple linear regression is fitted between $g_1(z/r^2+ g_2)$ and 1:1 metal tricarballylate complexes (MTri). The stability constant of uranyl tricarballylate (UO_2Tri^-) (6.29 or -2.75 when converted to the HARPHRQ code format by subtracting 9.04; see **Tables 11 and 12**), was estimated by substituting the value of $g_1(z/r^2+ g_2)$ for uranyl (48.1), derived using the ionic radii (r_M) of uranyl reacting with tricarballylic acid (see **Table 4** and Brown and Wanner (1987)), into the fitted linear regression equation.

Figure 8 provides an example of the LFER approach, where a simple linear regression is fitted between 1:1 copper-di- and tri-carboxylate complexes (CuL) and the corresponding uranyl complexes (UO_2L). The selected value for the stability constant of copper tricarballylate ($CuTri^-$) was substituted into the fitted linear regression equation to give an estimated value of 6.35 (or -2.69, see **Table 20**) for the stability constant of uranyl tricarballyate (UO_2Tri^-). This value was very similar to that estimated using the UTMIC method (6.29, see above example). Hence, a mean value of 6.32 (or -2.72) was selected for this study (**Table 5**). Copper di- and tri-carboxylate complexes were used in the LFER regression because they provided an abundant and internally consistent source of data relative to other metals. Using the same rationale, Zn was selected as a regressor to estimate cadmium tricarballylate ($CdTri^-$) (**Fig. 10**); Zn was selected because it has similar physicochemical properties to Cd (both Group 12 metals).

The estimation of stability constants for uncertain or unmeasured metal complexes does not necessarily imply that they form. However, the formation of metal complexes analogous to those that have been estimated would suggest their existence (e.g. $CdTri^-$, CdHTri), and verify that they do indeed form, based on the predictions of the HARPHRQ code under the prescribed experimental conditions. The UTMIC and LFER provide a more practical approach for determining the stability constant of a metal complex, based on the stoichiometry of the species and the electronic properties of the reacting ions, than experimentally verifying whether a given metal complex actually exists in solution.

3.6 Stability constant database

Selected stability constants for H, Na, Ca, Mg, Mn, Fe, Al, U, Pb, Zn, Cu and Cd are given in **Tables 6–20**, respectively, for inorganic and organic complexes and minerals.

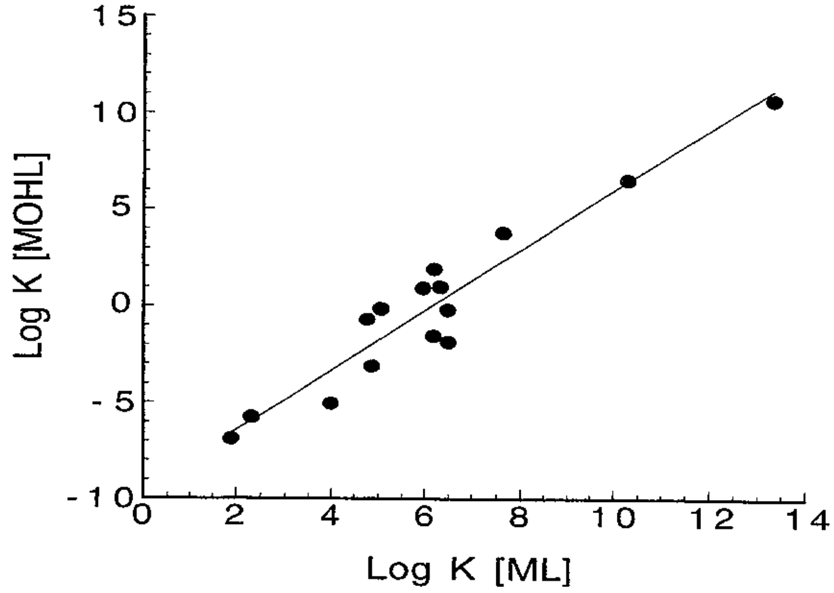

Figure 3. Linear free energy relationship (LFER) showing the log K of 1:1 metal di- and tri-carboxylate complexes [ML] regressed against the corresponding log K of 1:1:1 metal hydroxy di- and tri-carboxylate complexes [M(OH)L]. The regression equation is log K [M(OH)L] = 1.559log K [ML] - 9.523; $r^2 = 0.915$, $P \leq 0.001$, n = 15.

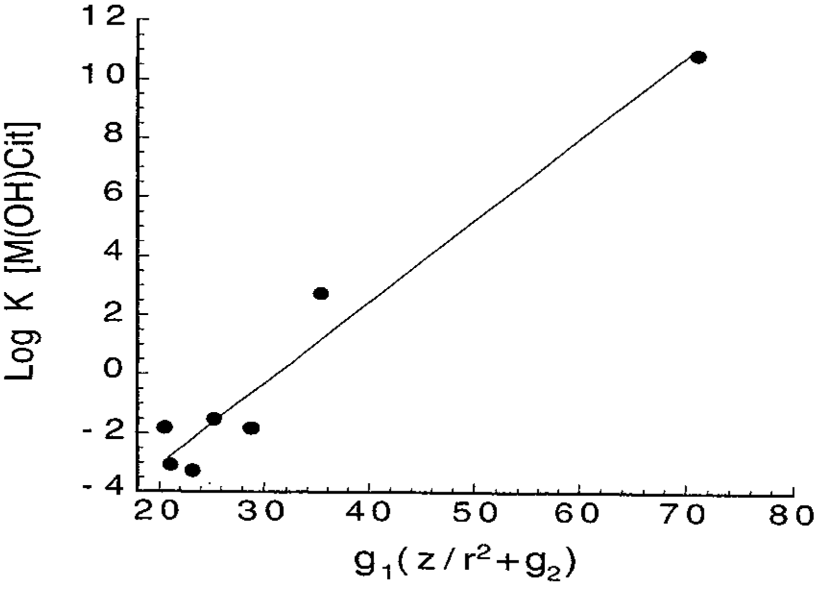

Figure 4. Simple linear regression showing the log K of 1:1:1 metal hydroxy-citrate complexes [M(OH)Cit] versus the corresponding function $[g_1(z/r^2 + g_2)]$ for each metal derived using the unified theory of metal ion complexation (UTMIC) (see **Table 5**). The regression equation is log K [M(OH)Cit] = $0.278[g_1(z/r^2 + g_2)] - 8.627$; $r^2 = 0.958$, $P \leq 0.001$, n = 7.

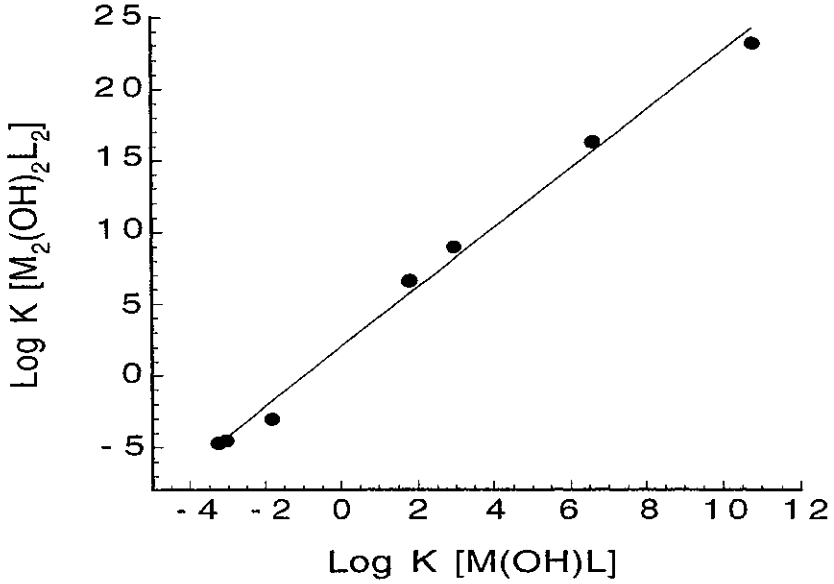

Figure 5. Linear free energy relationship (LFER) showing the log K of 1:1:1 metal hydroxy di- and tri-carboxylate complexes [M(OH)L] regressed against the corresponding log K of 2:2:2 metal hydroxy di- and tri-carboxylate complexes [$M_2(OH)_2L_2$]. The regression equation is log K [$M_2(OH)_2L_2$] = 2.070log K. [M(OH)L] + 2.006; $r^2 = 0.993$, $P \leq 0.001$, n = 9.

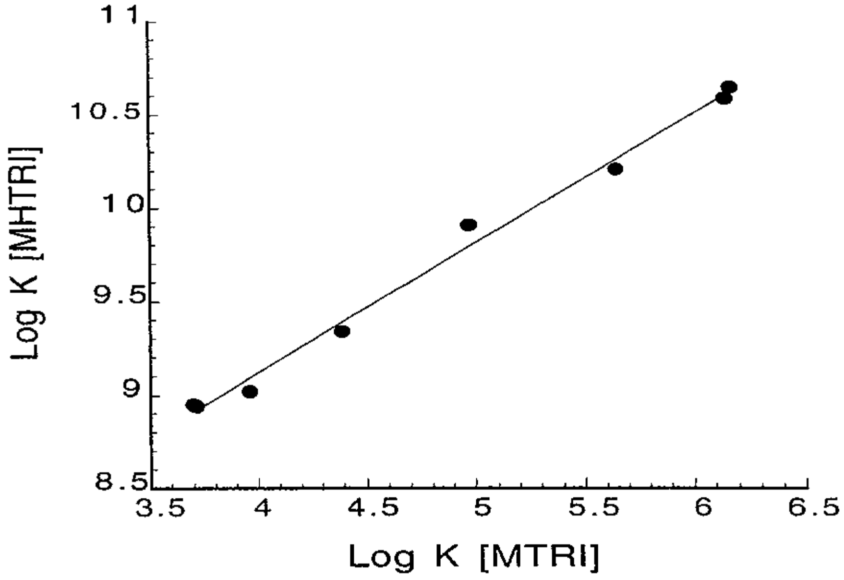

Figure 6. Linear free energy relationship (LFER) showing the log K of 1:1 metal tricarballylate complexes [MTri] regressed against the corresponding log K of 1:1:1 metal hydrogen tricarballylate complexes [MHTri]. The regression equation is log K [MHTri] = 0.696log K [MTri] + 6.336; $r^2 = 0.993$, $P \leq 0.001$, n = 8.

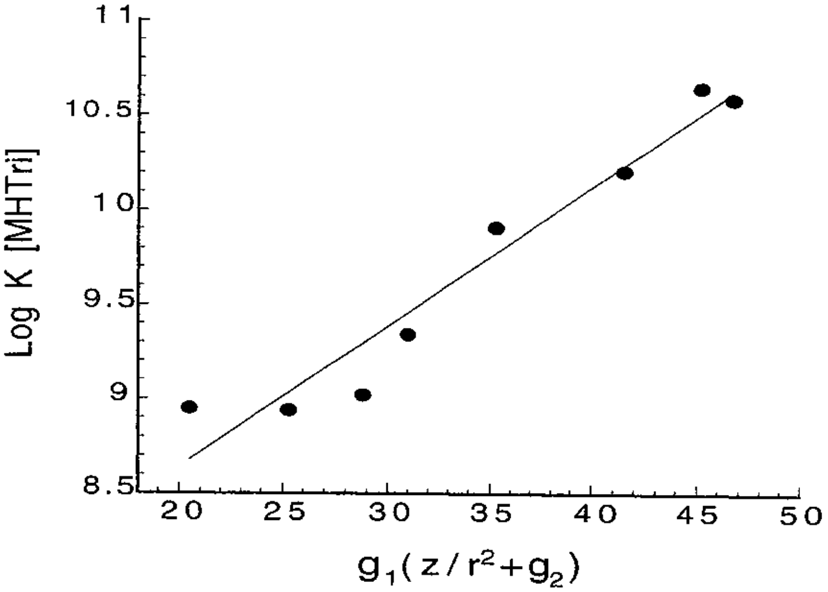

Figure 7. Simple linear regression showing the log K of 1:1:1 metal hydrogen tricarballylate complexes [MHTri] versus the corresponding function [$g_1(z/r^2 + g_2)$] for each metal derived using the unified theory of metal ion complexation (UTMIC) (see **Table 5**). The regression equation is log K [MHTri] = 0.074[$g_1(z/r^2 + g_2)$] + 7.154; $r^2 = 0.944$, $P \leq 0.001$, n = 8.

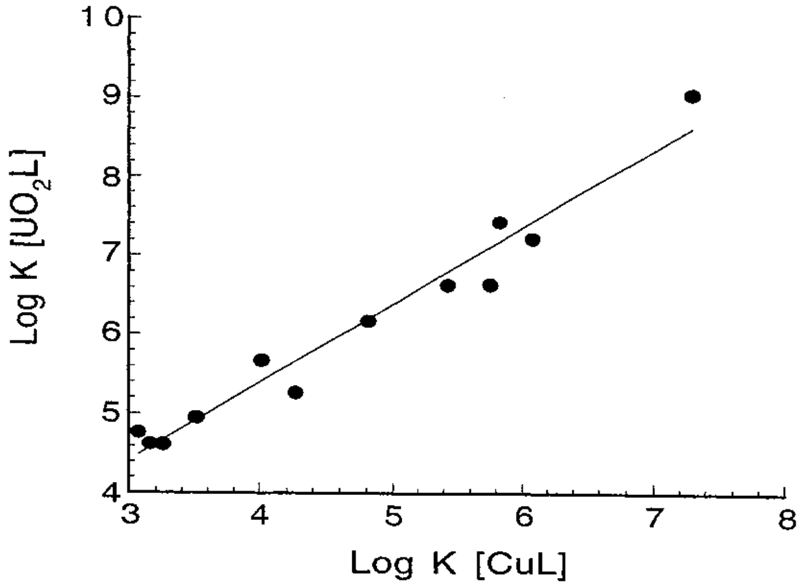

Figure 8. Simple linear regression showing the log K of 1:1 copper di- and tri-carboxylate complexes [CuL] versus the corresponding log K of 1:1 uranyl di- and tri-carboxylate complexes [UO_2L]. The regression equation is log K [UO_2L] = 0.981log K [CuL] + 1.470; $r^2 = 0.959$, $P \leq 0.001$, n = 12.

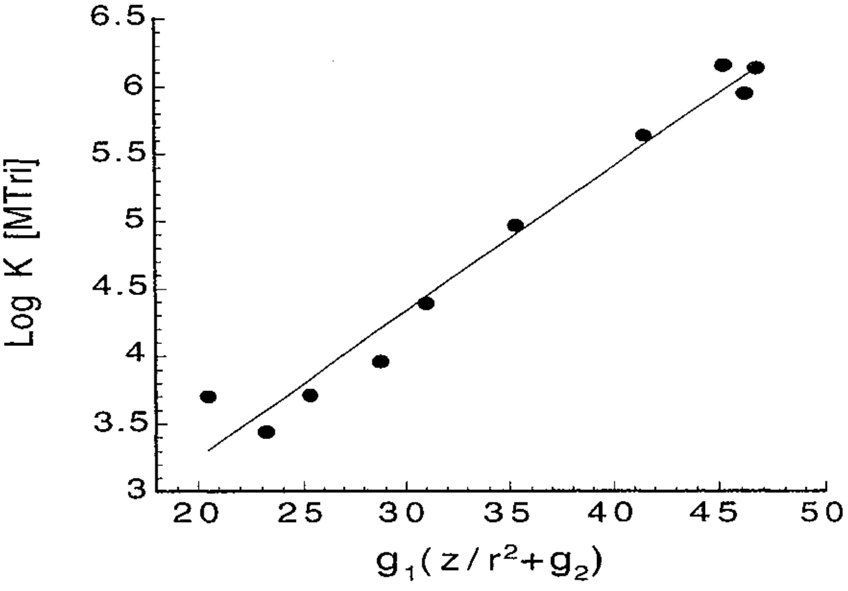

Figure 9. Simple linear regression showing the log K of 1:1 metal tricarballylate complexes [MTri] versus the corresponding function $[g_1(z/r^2 + g_2)]$ for each metal derived using the unified theory of metal ion complexation (UTMIC) (see **Table 5**). The regression equation is log K [MTri] = $0.108[g_1(z/r^2 + g_2)] + 1.098$; $r^2 = 0.971$, $P \leq 0.001$, n = 10.

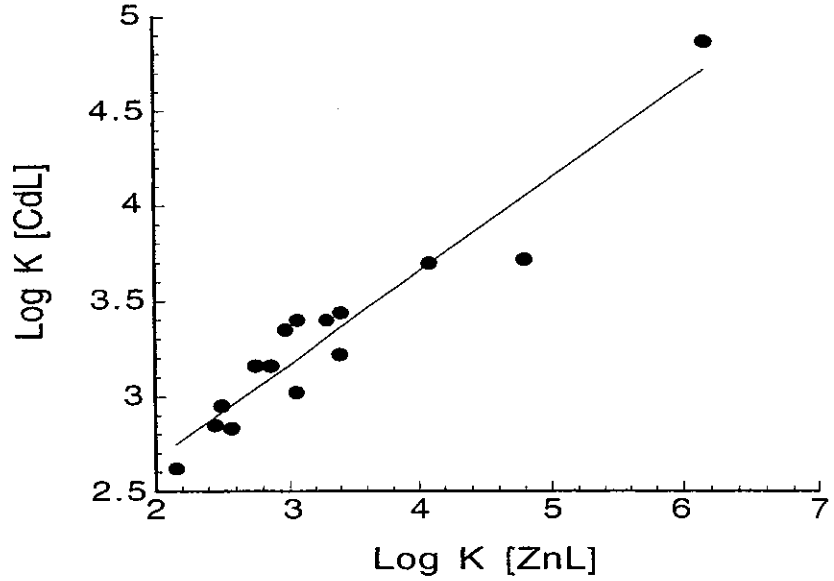

Figure 10. Linear free energy relationship (LFER) showing the log K of 1:1 zinc di- and tri-carboxylate complexes [ZnL] regressed against the corresponding log K of 1:1 cadmium di- and tri-carboxylate complexes [CdL]. The regression equation is log K [CdL] = 0.493log K [ZnL] + 1.686; $r^2 = 0.917$, $P \leq 0.001$, n = 15.

Table 6. Selected stability constants for hydrogen (H^+) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
OH^-	$H_2O \leftrightarrow H^+ + OH^-$	-13.998	Nordstrom and Munoz (1994)
HCl	$H^+ + Cl^- \leftrightarrow HCl$	-2.67	Petkovic (1982)
HSO_4^-	$H^+ + SO_4^{2-} \leftrightarrow HSO_4^-$	1.99	De Robertis *et al.* (1994)
HNO_3	$H^+ + NO_3^- \leftrightarrow HNO_3$	-2.19	Petkovic (1982)
HCO_3^-	$H^+ + CO_3^{2-} \leftrightarrow HCO_3^-$	10.33	Nordstrom and Munoz (1994)
H_2CO_3	$2H^+ + CO_3^{2-} \leftrightarrow H_2CO_3$	16.68	Nordstrom and Munoz (1994)
HPO_4^{2-}	$H^+ + PO_4^{3-} \leftrightarrow HPO_4^{2-}$	12.35	Grenthe *et al.* (1992)
$H_2PO_4^-$	$2H^+ + PO_4^{3-} \leftrightarrow H_2PO_4^-$	19.56	Grenthe *et al.* (1992)
H_3PO_4	$3H^+ + PO_4^{3-} \leftrightarrow H_3PO_4$	21.70	Grenthe *et al.* (1992)
Organic complexes			
$HAsp^-$	$H^+ + Asp^{2-} \leftrightarrow HAsp^-$	10.06	A
H_2Asp	$2H^+ + Asp^{2-} \leftrightarrow H_2Asp$	14.02	A
$HCit^{2-}$	$H^+ + Cit^{3-} \leftrightarrow HCit^{2-}$	6.37	A
H_2Cit^-	$2H^+ + Cit^{3-} \leftrightarrow H_2Cit^-$	11.16	A
H_3Cit	$3H^+ + Cit^{3-} \leftrightarrow H_3Cit$	14.29	A
$HMal^-$	$H^+ + Mal^{2-} \leftrightarrow HMal^-$	5.69	A
H_2Mal	$2H^+ + Mal^{2-} \leftrightarrow H_2Mal$	8.56	A

A Selected value was derived from a critical evaluation of data, obtained from publications listed in the bibliography of Smith *et al.* (1998), using the criteria outlined by Wanner (1991), Fuger *et al.* (1992) and Smith and Martell (1995)

Table 6 (cont.). Selected stability constants for hydrogen (H^+) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$HSal^-$	$H^+ + Sal^{2-} \leftrightarrow HSal^-$	13.79	A
H_2Sal	$2H^+ + Sal^{2-} \leftrightarrow H_2Sal$	16.83	A
$HTri^{2-}$	$H^+ + Tri^{3-} \leftrightarrow HTri^{2-}$	6.49	Section 5
H_2Tri^-	$2H^+ + Tri^{3-} \leftrightarrow H_2Tri^-$	11.37	Section 5
H_3Tri	$3H^+ + Tri^{3-} \leftrightarrow H_3Tri$	15.00	Section 5
Gases			
CO_2 (g)	$H_2O + CO_2 (g) \leftrightarrow H_2CO_3$	-1.47	Nordstrom and Munoz (1994)

A Selected value was derived from a critical evaluation of data, obtained from publications listed in the bibliography of Smith *et al.* (1998), using the criteria outlined by Wanner (1991), Fuger *et al.* (1992) and Smith and Martell (1995)

Table 7. Selected stability constants for sodium (Na^+) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
NaOH	$Na^+ + H_2O \leftrightarrow NaOH + H^+$	-14.08	De Robertis *et al.* (1994)
NaCl	$Na^+ + Cl^- \leftrightarrow NaCl$	-0.48	De Robertis *et al.* (1995)
$NaSO_4^-$	$Na^+ + SO_4^{2-} \leftrightarrow NaSO_4^-$	0.74	De Robertis *et al.* (1994)
Na_2SO_4	$2Na^+ + SO_4^{2-} \leftrightarrow Na_2SO_4$	0.81	Fisher (1975)
$NaHSO_4$	$Na^+ + H^+ + SO_4^{2-} \leftrightarrow NaHSO_4$	1.29	Dickson and Whitfield (1981)
$NaNO_3$	$Na^+ + NO_3^- \leftrightarrow NaNO_3$	-0.55	Smith *et al.* (1998)
$NaCO_3^-$	$Na^+ + CO_3^{2-} \leftrightarrow NaCO_3^-$	1.27	Smith *et al.* (1998)
$NaHCO_3$	$Na^+ + H^+ + CO_3^{2-} \leftrightarrow NaHCO_3$	10.45	De Robertis *et al.* (1995)
$NaPO_4^{2-}$	$Na^+ + PO_4^{3-} \leftrightarrow NaPO_4^{2-}$	1.43	De Stefano *et al.* (1998)
$NaHPO_4^-$	$Na^+ + H^+ + PO_4^{3-} \leftrightarrow NaHPO_4^-$	13.42	De Stefano *et al.* (1998)
NaH_2PO_4	$Na^+ + 2H^+ + PO_4^{3-} \leftrightarrow NaH_2PO_4$	19.84	De Stefano *et al.* (1998)
$Na_2PO_4^-$	$2Na^+ + PO_4^{3-} \leftrightarrow Na_2PO_4^-$	2.59	De Stefano *et al.* (1998)
Na_2HPO_4	$Na^+ + H^+ + PO_4^{3-} \leftrightarrow Na_2HPO_4$	13.34	De Stefano *et al.* (1998)
$NaKPO_4^-$	$Na^+ + K^+ + PO_4^{3-} \leftrightarrow NaKPO_4^-$	2.75	De Stefano *et al.* (1998)
Organic complexes			
$NaAsp^-$	$Na^+ + Asp^{2-} \leftrightarrow NaAsp^-$	0.42	De Stefano *et al.* (1995)
NaHAsp	$Na^+ + H^+ + Asp^{2-} \leftrightarrow NaHAsp$	9.75	De Stefano *et al.* (1995)
$NaCit^{2-}$	$Na^+ + Cit^{3-} \leftrightarrow NaCit^{2-}$	1.49	Section 5
Na_2Cit^-	$2Na^+ + Cit^{3-} \leftrightarrow Na_2Cit^-$	2.47	Section 5

Table 7 (cont.). Selected stability constants for sodium (Na^+) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$NaHCit^-$	$Na^+ + H^+ + Cit^{3-} \leftrightarrow NaHCit^-$	7.34	Section 5
NaH_2Cit	$Na^+ + 2H^+ + Cit^{3-} \leftrightarrow NaH_2Cit$	11.58	Section 5
Na_2HCit	$2Na^+ + H^+ + Cit^{3-} \leftrightarrow Na_2HCit$	7.0	De Stefano *et al.* (1999)
$NaKCit^-$	$Na^+ + K^+ + Cit^{3-} \leftrightarrow NaKCit^-$	2.47	De Stefano *et al.* (1999)
$NaKHCit$	$Na^+ + K^+ + H^+ + Cit^{3-} \leftrightarrow NaKHCit$	7.3	De Stefano *et al.* (1999)
$NaMal^-$	$Na^+ + Mal^{2-} \leftrightarrow NaMal^-$	0.82	Section 5
$NaHMal$	$Na^+ + H^+ + Mal^{2-} \leftrightarrow NaHMal$	5.66	Daniele *et al.* (1985a)
$NaSal^-$	$Na^+ + Sal^{2-} \leftrightarrow NaSal^-$	-0.07	Daniele *et al.* (1985a)
$NaHSal$	$Na^+ + H^+ + Sal^{2-} \leftrightarrow NaHSal$	13.81	Daniele *et al.* (1985a)
$NaTri^{2-}$	$Na^+ + Tri^{3-} \leftrightarrow NaTri^{2-}$	1.40	De Stefano *et al.* (1994)
$NaHTri^-$	$Na^+ + H^+ + Tri^{3-} \leftrightarrow NaHTri^-$	7.31	De Stefano *et al.* (1994)
NaH_2Tri	$Na^+ + 2H^+ + Tri^{3-} \leftrightarrow NaH_2Tri$	11.56	De Stefano *et al.* (1994)
Na_2Tri^-	$2Na^+ + Tri^{3-} \leftrightarrow Na_2Tri^-$	1.98	De Stefano *et al.* (1994)
Na_2HTri	$2Na^+ + H^+ + Tri^{3-} \leftrightarrow Na_2HTri$	6.96	De Stefano *et al.* (1994)

Table 8. Selected stability constants for potassium (K^+) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
KOH	$K^+ + H_2O \leftrightarrow KOH + H^+$	-14.18	De Robertis *et al.* (1995)
KCl	$K^+ + Cl^- \leftrightarrow KCl$	-0.42	De Robertis *et al.* (1995)
KSO_4^-	$K^+ + SO_4^{2-} \leftrightarrow KSO_4^-$	0.85	De Robertis *et al.* (1994)
K_2SO_4	$2K^+ + SO_4^{2-} \leftrightarrow K_2SO_4$	0.96	Fisher and Fox (1978)
KNO_3	$K^+ + NO_3^- \leftrightarrow KNO_3$	-0.18	Smith *et al.* (1998)
KPO_4^{2-}	$K^+ + PO_4^{3-} \leftrightarrow KPO_4^{2-}$	1.37	De Stefano *et al.* (1998)
$KHPO_4^-$	$K^+ + H^+ + PO_4^{3-} \leftrightarrow KHPO_4^-$	13.23	De Stefano *et al.* (1998)
KH_2PO_4	$K^+ + 2H^+ + PO_4^{3-} \leftrightarrow KH_2PO_4$	19.82	De Stefano *et al.* (1998)
$K_2PO_4^-$	$2K^+ + PO_4^{3-} \leftrightarrow K_2PO_4^-$	2.20	De Stefano *et al.* (1998)
K_2HPO_4	$K^+ + H^+ + PO_4^{3-} \leftrightarrow K_2HPO_4$	13.46	De Stefano *et al.* (1998)
$NaKPO_4^-$	$Na^+ + K^+ + PO_4^{3-} \leftrightarrow NaKPO_4^-$	2.75	De Stefano *et al.* (1998)
Organic complexes			
$KCit^{2-}$	$K^+ + Cit^{3-} \leftrightarrow KCit^{2-}$	1.33	Section 5
K_2Cit^-	$2K^+ + Cit^{3-} \leftrightarrow K_2Cit^-$	2.05	Section 5
$KHCit^-$	$K^+ + H^+ + Cit^{3-} \leftrightarrow KHCit^-$	7.00	Section 5
KH_2Cit	$K^+ + 2H^+ + Cit^{3-} \leftrightarrow KH_2Cit$	11.22	Section 5
$NaKCit^-$	$Na^+ + K^+ + Cit^{3-} \leftrightarrow NaKCit^-$	2.47	De Stefano *et al.* (1999)
K_2HCit	$2K^+ + H^+ + Cit^{3-} \leftrightarrow K_2HCit$	7.0	De Stefano *et al.* (1999)
NaKHCit	$Na^+ + K^+ + H^+ + Cit^{3-} \leftrightarrow NaKHCit$	7.3	De Stefano *et al.* (1999)

Table 8 (cont.). Selected stability constants for potassium (K^+) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$KMal^-$	$K^+ + Mal^{2-} \leftrightarrow KMal^-$	0.90	Section 5
$KHMal$	$K^+ + H^+ + Mal^{2-} \leftrightarrow KHMal$	5.82	Daniele *et al.* (1985a)
$KSal^-$	$K^+ + Sal^{2-} \leftrightarrow KSal^-$	-0.07	Daniele *et al.* (1985a)
$KHSal$	$K^+ + H^+ + Sal^{2-} \leftrightarrow KHSal$	13.81	Daniele *et al.* (1985a)
$KTri^{2-}$	$K^+ + Tri^{3-} \leftrightarrow KTri^{2-}$	1.39	De Stefano *et al.* (1994)
$KHTri^-$	$K^+ + H^+ + Tri^{3-} \leftrightarrow KHTri^-$	7.27	De Stefano *et al.* (1994)
KH_2Tri	$K^+ + 2H^+ + Tri^{3-} \leftrightarrow KH_2Tri$	11.50	De Stefano *et al.* (1994)
K_2Tri^-	$2K^+ + Tri^{3-} \leftrightarrow K_2Tri^-$	1.75	De Stefano *et al.* (1994)
K_2HTri	$2K^+ + H^+ + Tri^{3-} \leftrightarrow K_2HTri$	6.66	De Stefano *et al.* (1994)

Table 9. Selected stability constants for calcium (Ca^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$CaOH^+$	$Ca^{2+} + H_2O \leftrightarrow CaOH^+ + H^+$	-12.72	De Robertis *et al.* (1994)
$CaCl^+$	$Ca^{2+} + Cl^- \leftrightarrow CaCl^+$	0.46	De Robertis *et al.* (1995)
$CaSO_4$	$Ca^{2+} + SO_4^{2-} \leftrightarrow CaSO_4$	2.30	De Robertis *et al.* (1994)
$CaNO_3^+$	$Ca^{2+} + NO_3^- \leftrightarrow CaNO_3^+$	0.70	De Robertis *et al.* (1995)
$CaCO_3$	$Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_3$	3.20	Smith *et al.* (1998)
$CaHCO_3^+$	$Ca^{2+} + H^+ + CO_3^{2-} \leftrightarrow CaHCO_3^+$	11.44	Nordstrom *et al.* (1990)
$Ca_2[UO_2(CO_3)_3]$	$2Ca^{2+} + U^{4+} + 2H_2O + 3CO_3^{2-} \leftrightarrow Ca_2[UO_2(CO_3)_3] + 4H^+ + 2e^-$	20.33	Bernhard *et al.* (1996)
$CaPO_4^-$	$Ca^{2+} + PO_4^{3-} \leftrightarrow CaPO_4^-$	6.46	De Stefano *et al.* (1998)
$CaHPO_4$	$Ca^{2+} + H^+ + PO_4^{3-} \leftrightarrow CaHPO_4$	15.03	De Stefano *et al.* (1998)
$Ca(HPO_4)_2^{2-}$	$Ca^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Ca(HPO_4)_2^{2-}$	27.74	May *et al.* (1977)
$CaH_2PO_4^+$	$Ca^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow CaH_2PO_4^+$	20.97	De Stefano *et al.* (1998)
$Ca(H_2PO_4)_2$	$Ca^{2+} + 4H^+ + 2PO_4^{3-} \leftrightarrow Ca(H_2PO_4)_2$	40.48	Ciavatta *et al.* (1991)
Organic complexes			
$CaAsp$	$Ca^{2+} + Asp^{2-} \leftrightarrow CaAsp$	2.51	Section 5
Ca_2Asp^{2+}	$2Ca^{2+} + Asp^{2-} \leftrightarrow Ca_2Asp^{2+}$	4.83	Blaquiere and Berthon (1987)
$CaHAsp^+$	$Ca^{2+} + H^+ + Asp^{2-} \leftrightarrow CaHAsp^+$	11.52	Section 5
CaH_2Asp^{2+}	$Ca^{2+} + 2H^+ + Asp^{2-} \leftrightarrow CaH_2Asp^{2+}$	14.60	Section 5
$CaOHAsp^-$	$Ca^{2+} + H_2O + Asp^{2-} \leftrightarrow CaOHAsp^- + H^+$	-8.51	Blaquiere and Berthon (1987)
$CaCit^-$	$Ca^{2+} + Cit^{3-} \leftrightarrow CaCit^-$	4.77	Section 5

Table 9 (cont.). Selected stability constants for calcium (Ca^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Ca(Cit)_2^{4-}$	$Ca^{2+} + 2Cit^{3-} \leftrightarrow Ca(Cit)_2^{4-}$	5.79	Section 5
CaHCit	$Ca^{2+} + H^+ + Cit^{3-} \leftrightarrow CaHCit$	9.39	Section 5
CaH_2Cit^+	$Ca^{2+} + 2H^+ + Cit^{3-} \leftrightarrow CaH_2Cit^+$	12.64	Section 5
$CaH(Cit)_2^{3-}$	$Ca^{2+} + H^+ + 2Cit^{3-} \leftrightarrow CaH(Cit)_2^{3-}$	12.11	Blaquiere and Berthon (1987)
$Ca(HCit)_2^{2-}$	$Ca^{2+} + 2H^+ + 2Cit^{3-} \leftrightarrow Ca(HCit)_2^{2-}$	18.99	Section 5
$CaOHCit^{2-}$	$Ca^{2+} + H_2O + Cit^{3-} \leftrightarrow CaOHCit^{2-} + H^+$	-7.43	Blaquiere and Berthon (1987)
$Ca(OH)_2(Cit)_2^{6-}$	$Ca^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Ca(OH)_2(Cit)_2^{6-} + 2H^+$	-11.14	Blaquiere and Berthon (1987)
$CaCitHPO_4^{3-}$	$Ca^{2+} + Cit^{3-} + H^+ + PO_4^{3-} \leftrightarrow CaCitHPO_4^{3-}$	23.93	Ramamoorthy and Manning (1975)
CaMal	$Ca^{2+} + Mal^{2-} \leftrightarrow CaMal$	2.46	Section 5
$CaHMal^+$	$Ca^{2+} + H^+ + Mal^{2-} \leftrightarrow CaHMal^+$	6.70	Section 5
CaSal	$Ca^{2+} + Sal^{2-} \leftrightarrow CaSal$	4.33	Section 5
$Ca(Sal)_2^{2-}$	$Ca^{2+} + 2Sal^{2-} \leftrightarrow Ca(Sal)_2^{2-}$	8.45	May *et al.* (1977)
$CaHSal^+$	$Ca^{2+} + H^+ + Sal^{2-} \leftrightarrow CaHSal^+$	14.34	Section 5
$CaTri^-$	$Ca^{2+} + Tri^{3-} \leftrightarrow CaTri^-$	3.33	Section 5
CaHTri	$Ca^{2+} + H^+ + Tri^{3-} \leftrightarrow CaHTri$	8.74	Section 5
CaH_2Tri^+	$Ca^{2+} + 2H^+ + Tri^{3-} \leftrightarrow CaH_2Tri^+$	12.57	Section 5
Ca_2Tri^+	$2Ca^{2+} + Tri^{3-} \leftrightarrow Ca_2Tri^+$	4.46	De Stefano *et al.* (1994)

Table 10 (cont.). Selected stability constants for magnesium (Mg^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes			
MgH_2Cit^+	$Mg^{2+} + 2H^+ + Cit^{3-} \leftrightarrow MgH_2Cit^+$	12.48	Section 5
$MgH(Cit)_2^{3-}$	$Mg^{2+} + H^+ + 2Cit^{3-} \leftrightarrow MgH(Cit)_2^{3-}$	12.11	Blaquiere and Berthon (1987)
$Mg(OH)_2Cit^{3-}$	$Mg^{2+} + 2H_2O + Cit^{3-} \leftrightarrow Mg(OH)_2Cit^{3-} + 2H^+$	-18.23	Blaquiere and Berthon (1987)
$Mg_2(OH)_2(Cit)_2^{4-}$	$2Mg^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Mg_2(OH)_2(Cit)_2^{4-} + 2H^+$	-11.67	Blaquiere and Berthon (1987)
$CuMg(OH)_2(Cit)_2^{4-}$	$Cu^{2+} + Mg^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CuMg(OH)_2(Cit)_2^{4-} + 2H^+$	-0.24	Blomqvist and Still (1984)
MgMal	$Mg^{2+} + Mal^{2-} \leftrightarrow MgMal$	2.86	Section 5
$MgHMal^+$	$Mg^{2+} + H^+ + Mal^{2-} \leftrightarrow MgHMal^+$	6.89	Section 5
MgSal	$Mg^{2+} + Sal^{2-} \leftrightarrow MgSal$	5.95	Section 5
$Mg(Sal)_2^{2-}$	$Mg^{2+} + 2Sal^{2-} \leftrightarrow Mg(Sal)_2^{2-}$	9.46	May *et al.* (1977)
$MgHSal^+$	$Mg^{2+} + H^+ + Sal^{2-} \leftrightarrow MgHSal^+$	14.87	May *et al.* (1977)
$MgTri^-$	$Mg^{2+} + Tri^{3-} \leftrightarrow MgTri^-$	3.34	Section 5
MgHTri	$Mg^{2+} + H^+ + Tri^{3-} \leftrightarrow MgHTri$	8.50	Section 5
MgH_2Tri^+	$Mg^{2+} + 2H^+ + Tri^{3-} \leftrightarrow MgH_2Tri^+$	12.48	Section 5
Mg_2Tri^+	$2Mg^{2+} + Tri^{3-} \leftrightarrow Mg_2Tri^+$	4.21	De Stefano *et al.* (1994)
Minerals			
$CaMg(CO_3)_2$ [dolomite]	$CaMg(CO_3)_2 \leftrightarrow Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	-17.09	Nordstrom *et al.* (1990)
$Mg(OH)_2$ [brucite]	$Mg(OH)_2 + 2H^+ \leftrightarrow Mg^{2+} + 2H_2O$	17.13	Brown *et al.* (1996a)
$MgCO_3$ [magnesite]	$MgCO_3 \leftrightarrow Mg^{2+} + CO_3^{2-}$	-7.46	Smith *et al.* (1998)
$MgHPO_4{\cdot}3H_2O$ [newberyite]	$MgHPO_4{\cdot}3H_2O \leftrightarrow Mg^{2+} + HPO_4^{2-} + 3H_2O$	-5.75	Brown *et al.* (1996b)

Table 11. Selected stability constants for iron (Fe^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$FeOH^+$	$Fe^{2+} + H_2O \leftrightarrow FeOH^+ + H^+$	-9.56	A
$Fe(OH)_2$	$Fe^{2+} + 2H_2O \leftrightarrow Fe(OH)_2 + 2H^+$	-20.35	A
$Fe(OH)_3^-$	$Fe^{2+} + 3H_2O \leftrightarrow Fe(OH)_3^- + 3H^+$	-32.24	A
$Fe(OH)_4^{2-}$	$Fe^{2+} + 4H_2O \leftrightarrow Fe(OH)_4^{2-} + 4H^+$	-45.18	A
$FeCl^+$	$Fe^{2+} + Cl^- \leftrightarrow FeCl^+$	0.14	Nordstrom *et al.* (1990)
$FeSO_4$	$Fe^{2+} + SO_4^{2-} \leftrightarrow FeSO_4$	2.25	Nordstrom *et al.* (1990)
$FeHSO_4^+$	$Fe^{2+} + H^+ + SO_4^{2-} \leftrightarrow FeHSO_4^+$	3.07	Nordstrom *et al.* (1990)
$FeCO_3$	$Fe^{2+} + CO_3^{2-} \leftrightarrow FeCO_3$	5.45	Bruno *et al.* (1992b)
$Fe(CO_3)_2^{2-}$	$Fe^{2+} + CO_3^{2-} \leftrightarrow Fe(CO_3)_2^{2-}$	7.17	Bruno *et al.* (1992b)
$FeHCO_3^+$	$Fe^{2+} + H^+ + CO_3^{2-} \leftrightarrow FeHCO_3^+$	11.43	Smith *et al.* (1998)
$FeHPO_4$	$Fe^{2+} + H^+ + PO_4^{3-} \leftrightarrow FeHPO_4$	16.19	B
$Fe(HPO_4)_2^{2-}$	$Fe^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Fe(HPO_4)_2^{2-}$	28.43	May *et al.* (1977)
$FeH_2PO_4^+$	$Fe^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow FeH_2PO_4^+$	20.57	Ciavatta *et al.* (1992a)
$Fe(H_2PO_4)_2$	$Fe^{2+} + 4H^+ + 2PO_4^{3-} \leftrightarrow Fe(H_2PO_4)_2$	41.83	Ciavatta *et al.* (1992a)
Oxidation-reduction			
Fe^{3+}	$Fe^{2+} \leftrightarrow Fe^{3+} + e^-$	-13.02	Nordstrom *et al.* (1990)

A Selected value predicted using the unified theory of metal ion complexation [UTMIC] (see Section 3.5)

B Mean value selected from Nriagu (1972a) and Ciavatta *et al.* (1992a)

Table 11 (cont.). Selected stability constants for iron (Fe^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes			
FeAsp	$Fe^{2+} + Asp^{2-} \leftrightarrow FeAsp$	5.39	Section 5
$Fe(Asp)_2^{2-}$	$Fe^{2+} + 2Asp^{2-} \leftrightarrow Fe(Asp)_2^{2-}$	8.84	Section 5
$FeCit^-$	$Fe^{2+} + Cit^{3-} \leftrightarrow FeCit^-$	5.86	Section 5
$Fe(Cit)_2^{4-}$	$Fe^{2+} + 2Cit^{3-} \leftrightarrow Fe(Cit)_2^{4-}$	6.73	May *et al.* (1977)
FeHCit	$Fe^{2+} + H^+ + Cit^{3-} \leftrightarrow FeHCit$	9.98	Section 5
FeH_2Cit^+	$Fe^{2+} + 2H^+ + Cit^{3-} \leftrightarrow FeH_2Cit^+$	12.74	Section 5
$FeH(Cit)_2^{3-}$	$Fe^{2+} + H^+ + 2Cit^{3-} \leftrightarrow FeH(Cit)_2^{3-}$	13.61	Amico *et al.* (1979)
$Fe_2(OH)_2(Cit)_2^{4-}$	$2Fe^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Fe_2(OH)_2(Cit)_2^{4-} + 2H^+$	-4.43	Amico *et al.* (1979)
FeMal	$Fe^{2+} + Mal^{2-} \leftrightarrow FeMal$	3.03	Section 5
$Fe(Mal)_2^{2-}$	$Fe^{2+} + 2Mal^{2-} \leftrightarrow Fe(Mal)_2^{2-}$	3.25	Section 5
FeSal	$Fe^{2+} + Sal^{2-} \leftrightarrow FeSal$	7.51	Section 5
$Fe(Sal)_2^{2-}$	$Fe^{2+} + 2Sal^{2-} \leftrightarrow Fe(Sal)_2^{2-}$	12.21	Section 5
Minerals			
$Fe(OH)_2$	$Fe(OH)_2 + 2H^+ \leftrightarrow Fe^{2+} + 2H_2O$	13.57	Smith *et al.* (1998)
$FeCO_3$ [siderite]	$FeCO_3 \leftrightarrow Fe^{2+} + CO_3^{2-}$	-10.74	A
$Fe_3(PO_4)_2 \cdot 8H_2O$ [vivianite]	$Fe_3(PO_4)_2 \cdot 8H_2O \leftrightarrow 3Fe^{2+} + 2PO_4^{3-} + 8H_2O$	-36.0	Smith *et al.* (1998)

A Mean selected value derived from Latimer (1952), Langmuir (1969), Singer and Stumm (1970), Reiterer *et al.* (1981), Bruno *et al.* (1992b) and Ptacek and Reardon (1992). See latter two references for a literature comparison

Table 12. Selected stability constants for iron (Fe^{3+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$FeOH^{2+}$	$Fe^{2+} + H_2O \leftrightarrow FeOH^{2+} + H^+ + e^-$	-15.21	Daniele *et al.* (1994)
$Fe(OH)_2^+$	$Fe^{2+} + 2H_2O \leftrightarrow Fe(OH)_2^+ + 2H^+ + e^-$	-18.72	Daniele *et al.* (1994)
$Fe(OH)_3$	$Fe^{2+} + 3H_2O \leftrightarrow Fe(OH)_3 + 3H^+ + e^-$	-25.58	Nordstrom *et al.* (1990)
$Fe(OH)_4^-$	$Fe^{2+} + 4H_2O \leftrightarrow Fe(OH)_4^- + 4H^+ + e^-$	-34.62	Nordstrom *et al.* (1990)
$Fe_2(OH)_2^{4+}$	$2Fe^{2+} + 2H_2O \leftrightarrow Fe_2(OH)_2^{4+} + 2H^+ + 2e^-$	-28.95	Daniele *et al.* (1994)
$Fe_3(OH)_4^{5+}$	$3Fe^{2+} + 4H_2O \leftrightarrow Fe_3(OH)_4^{5+} + 4H^+ + 3e^-$	-45.36	Nordstrom *et al.* (1990)
$Fe_{12}(OH)_{34}^{2+}$	$12Fe^{2+} + 34H_2O \leftrightarrow Fe_{12}(OH)_{34}^{2+} + 34H^+ + 12e^-$	-205.1	Daniele *et al.* (1994)
$FeCl^{2+}$	$Fe^{2+} + Cl^- \leftrightarrow FeCl^{2+} + e^-$	-11.52	Tagirov *et al.* (2000)
$FeCl_2^+$	$Fe^{2+} + 2Cl^- \leftrightarrow FeCl_2^+ + e^-$	-10.64	Tagirov *et al.* (2000)
$FeCl_3$	$Fe^{2+} + 3Cl^- \leftrightarrow FeCl_3 + e^-$	-11.71	Bjerrum and Lukés (1986)
$FeCl_4^-$	$Fe^{2+} + 4Cl^- \leftrightarrow FeCl_4^- + e^-$	-13.82	Bjerrum and Lukés (1986)
$FeSO_4^+$	$Fe^{2+} + SO_4^{2-} \leftrightarrow FeSO_4^+ + e^-$	-8.98	Smith *et al.* (1998)
$Fe(SO_4)_2^-$	$Fe^{2+} + 2SO_4^{2-} \leftrightarrow Fe(SO_4)_2^- + e^-$	-7.64	Smith *et al.* (1998)
$FeHSO_4^{2+}$	$Fe^{2+} + H^+ + SO_4^{2-} \leftrightarrow FeHSO_4^{2+} + e^-$	-8.55	Nordstrom *et al.* (1990)
$Fe(OH)SO_4$	$Fe^{2+} + H_2O + SO_4^{2-} \leftrightarrow Fe(OH)SO_4 + H^+ + e^-$	-12.91	Stipp (1990)
$Fe(OH)_2SO_4^-$	$Fe^{2+} + 2H_2O + SO_4^{2-} \leftrightarrow Fe(OH)_2SO_4^- + 2H^+ + e^-$	-17.92	Stipp (1990)
$Fe_3(OH)_4SO_4^{3+}$	$3Fe^{2+} + 4H_2O + SO_4^{2-} \leftrightarrow Fe_3(OH)_4SO_4^{3+} + 4H^+ + 3e^-$	-42.67	Khoe and Robbins (1988)
$FeNO_3^{2+}$	$Fe^{2+} + NO_3^- \leftrightarrow FeNO_3^{2+} + e^-$	-12.02	Smith *et al.* (1998)
$Fe(CO_3)_2^-$	$Fe^{2+} + 2CO_3^{2-} \leftrightarrow Fe(CO_3)_2^- + e^-$	-5.62	Bruno *et al.* (1992a)
$Fe(OH)CO_3$	$Fe^{2+} + H_2O + CO_3^{2-} \leftrightarrow Fe(OH)CO_3 + H^+ + e^-$	-10.14	A

A Corrected value from Bruno *et al.* (1992a)

Table 12 (cont.). Selected stability constants for iron (Fe^{3+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$FePO_4$	$Fe^{2+} + PO_4^{3-} \leftrightarrow FePO_4 + e^-$	8.31	Khoe and Robbins (1988)
$Fe(OH)PO_4^-$	$Fe^{2+} + H_2O + PO_4^{3-} \leftrightarrow Fe(OH)PO_4^- + H^+ + e^-$	3.09	Filatova (1974)
$Fe(PO_4)_2^{3-}$	$Fe^{2+} + 2PO_4^{3-} \leftrightarrow Fe(PO_4)_2^{3-} + e^-$	21.85	Filatova (1974)
$FeHPO_4^+$	$Fe^{2+} + H^+ + PO_4^{3-} \leftrightarrow FeHPO_4^+ + e^-$	9.24	Smith *et al.* (1998)
$Fe_2HPO_4^{4+}$	$2Fe^{2+} + H^+ + PO_4^{3-} \leftrightarrow Fe_2HPO_4^{4+} + 2e^-$	15.09	Ramamoorthy and Manning (1974a)
$Fe(HPO_4)_2^-$	$Fe^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Fe(HPO_4)_2^- + e^-$	18.38	May *et al.* (1977)
$FeH_2PO_4^{2+}$	$Fe^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow FeH_2PO_4^{2+} + e^-$	10.82	Smith *et al.* (1998)
Oxidation-reduction			
Fe^{3+}	$Fe^{2+} \leftrightarrow Fe^{3+} + e^-$	-13.02	Nordstrom *et al.* (1990)
Organic complexes			
$FeAsp^+$	$Fe^{2+} + Asp^{2-} \leftrightarrow FeAsp^+ + e^-$	-0.41	Perrin (1959)
FeCit	$Fe^{2+} + Cit^{3-} \leftrightarrow FeCit + e^-$	0.40	Section 5
$Fe(Cit)_2^{3-}$	$Fe^{2+} + 2Cit^{3-} \leftrightarrow Fe(Cit)_2^{3-} + e^-$	6.07	Section 5
$Fe_2(Cit)_2$	$2Fe^{2+} + 2Cit^{3-} \leftrightarrow Fe_2(Cit)_2 + 2e^-$	1.50	Sal'nikov and Zhuravleva (1986)
$FeHCit^+$	$Fe^{2+} + H^+ + Cit^{3-} \leftrightarrow FeHCit^+ + e^-$	1.19	Section 5
FeH_2Cit^{2+}	$Fe^{2+} + 2H^+ + Cit^{3-} \leftrightarrow FeH_2Cit^{2+} + e^-$	1.22	Sal'nikov and Zhuravleva (1986)
$FeH(Cit)_2^{2-}$	$Fe^{2+} + H^+ + 2Cit^{3-} \leftrightarrow FeH(Cit)_2^{2-} + e^-$	10.41	Ribas *et al.* (1989)

Table 12 (cont.). Selected stability constants for iron (Fe^{3+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Fe(HCit)_2^-$	$Fe^{2+} + 2H^+ + 2Cit^{3-} \leftrightarrow Fe(HCit)_2^- + e^-$	13.35	Section 5
$FeOHCit^-$	$Fe^{2+} + H_2O + Cit^{3-} \leftrightarrow FeOHCit^- + H^+ + e^-$	-2.50	Section 5
$Fe(OH)_2Cit^{2-}$	$Fe^{2+} + 2H_2O + Cit^{3-} \leftrightarrow Fe(OH)_2Cit^{2-} + 2H^+ + e^-$	-10.03	Section 5
$FeOH(Cit)_2^{4-}$	$Fe^{2+} + H_2O + 2Cit^{3-} \leftrightarrow FeOH(Cit)_2^{4-} + H^+ + e^-$	0.50	Ribas *et al.* (1989)
$Fe(OH)_2(Cit)_2^{5-}$	$Fe^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Fe(OH)_2(Cit)_2^{5-} + 2H^+ + e^-$	-6.44	Ribas *et al.* (1989)
$Fe(OH)_3(Cit)_2^{6-}$	$Fe^{2+} + 3H_2O + 2Cit^{3-} \leftrightarrow Fe(OH)_3(Cit)_2^{6-} + 3H^+ + e^-$	-13.28	Ribas *et al.* (1989)
$Fe_2OH(Cit)_2^-$	$2Fe^{2+} + H_2O + 2Cit^{3-} \leftrightarrow Fe_2OH(Cit)_2^- + H^+ + 2e^-$	-0.27	Glebov *et al.* (1990)
$Fe_2(OH)_2(Cit)_2^{2-}$	$2Fe^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Fe_2(OH)_2(Cit)_2^{2-} + 2H^+ + 2e^-$	-2.75	Section 5
$Fe_2(OH)_3(Cit)_2^{3-}$	$2Fe^{2+} + 3H_2O + 2Cit^{3-} \leftrightarrow Fe_2(OH)_3(Cit)_2^{3-} + 3H^+ + 2e^-$	-7.75	Section 5
$CuFe(Cit)_2^-$	$Cu^{2+} + Fe^{2+} + 2Cit^{3-} \leftrightarrow CuFe(Cit)_2^- + e^-$	11.66	Sal'nikov and Zhuravleva (1986)
$CuFe(OH)_2(Cit)_2^{3-}$	$Cu^{2+} + Fe^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CuFe(OH)_2(Cit)_2^{3-} + 2H^+ + e^-$	3.63	Sal'nikov and Zhuravleva (1986)
$CuFe(OH)_3(Cit)_2^{4-}$	$Cu^{2+} + Fe^{2+} + 3H_2O + 2Cit^{3-} \leftrightarrow CuFe(OH)_3(Cit)_2^{4-} + 3H^+ + e^-$	-4.17	Sal'nikov and Zhuravleva (1986)
$FeMal^+$	$Fe^{2+} + Mal^{2-} \leftrightarrow FeMal^+ + e^-$	-3.85	Section 5
$Fe(Mal)_2^-$	$Fe^{2+} + 2Mal^{2-} \leftrightarrow Fe(Mal)_2^- + e^-$	2.29	Section 5
$Fe(Mal)_3^{3-}$	$Fe^{2+} + 3Mal^{2-} \leftrightarrow Fe(Mal)_3^{3-} + e^-$	5.93	Section 5
$FeHMal^{2+}$	$Fe^{2+} + H^+ + Mal^{2-} \leftrightarrow FeHMal^{2+} + e^-$	-2.60	A
$FeSal^+$	$Fe^{2+} + Sal^{2-} \leftrightarrow FeSal^+ + e^-$	4.58	Section 5
$Fe(Sal)_2^-$	$Fe^{2+} + 2Sal^{2-} \leftrightarrow Fe(Sal)_2^- + e^-$	16.68	Section 5
$Fe(Sal)_3^{3-}$	$Fe^{2+} + 3Sal^{2-} \leftrightarrow Fe(Sal)_3^{3-} + e^-$	24.20	Section 5
$FeHSal^{2+}$	$Fe^{2+} + H^+ + Sal^{2-} \leftrightarrow FeHSal^{2+} + e^-$	5.51	Park (1966)

A Selected value was derived using the value of $FeMal^+$ provided here, added to the original authors difference between $FeMal^+$ and $FeHMal^{2+}$

Table 12 (cont.). Selected stability constants for iron (Fe^{3+}) complexes

Species	Reaction	log K_o	Reference
Minerals			
$Fe(OH)_3$ [ferrihydrite]	$Fe(OH)_3 + 3H^+ \leftrightarrow Fe^{3+} + 3H_2O$	3.20	Smith *et al.* (1998)
$FePO_4{\cdot}2H_2O$ [strengite]	$FePO_4{\cdot}2H_2O \leftrightarrow Fe^{3+} + PO_4^{3-} + 2H_2O$	-26.07	A

A Mean selected value derived from Egan *et al.* (1961), Nriagu (1972b) and Ciavatta *et al.* (1992b)

Table 13. Selected stability constants for manganese (Mn^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$MnOH^+$	$Mn^{2+} + H_2O \leftrightarrow MnOH^+ + H^+$	-10.59	Baes and Mesmer (1976)
$Mn(OH)_2$	$Mn^{2+} + 2H_2O \leftrightarrow Mn(OH)_2 + 2H^+$	-22.20	Baes and Mesmer (1976)
$Mn(OH)_3^-$	$Mn^{2+} + 3H_2O \leftrightarrow Mn(OH)_3^- + 3H^+$	-34.80	Baes and Mesmer (1976)
$Mn(OH)_4^{2-}$	$Mn^{2+} + 4H_2O \leftrightarrow Mn(OH)_4^{2-} + 4H^+$	-48.30	Smith *et al.* (1998)
Mn_2OH^{3+}	$2Mn^{2+} + H_2O \leftrightarrow Mn_2OH^{3+} + H^+$	-10.14	Falck (1992)
$Mn_2(OH)_3^+$	$2Mn^{2+} + 3H_2O \leftrightarrow Mn_2(OH)_3^+ + 3H^+$	-23.90	Smith *et al.* (1998)
$Mn_4(OH)_4^{4+}$	$4Mn^{2+} + 4H_2O \leftrightarrow Mn_4(OH)_4^{4+} + 4H^+$	-48.30	Smith *et al.* (1998)
$MnCl^+$	$Mn^{2+} + Cl^- \leftrightarrow MnCl^+$	-0.61	Gammons and Seward (1996)
$MnSO_4$	$Mn^{2+} + SO_4^{2-} \leftrightarrow MnSO_4$	2.26	Smith *et al.* (1998)
$MnNO_3^+$	$Mn^{2+} + CO_3^{2-} \leftrightarrow MnNO_3^+$	0.18	Smith *et al.* (1998)
$Mn(NO_3)_2$	$Mn^{2+} + 2NO_3^- \leftrightarrow Mn(NO_3)_2$	0.55	Smith *et al.* (1998)
$MnCO_3$	$Mn^{2+} + CO_3^{2-} \leftrightarrow MnCO_3$	4.70	Néher-Neumann (1994)
$MnHCO_3^+$	$Mn^{2+} + H^+ + CO_3^{2-} \leftrightarrow MnHCO_3^+$	11.09	Néher-Neumann (1994)
$MnHPO_4$	$Mn^{2+} + H^+ + PO_4^{3-} \leftrightarrow MnHPO_4$	16.32	Falck (1992)
$Mn(HPO_4)_2^{2-}$	$Mn^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Mn(HPO_4)_2^{2-}$	29.97	Falck (1992)
$MnH_2PO_4^+$	$Mn^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow MnH_2PO_4^+$	21.01	Falck (1992)
Organic complexes			
MnAsp	$Mn^{2+} + Asp^{2-} \leftrightarrow MnAsp$	4.50	Section 5
$Mn(Asp)_2^{2-}$	$Mn^{2+} + 2Asp^{2-} \leftrightarrow Mn(Asp)_2^{2-}$	7.00	Benedikovic *et al.* (1991)

Table 13 (cont.). Selected stability constants for manganese (Mn^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$MnCit^-$	$Mn^{2+} + Cit^{3-} \leftrightarrow MnCit^-$	5.12	Section 5
$Mn(Cit)_2^{4-}$	$Mn^{2+} + 2Cit^{3-} \leftrightarrow Mn(Cit)_2^{4-}$	6.50	Section 5
$MnHCit$	$Mn^{2+} + H^+ + Cit^{3-} \leftrightarrow MnHCit$	9.48	Section 5
MnH_2Cit^+	$Mn^{2+} + 2H^+ + Cit^{3-} \leftrightarrow MnH_2Cit^+$	13.14	Section 5
$MnOHCit^{2-}$	$Mn^{2+} + H_2O + Cit^{3-} \leftrightarrow MnOHCit^{2-} + H^+$	-3.27	Section 5
Mn_2OHCit	$2Mn^{2+} + H_2O + Cit^{3-} \leftrightarrow Mn_2OHCit + H^+$	1.88	Roos and Williams (1977)
$Mn_2(OH)_2(Cit)_2^{4-}$	$2Mn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Mn_2(OH)_2(Cit)_2^{4-} + 2H^+$	-4.69	Amico *et al.* (1979)
$CdMn(OH)_2(Cit)_2^{4-}$	$Cd^{2+} + Mn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CdMn(OH)_2(Cit)_2^{4-} + 2H^+$	-4.89	Amico *et al.* (1985)
$MnMal$	$Mn^{2+} + Mal^{2-} \leftrightarrow MnMal$	3.38	Section 5
$Mn(Mal)_2^{2-}$	$Mn^{2+} + 2Mal^{2-} \leftrightarrow Mn(Mal)_2^{2-}$	4.29	Nozaki *et al.* (1970)
$MnOHMal^-$	$Mn^{2+} + H_2O + Mal^{2-} \leftrightarrow MnOHMal^+ + H^+$	-4.27	A
$MnSal$	$Mn^{2+} + Sal^{2-} \leftrightarrow MnSal$	6.88	Section 5
$Mn(Sal)_2^{2-}$	$Mn^{2+} + 2Sal^{2-} \leftrightarrow Mn(Sal)_2^{2-}$	10.78	Perrin (1958)
$MnTri^-$	$Mn^{2+} + Tri^{3-} \leftrightarrow MnTri^-$	3.44	Li *et al.* (1959)

A Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

Table 13 (cont.). Selected stability constants for manganese (Mn^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
MnHTri	$Mn^{2+} + H^+ + Tri^{3-} \leftrightarrow MnHTri$	8.81	A
$MnOHTri^{2-}$	$Mn^{2+} + H_2O + Tri^{3-} \leftrightarrow MnOHTri^{2-} + H^+$	-4.16	B
Minerals			
$Mn(OH)_2$ [pyrochroite]	$Mn(OH)_2 + 2H^+ \leftrightarrow Mn^{2+} + 2H_2O$	15.20	Smith *et al.* (1998)
$MnCO_3$ [rhodocrosite]	$MnCO_3 \leftrightarrow Mn^{2+} + CO_3^{2-}$	-10.58	Smith *et al.* (1998)
$MnHPO_4{\cdot}3H_2O$	$MnHPO_4{\cdot}3H_2O \leftrightarrow Mn^{2+} + HPO_4^{2-} + 3H_2O$	-7.44	Brown *et al.* (1996b)

A Selected value was derived from two independent methods: (i) the linear free energy relationship (LFER) between 1:1 metal tricarballylate complexes (ML) and 1:1:1 metal hydrogen tricarballylate (MHL) complexes and (ii) the unified theory of metal complexation (UTMIC), whereby available 1:1:1 metal hydrogen tricarballylate complexes are regressed against a corresponding value of $g_1(z_M/r_M{}^2 + g_2)$

B Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

Table 14. Selected stability constants for uranium (U^{4+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
UOH^{3+}	$U^{4+} + H_2O \leftrightarrow UOH^{3+} + H^+$	-0.4	Neck and Kim (1999)
$U(OH)_2^{2+}$	$U^{4+} + 2H_2O \leftrightarrow U(OH)_2^{2+} + 2H^+$	-0.5	Neck and Kim (1999)
$U(OH)_3^{2+}$	$U^{4+} + 3H_2O \leftrightarrow U(OH)_3^{+} + 3H^+$	-3.8	Neck and Kim (1999)
$U(OH)_4$	$U^{4+} + 4H_2O \leftrightarrow U(OH)_4 + 4H^+$	-9.3	Neck and Kim (1999)
$U_6(OH)_{15}^{9+}$	$6U^{4+} + 15H_2O \leftrightarrow U_6(OH)_{15}^{9+} + 15H^+$	-16.90	Grenthe *et al.* (1992)
UCl^{3+}	$U^{4+} + Cl^- \leftrightarrow UCl^{3+}$	1.72	Grenthe *et al.* (1992)
USO_4^{2+}	$U^{4+} + SO_4^{2-} \leftrightarrow USO_4^{2+}$	6.58	Grenthe *et al.* (1992)
$U(SO_4)_2$	$U^{4+} + 2SO_4^{2-} \leftrightarrow U(SO_4)_2$	10.51	Grenthe *et al.* (1992)
UNO_3^{3+}	$U^{4+} + NO_3^- \leftrightarrow UNO_3^{3+}$	1.47	Grenthe *et al.* (1992)
$U(NO_3)_2^{2+}$	$U^{4+} + 2NO_3^- \leftrightarrow U(NO_3)_2^{2+}$	2.30	Grenthe *et al.* (1992)
$U(CO_3)_4^{4-}$	$U^{4+} + 4CO_3^{2-} \leftrightarrow U(CO_3)_4^{4-}$	32.90	Grenthe *et al.* (1992)
$U(CO_3)_5^{6-}$	$U^{4+} + 5CO_3^{2-} \leftrightarrow U(CO_3)_5^{6-}$	33.0	Neck and Kim (1999)
Oxidation-reduction			
UO_2^{2+}	$U^{4+} + 2H_2O \leftrightarrow UO_2^{2+} + 4H^+ + 2e^-$	-9.04	Grenthe *et al.* (1992)

Table 15. Selected stability constants for uranium (UO_2^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
UO_2OH^+	$U^{4+} + 3H_2O \leftrightarrow UO_2OH^+ + 5H^+ + 2e^-$	-14.24	Grenthe *et al.* (1992)
$UO_2(OH)_2$	$U^{4+} + 4H_2O \leftrightarrow UO_2(OH)_2 + 6H^+ + 2e^-$	-21.20	Choppin and Mathur (1991)
$UO_2(OH)_3^-$	$U^{4+} + 5H_2O \leftrightarrow UO_2(OH)_3^- + 7H^+ + 2e^-$	-28.24	Grenthe *et al.* (1992)
$UO_2(OH)_4^{2-}$	$U^{4+} + 6H_2O \leftrightarrow UO_2(OH)_4^{2-} + 8H^+ + 2e^-$	-44.50	Baston *et al.* (1993)
$(UO_2)_2OH^{3+}$	$2U^{4+} + 5H_2O \leftrightarrow (UO_2)_2OH^{3+} + 9H^+ + 4e^-$	-20.78	Grenthe *et al.* (1992)
$(UO_2)_2(OH)_2^{2+}$	$2U^{4+} + 6H_2O \leftrightarrow (UO_2)_2(OH)_2^{2+} + 10H^+ + 4e^-$	-23.70	Grenthe *et al.* (1992)
$(UO_2)_3(OH)_4^{2+}$	$3U^{4+} + 10H_2O \leftrightarrow (UO_2)_3(OH)_4^{2+} + 16H^+ + 6e^-$	-39.01	Grenthe *et al.* (1992)
$(UO_2)_3(OH)_5^+$	$3U^{4+} + 11H_2O \leftrightarrow (UO_2)_3(OH)_5^+ + 17H^+ + 6e^-$	-42.66	Grenthe *et al.* (1992)
$(UO_2)_3(OH)_7^-$	$3U^{4+} + 13H_2O \leftrightarrow (UO_2)_3(OH)_7^- + 19H^+ + 6e^-$	-58.12	Grenthe *et al.* (1992)
$(UO_2)_3(OH)_8^{2-}$	$3U^{4+} + 14H_2O \leftrightarrow (UO_2)_3(OH)_8^{2-} + 20H^+ + 6e^-$	-64.76	Palmer and Nguyen-Trung (1995)
$(UO_2)_3(OH)_{10}^{4-}$	$3U^{4+} + 16H_2O \leftrightarrow (UO_2)_3(OH)_{10}^{4-} + 22H^+ + 6e^-$	-89.51	Palmer and Nguyen-Trung (1995)
$(UO_2)_4(OH)_7^+$	$4U^{4+} + 15H_2O \leftrightarrow (UO_2)_4(OH)_7^+ + 23H^+ + 8e^-$	-58.05	Grenthe *et al.* (1992)
UO_2Cl^+	$U^{4+} + 2H_2O + Cl^- \leftrightarrow UO_2Cl^+ + 4H^+ + 2e^-$	-8.87	Grenthe *et al.* (1992)
UO_2Cl_2	$U^{4+} + 2H_2O + 2Cl^- \leftrightarrow UO_2Cl_2 + 4H^+ + 2e^-$	-10.14	Grenthe *et al.* (1992)
UO_2SO_4	$U^{4+} + 2H_2O + SO_4^{2-} \leftrightarrow UO_2SO_4 + 4H^+ + 2e^-$	-5.89	Grenthe *et al.* (1992)
$UO_2(SO_4)_2^{2-}$	$U^{4+} + 2H_2O + 2SO_4^{2-} \leftrightarrow UO_2(SO_4)_2^{2-} + 4H^+ + 2e^-$	-4.91	Grenthe *et al.* (1992)
$UO_2(SO_4)_3^{4-}$	$U^{4+} + 2H_2O + 3SO_4^{2-} \leftrightarrow UO_2(SO_4)_3^{4-} + 4H^+ + 2e^-$	-6.42	Geipel *et al.* (1996)
$(UO_2)_2(OH)_2(SO_4)_2^{2-}$	$2U^{4+} + 6H_2O + 2SO_4^{2-} \leftrightarrow (UO_2)_2(OH)_2(SO_4)_2^{2-} + 10H^+ + 4e^-$	-18.77	Comarmond and Brown (2000)
$(UO_2)_3(OH)_4(SO_4)_4^{6-}$	$3U^{4+} + 10H_2O + 4SO_4^{2-} \leftrightarrow (UO_2)_3(OH)_4(SO_4)_4^{6-} + 16H^+ + 6e^-$	-33.11	Comarmond and Brown (2000)
$(UO_2)_4(OH)_7(SO_4)_4^{7-}$	$4U^{4+} + 15H_2O + 4SO_4^{2-} \leftrightarrow (UO_2)_4(OH)_7(SO_4)_4^{7-} + 23H^+ + 8e^-$	-55.16	Comarmond and Brown (2000)

Table 15 (cont.). Selected stability constants for uranium (UO_2^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$UO_2NO_3^+$	$U^{4+} + 2H_2O + NO_3^- \leftrightarrow UO_2NO_3^+ + 4H^+ + 2e^-$	-8.74	Grenthe *et al.* (1992)
UO_2CO_3	$U^{4+} + 2H_2O + CO_3^{2-} \leftrightarrow UO_2CO_3 + 4H^+ + 2e^-$	0.63	Grenthe *et al.* (1995)
$UO_2(CO_3)_2^{2-}$	$U^{4+} + 2H_2O + 2CO_3^{2-} \leftrightarrow UO_2(CO_3)_2^{2-} + 4H^+ + 2e^-$	7.90	Grenthe *et al.* (1992)
$UO_2(CO_3)_3^{4-}$	$U^{4+} + 2H_2O + 3CO_3^{2-} \leftrightarrow UO_2(CO_3)_3^{4-} + 4H^+ + 2e^-$	12.56	Grenthe *et al.* (1992)
$(UO_2)_3(CO_3)_6^{6-}$	$3U^{4+} + 6H_2O + 6CO_3^{2-} \leftrightarrow (UO_2)_3(CO_3)_6^{6-} + 4H^+ + 2e^-$	26.88	Grenthe *et al.* (1992)
$(UO_2)_2(OH)_3CO_3^-$	$2U^{4+} + 7H_2O + CO_3^{2-} \leftrightarrow (UO_2)_2(OH)_3CO_3^- + 11H^+ + 4e^-$	-18.94	Grenthe *et al.* (1992)
$(UO_2)_3(OH)_4HCO_3^+$	$3U^{4+} + 9H_2O + CO_3^{2-} \leftrightarrow (UO_2)_3(OH)_4HCO_3^+ + 14H^+ + 6e^-$	-26.47	Grenthe *et al.* (1992)
$Ca_2[UO_2(CO_3)_3]$	$2Ca^{2+} + U^{4+} + 2H_2O + 3CO_3^{2-} \leftrightarrow Ca_2[UO_2(CO_3)_3] + 4H^+ + 2e^-$	20.33	Bernhard *et al.* (1996)
$UO_2PO_4^-$	$U^{4+} + 2H_2O + PO_4^{3-} \leftrightarrow UO_2PO_4^- + 4H^+ + 2e^-$	4.19	Grenthe *et al.* (1992)
UO_2HPO_4	$U^{4+} + 2H_2O + PO_4^{3-} \leftrightarrow UO_2HPO_4 + 3H^+ + 2e^-$	10.64	Brendler *et al.* (1996)
$UO_2H_2PO_4^+$	$U^{4+} + 2H_2O + PO_4^{3-} \leftrightarrow UO_2H_2PO_4^+ + 2H^+ + 2e^-$	13.74	Brendler *et al.* (1996)
$UO_2(H_2PO_4)_2^+$	$U^{4+} + 2H_2O + 2PO_4^{3-} \leftrightarrow UO_2(H_2PO_4)_2^+ + 2e^-$	36.03	Brendler *et al.* (1996)
$UO_2H_3PO_4^{2+}$	$U^{4+} + 2H_2O + PO_4^{3-} \leftrightarrow UO_2H_3PO_4^{2+} + 2e^-$	13.44	Grenthe *et al.* (1992)
Oxidation-reduction			
UO_2^{2+}	$U^{4+} + 2H_2O \leftrightarrow UO_2^{2+} + 4H^+ + 2e^-$	-9.04	Grenthe *et al.* (1992)

Table 15 (cont.). Selected stability constants for uranium (UO_2^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes			
UO_2Asp	$U^{4+} + 2H_2O + Asp^{2-} \leftrightarrow UO_2Asp + 4H^+ + 2e^-$	-4.54	Saito and Choppin (1984)
UO_2HAsp^+	$U^{4+} + 2H_2O + Asp^{2-} \leftrightarrow UO_2HAsp^+ + 3H^+ + 2e^-$	4.00	Section 5
$UO_2(HAsp)_2$	$U^{4+} + 2H_2O + 2Asp^{2-} \leftrightarrow UO_2(HAsp)_2 + 2H^+ + 2e^-$	15.46	Section 5
UO_2Cit^-	$U^{4+} + 2H_2O + Cit^{3-} \leftrightarrow UO_2Cit^- + 4H^+ + 2e^-$	0.10	Section 5
$UO_2(Cit)_2^{4-}$	$U^{4+} + 2H_2O + 2Cit^{3-} \leftrightarrow UO_2(Cit)_2^{4-} + 4H^+ + 2e^-$	3.32	Hummel (1993)
$(UO_2)_2(Cit)_2^{2-}$	$2U^{4+} + 4H_2O + 2Cit^{3-} \leftrightarrow (UO_2)_2(Cit)_2^{2-} + 8H^+ + 4e^-$	2.62	Section 5
UO_2HCit	$U^{4+} + 2H_2O + Cit^{3-} \leftrightarrow UO_2HCit + 3H^+ + 2e^-$	2.28	Section 5
$UO_2H_2Cit^+$	$U^{4+} + 2H_2O + Cit^{3-} \leftrightarrow UO_2H_2Cit^+ + 2H^+ + 2e^-$	4.57	Section 5
UO_2OHCit^{2-}	$U^{4+} + 3H_2O + Cit^{3-} \leftrightarrow UO_2OHCit^{2-} + 5H^+ + 2e^-$	-4.29	A
$(UO_2)_2(OH)_2(Cit)_2^{4-}$	$2U^{4+} + 6H_2O + 2Cit^{3-} \leftrightarrow (UO_2)_2(OH)_2(Cit)_2^{4-} + 10H^+ + 4e^-$	-6.24	B
UO_2Mal	$U^{4+} + 2H_2O + Mal^{2-} \leftrightarrow UO_2Mal + 4H^+ + 2e^-$	-2.75	Section 5
$UO_2(Mal)_2^{2-}$	$U^{4+} + 2H_2O + 2Mal^{2-} \leftrightarrow UO_2(Mal)_2^{2-} + 4H^+ + 2e^-$	1.22	Section 5
UO_2OHMal^-	$U^{4+} + 3H_2O + 2Mal^{2-} \leftrightarrow UO_2OHMal^- + 5H^+ + 2e^-$	-8.04	Vanni *et al.* (1969)
$UO_2MalAsp^{2-}$	$U^{4+} + 2H_2O + Mal^{2-} + Asp^{2-} \leftrightarrow UO_2MalAsp^{2-} + 4H^+ + 2e^-$	1.88	Janarthanam *et al.* (1995)
UO_2Sal	$U^{4+} + 2H_2O + Sal^{2-} \leftrightarrow UO_2Sal + 4H^+ + 2e^-$	3.98	Section 5
$UO_2(Sal)_2^{2-}$	$U^{4+} + 2H_2O + 2Sal^{2-} \leftrightarrow UO_2(Sal)_2^{2-} + 4H^+ + 2e^-$	13.69	Section 5

A Selected value was derived using two independent methods: (i) the linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL) and (ii) the unified theory of metal complexation (UTMIC), whereby available 1:1:1 metal hydroxy citrate complexes (MOHCit) are regressed against a corresponding value of $g_1(z_M/r_M^2 + g_2)$

B Selected value was derived using the linear free energy relationship (LFER) between 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL) and 2:2:2 metal hydroxy di- and tri-carboxylate complexes ($M_2(OH)_2L_2$)

Table 15 (cont.). Selected stability constants for uranium (UO_2^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
UO_2HSal^+	$U^{4+} + 2H_2O + 2Mal^{2-} \leftrightarrow UO_2HSal^+ + 3H^+ + 2e^-$	6.92	Section 5
UO_2OHSal^-	$U^{4+} + 3H_2O + 2Sal^{2-} \leftrightarrow UO_2OHSal^- + 5H^+ + 2e^-$	-2.30	Simões-Gonçalves and Mota (1987)
UO_2Tri^-	$U^{4+} + 2H_2O + Tri^{3-} \leftrightarrow UO_2Tri^- + 4H^+$	-2.72	A
UO_2HTri	$U^{4+} + 2H_2O + Tri^{3-} \leftrightarrow UO_2HTri + 3H^+$	1.70	B
UO_2OHTri^{2-}	$U^{4+} + 2H_2O + Tri^{3-} \leftrightarrow UO_2OHTri^{2-} + 5H^+$	-8.71	C
Minerals			
β-$UO_2(OH)_2$	β-$UO_2(OH)_2 + 2H^+ \leftrightarrow UO_2^{2+} + 2H_2O$	4.94	Grenthe *et al.* (1992)
UO_2CO_3 [rutherfordine]	$UO_2CO_3 \leftrightarrow UO_2^{2+} + CO_3^{2-}$	-14.32	D
$UO_2HPO_4{\cdot}4H_2O$	$UO_2HPO_4{\cdot}4H_2O \leftrightarrow UO_2^{2+} + HPO_4^{2-} + 4H_2O$	-11.86	Grenthe *et al.* (1992)

A Selected value was derived from two independent methods: (i) the LFER between 1:1 Cu di- and tri-carboxylate complexes (CuL) and their corresponding uranyl (UO_2L) complexes and (ii) the UTMIC, whereby available 1:1 metal tricarballylate (MTri) complexes are regressed against a corresponding value of $g_1(z_M/r_M^2 + g_2)$

B Selected value was derived from two independent methods: (i) the LFER between 1:1 metal tricarballylate complexes (ML) and 1:1:1 metal hydrogen tricarballylate (MHL) complexes and (ii) the unified theory of metal complexation (UTMIC), whereby available 1:1:1 metal hydrogen tricarballylate complexes are regressed against a corresponding value of $g_1(z_M/r_M^2 + g_2)$

C Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

D Mean selected value derived from Sergeyeva *et al.* (1972), Nikolaeva (1976), Grenthe *et al.* (1984), Kramer-Schnabel *et al.* (1992), Pashalidis *et al.* (1993) and Meinrath *et al.* (1996)

Table 16. Selected stability constants for aluminium (Al^{3+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$AlOH^{2+}$	$Al^{3+} + H_2O \leftrightarrow AlOH^{2+} + H^+$	-4.95	Palmer and Wesolowski (1993)
$Al(OH)_2^+$	$Al^{3+} + 2H_2O \leftrightarrow Al(OH)_2^+ + 2H^+$	-10.56	Wesolowski and Palmer (1994)
$Al(OH)_3$	$Al^{3+} + 3H_2O \leftrightarrow Al(OH)_3 + 3H^+$	-16.99	Plyasunova and Grenthe (1994)
$Al(OH)_4^-$	$Al^{3+} + 4H_2O \leftrightarrow Al(OH)_4^- + 4H^+$	-22.87	Wesolowski and Palmer (1994)
$Al_2(OH)_2^{4+}$	$2Al^{3+} + 2H_2O \leftrightarrow Al_2(OH)_2^{4+} + 2H^+$	-7.69	Baes and Mesmer (1976)
$Al_3(OH)_4^{5+}$	$3Al^{3+} + 4H_2O \leftrightarrow Al_3(OH)_4^{5+} + 4H^+$	-13.89	Baes and Mesmer (1976)
$Al_{13}O_4(OH)_{24}^{7+}$	$13Al^{3+} + 28H_2O \leftrightarrow Al_{13}O_4(OH)_{24}^{7+} + 32H^+$	-101.6	A
$AlSO_4^+$	$Al^{3+} + SO_4^{2-} \leftrightarrow AlSO_4^+$	4.2	B
$Al(SO_4)_2^-$	$Al^{3+} + 2SO_4^{2-} \leftrightarrow Al(SO_4)_2^-$	5.9	B
$AlHSO_4^{2+}$	$Al^{3+} + H^+ + SO_4^{2-} \leftrightarrow AlHSO_4^{2+}$	2.45	Nordstrom *et al.* (1990)
$Al_2(OH)_2CO_3^{2+}$	$2Al^{3+} + 2H_2O + CO_3^{2-} \leftrightarrow Al_2(OH)_2CO_3^{2+} + 2H^+$	4.19	Smith *et al.* (1998)
$Al_3(OH)_3CO_3^{4+}$	$3Al^{3+} + 3H_2O + CO_3^{2-} \leftrightarrow Al_3(OH)_3CO_3^{4+} + 3H^+$	1.50	Smith *et al.* (1998)
$AlPO_4$	$Al^{3+} + PO_4^{3-} \leftrightarrow AlPO_4$	18.09	Smith *et al.* (1998)
$Al_2PO_4^{3+}$	$2Al^{3+} + PO_4^{3-} \leftrightarrow Al_2PO_4^{3+}$	23.29	Smith *et al.* (1998)
$AlHPO_4^+$	$Al^{3+} + H^+ + PO_4^{3-} \leftrightarrow AlHPO_4^+$	21.51	Smith *et al.* (1998)
$AlH_2PO_4^{2+}$	$Al^{3+} + 2H^+ + PO_4^{3-} \leftrightarrow AlH_2PO_4^{2+}$	24.54	Smith *et al.* (1998)
$Al_2(OH)_2PO_4^+$	$2Al^{3+} + 2H_2O + PO_4^{3-} \leftrightarrow Al_2(OH)_2PO_4^+ + 2H^+$	18.72	Smith *et al.* (1998)
$Al_2(OH)_3PO_4$	$2Al^{3+} + 3H_2O + PO_4^{3-} \leftrightarrow Al_2(OH)_3PO_4 + 3H^+$	9.62	Smith *et al.* (1998)

A Mean selected value derived from Turner (1975), Baes and Mesmer (1976), Öhman and Forsling (1981), Brown *et al.* (1985) and Markland and Öhman (1990)

B Estimated from data at higher temperatures given in Ridley *et al.* (1999)

Table 16 (cont.). Selected stability constants for aluminium (Al^{3+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes			
$AlAsp^+$	$Al^{3+} + Asp^{2-} \leftrightarrow AlAsp^+$	8.93	Section 5
$AlHAsp^{2+}$	$Al^{3+} + H^+ + Asp^{2-} \leftrightarrow AlHAsp^{2+}$	12.75	Section 5
AlH_2Asp^{3+}	$Al^{3+} + 2H^+ + Asp^{2-} \leftrightarrow AlH_2Asp^{3+}$	15.21	Berthon and Daydé (1992)
$Al_2(OH)Asp^{3+}$	$2Al^{3+} + H_2O + Asp^{2-} \leftrightarrow Al_2(OH)Asp^{3+} + H^+$	7.61	Berthon and Daydé (1992)
$Al_2(OH)_2Asp^{2+}$	$2Al^{3+} + 2H_2O + Asp^{2-} \leftrightarrow Al_2(OH)_2Asp^{2+} + 2H^+$	4.02	Berthon and Daydé (1992)
$Al_2(OH)_4Asp$	$2Al^{3+} + 4H_2O + Asp^{2-} \leftrightarrow Al_2(OH)_4Asp + 4H^+$	-4.48	Berthon and Daydé (1992)
$AlCit$	$Al^{3+} + Cit^{3-} \leftrightarrow AlCit$	10.27	Section 5
$Al(Cit)_2{}^{3-}$	$Al^{3+} + 2Cit^{3-} \leftrightarrow Al(Cit)_2{}^{3-}$	15.22	Section 5
$AlHCit^+$	$Al^{3+} + H^+ + Cit^{3-} \leftrightarrow AlHCit^+$	12.67	Section 5
AlH_2Cit^{2+}	$Al^{3+} + 2H^+ + Cit^{3-} \leftrightarrow AlH_2Cit^{2+}$	13.93	Section 5
$AlH(Cit)_2{}^{2-}$	$Al^{3+} + H^+ + 2Cit^{3-} \leftrightarrow AlH(Cit)_2{}^{2-}$	19.81	Gregor and Powell (1986)
$AlOHCit^-$	$Al^{3+} + H_2O + Cit^{3-} \leftrightarrow AlOHCit^- + H^+$	6.56	Section 5
$Al(OH)_2Cit^{2-}$	$Al^{3+} + 2H_2O + Cit^{3-} \leftrightarrow Al(OH)_2Cit^{2-} + 2H^+$	-0.25	Section 5
$AlOH(Cit)_2{}^{4-}$	$Al^{3+} + H_2O + 2Cit^{3-} \leftrightarrow AlOH(Cit)_2{}^{4-} + H^+$	8.29	Section 5
$Al(OH)_2(Cit)_2{}^{5-}$	$Al^{3+} + 2H_2O + 2Cit^{3-} \leftrightarrow Al(OH)_2(Cit)_2{}^{5-} + 2H^+$	-0.18	Section 5
$Al_2(OH)_2(Cit)_2{}^{2-}$	$2Al^{3+} + 2H_2O + 2Cit^{3-} \leftrightarrow Al_2(OH)_2(Cit)_2{}^{2-} + 2H^+$	16.34	Venturini and Berthon (1989)
$Al_3(OH)_4(Cit)_2{}^{4-}$	$3Al^{3+} + 4H_2O + 2Cit^{3-} \leftrightarrow Al_3(OH)_4(Cit)_2{}^{4-} + 4H^+$	20.17	Section 5
$Al_3(OH)_7(Cit)_3{}^{7-}$	$3Al^{3+} + 7H_2O + 3Cit^{3-} \leftrightarrow Al_3(OH)_7(Cit)_3{}^{7-} + 7H^+$	-9.21	Öhman (1988)
$AlMal^+$	$Al^{3+} + Mal^{2-} \leftrightarrow AlMal^+$	7.74	Section 5
$Al(Mal)_2{}^-$	$Al^{3+} + 2Mal^{2-} \leftrightarrow Al(Mal)_2{}^-$	12.95	Section 5

Table 16 (cont.). Selected stability constants for aluminium (Al^{3+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Al(Mal)_3^{3-}$	$Al^{3+} + 3Mal^{2-} \leftrightarrow Al(Mal)_3^{3-}$	14.96	Section 5
$AlHMal^{2+}$	$Al^{3+} + H^+ + Mal^{2-} \leftrightarrow AlHMal^{2+}$	9.88	Tedesco and González-Quitana (1974)
$Al(HMal)_2^+$	$Al^{3+} + 2H^+ + 2Mal^{2-} \leftrightarrow Al(HMal)_2^+$	18.38	Tedesco and González-Quitana (1974)
$AlOH(Mal)_2^{2-}$	$Al^{3+} + H_2O + 2Mal^{2-} \leftrightarrow AlOH(Mal)_2^{2-} + H^+$	5.95	Powell and Town (1993)
$Al(OH)_2Mal^{2+}$	$Al^{3+} + 2H_2O + Mal^{2-} \leftrightarrow Al(OH)_2Mal^{2+} + 2H^+$	-4.08	Kiss *et al.* (1994)
$AlSal^+$	$Al^{3+} + Sal^{2-} \leftrightarrow AlSal^+$	14.74	Section 5
$Al(Sal)_2^-$	$Al^{3+} + 2Sal^{2-} \leftrightarrow Al(Sal)_2^-$	25.67	Section 5
$Al(Sal)_3^{3-}$	$Al^{3+} + 3Sal^{2-} \leftrightarrow Al(Sal)_3^{3-}$	34.95	Section 5
$AlOH(Sal)_2^{2-}$	$Al^{3+} + H_2O + 2Sal^{2-} \leftrightarrow AlOH(Sal)_2^{2-} + H^+$	17.90	Section 5
$Al(OH)_2Sal^-$	$Al^{3+} + 2H_2O + Sal^{2-} \leftrightarrow Al(OH)_2Sal^- + 2H^+$	3.93	Rajan *et al.* (1981)
$Al(OH)_3Sal^{2-}$	$Al^{3+} + 3H_2O + Sal^{2-} \leftrightarrow Al(OH)_3Sal^{2-} + 3H^+$	-5.89	Rajan *et al.* (1981)
$Al(OH)_2(Sal)_2^{3-}$	$Al^{3+} + 2H_2O + 2Sal^{2-} \leftrightarrow Al(OH)_2(Sal)_2^{3-} + 2H^+$	7.57	Öhman and Sjöberg (1983b)
$Al_2(OH)_2(Sal)_2$	$2Al^{3+} + 2H_2O + 2Sal^{2-} \leftrightarrow Al_2(OH)_2(Sal)_2 + 2H^+$	20.94	Kiss *et al.* (1993)
$AlTri$	$Al^{3+} + Tri^{3-} \leftrightarrow AlTri$	7.63	Jackson (1982)
$AlHTri^+$	$Al^{3+} + H^+ + Tri^{3-} \leftrightarrow AlHTri^+$	11.08	Jackson (1982)
$AlOHTri^-$	$Al^{3+} + H_2O + Tri^{3-} \leftrightarrow AlOHTri^- + H^+$	3.83	Jackson (1982)

Table 16 (cont.). Selected stability constants for aluminium (Al^{3+}) complexes

Species	Reaction	log K_o	Reference
Minerals			
$Al(OH)_{3(am)}$	$Al(OH)_3 + 3H^+ \leftrightarrow Al^{3+} + 3H_2O$	3.20	Nordstrom *et al.* (1990)
$AlPO_4$	$AlPO_4 \leftrightarrow Al^{3+} + PO_4^{3-} + 2H_2O$	-21.29	Smith *et al.* (1998)

Table 17. Selected stability constants for lead (Pb^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$PbOH^+$	$Pb^{2+} + H_2O \leftrightarrow PbOH^+ + H^+$	-7.60	Smith *et al.* (1998)
$Pb(OH)_2$	$Pb^{2+} + 2H_2O \leftrightarrow Pb(OH)_2 + 2H^+$	-16.93	Falck (1992)
$Pb(OH)_3^-$	$Pb^{2+} + 3H_2O \leftrightarrow Pb(OH)_3^- + 3H^+$	-27.74	A
$Pb(OH)_4^{2-}$	$Pb^{2+} + 4H_2O \leftrightarrow Pb(OH)_4^{2-} + 4H^+$	-39.70	Falck (1992)
Pb_2OH^{3+}	$2Pb^{2+} + H_2O \leftrightarrow Pb_2OH^{3+} + H^+$	-6.40	Smith *et al.* (1998)
$Pb_3(OH)_4^{2+}$	$3Pb^{2+} + 4H_2O \leftrightarrow Pb_3(OH)_4^{2+} + 4H^+$	-22.87	B
$Pb_3(OH)_5^+$	$3Pb^{2+} + 5H_2O \leftrightarrow Pb_3(OH)_5^+ + 5H^+$	-30.65	C
$Pb_4(OH)_4^{4+}$	$4Pb^{2+} + 4H_2O \leftrightarrow Pb_4(OH)_4^{4+} + 4H^+$	-20.10	Smith *et al.* (1998)
$Pb_6(OH)_8^{4+}$	$6Pb^{2+} + 8H_2O \leftrightarrow Pb_6(OH)_8^{4+} + 8H^+$	-42.87	B
$PbCl^+$	$Pb^{2+} + Cl^- \leftrightarrow PbCl^+$	1.44	Sverjensky *et al.* (1997)
$PbCl_2$	$Pb^{2+} + 2Cl^- \leftrightarrow PbCl_2$	2.00	Sverjensky *et al.* (1997)
$PbCl_3^-$	$Pb^{2+} + 3Cl^- \leftrightarrow PbCl_3^-$	1.69	Sverjensky *et al.* (1997)
PbOHCl	$Pb^{2+} + H_2O + Cl^- \leftrightarrow PbOHCl + H^+$	-7.20	D
$PbSO_4$	$Pb^{2+} + SO_4^{2-} \leftrightarrow PbSO_4$	2.69	Smith *et al.* (1998)
$Pb(SO_4)_2^{2-}$	$Pb^{2+} + 2SO_4^{2-} \leftrightarrow Pb(SO_4)_2^{2-}$	4.00	Phillips (1982)
$PbNO_3^+$	$Pb^{2+} + CO_3^{2-} \leftrightarrow PbNO_3^+$	0.88	Smith *et al.* (1998)
$Pb(NO_3)_2$	$Pb^{2+} + 2NO_3^- \leftrightarrow Pb(NO_3)_2$	1.17	Smith *et al.* (1998)

A Mean selected value derived from Carell and Olin (1960), Azab (1987), Cross *et al.* (1987) and Ferri *et al.* (1987b, 1989)

B Mean selected value derived from Olin (1960), Sylva and Brown (1980) and Cruwagen and Van de Water (1993)

C Mean selected value derived from Sylva and Brown (1980) and Cruwagen and Van de Water (1993)

D Selected value extrapolated from the statistical calculation by Gunneriusson *et al.* (1994) using the values of $PbOH^+$ and $PbCl^+$ from Smith *et al.* (1998)

Table 17 (cont.). Selected stability constants for lead (Pb^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$PbCO_3$	$Pb^{2+} + CO_3^{2-} \leftrightarrow PbCO_3$	6.98	Millero and Hawke (1992)
$Pb_2CO_3^{2+}$	$2Pb^{2+} + CO_3^{2-} \leftrightarrow Pb_2CO_3^{2+}$	8.28	Néher-Neumann (1992)
$Pb_3CO_3^{4+}$	$3Pb^{2+} + CO_3^{2-} \leftrightarrow Pb_3CO_3^{4+}$	7.19	Néher-Neumann (1992)
$Pb(CO_3)_2^{2-}$	$Pb^{2+} + 2CO_3^{2-} \leftrightarrow Pb(CO_3)_2^{2-}$	10.23	Millero and Hawke (1992)
$PbHCO_3^+$	$Pb^{2+} + H^+ + CO_3^{2-} \leftrightarrow PbHCO_3^+$	12.72	Néher-Neumann (1992)
$Pb(OH)CO_3^-$	$Pb^{2+} + H_2O + CO_3^{2-} \leftrightarrow Pb(OH)CO_3^- + H^+$	-1.75	A
$PbHPO_4$	$Pb^{2+} + H^+ + PO_4^{3-} \leftrightarrow PbHPO_4$	15.45	Smith *et al.* (1998)
$Pb(HPO_4)_2^{2-}$	$Pb^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Pb(HPO_4)_2^{2-}$	28.74	May *et al.* (1977)
$PbH_2PO_4^+$	$Pb^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow PbH_2PO_4^+$	21.06	Smith *et al.* (1998)
Organic complexes			
PbAsp	$Pb^{2+} + Asp^{2-} \leftrightarrow PbAsp$	6.88	Section 5
$Pb(Asp)_2^{2-}$	$Pb^{2+} + 2Asp^{2-} \leftrightarrow Pb(Asp)_2^{2-}$	9.62	Section 5
$PbHAsp^+$	$Pb^{2+} + H^+ + Asp^{2-} \leftrightarrow PbHAsp^+$	12.20	Section 5
PbH_2Asp^{2+}	$Pb^{2+} + 2H^+ + Asp^{2-} \leftrightarrow PbH_2Asp^{2+}$	14.94	Bottari *et al.* (1989a)
$PbH(Asp)_2^-$	$Pb^{2+} + H^+ + 2Asp^{2-} \leftrightarrow PbH(Asp)_2^-$	17.52	Bottari *et al.* (1989a)
$Pb(HAsp)_2$	$Pb^{2+} + 2H^+ + 2Asp^{2-} \leftrightarrow Pb(HAsp)_2$	23.78	Bottari *et al.* (1989a)
$PbOHAsp^-$	$Pb^{2+} + H_2O + Asp^{2-} \leftrightarrow PbOHAsp^- + H^+$	-1.99	Diez-Cabellero *et al.* (1985b)

A Selected value derived from a knowledge of the stoichiometric ratios between $Pb(CO_3)_2^{2-}$, $Pb(OH)_3^-$ and $Pb(OH)CO_3^-$ established by Ferri *et al.* (1987b), together with the two former selected stability constants as given by Smith *et al.* (1998)

Table 17 (cont.). Selected stability constants for lead (Pb^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Pb(Asp)_2CO_3^{4-}$	$Pb^{2+} + 2Asp^{2-} + CO_3^{2-} \leftrightarrow Pb(Asp)_2CO_3^{4-}$	10.12	Rao and Subrahmanya (1964a)[A]
$PbCit^-$	$Pb^{2+} + Cit^{3-} \leftrightarrow PbCit^-$	5.47	Section 5
Pb_2Cit^+	$2Pb^{2+} + Cit^{3-} \leftrightarrow Pb_2Cit^+$	8.07	Ekström and Olin (1978)
$Pb(Cit)_2^{4-}$	$Pb^{2+} + 2Cit^{3-} \leftrightarrow Pb(Cit)_2^{4-}$	6.48	Section 5
$Pb_2(Cit)_2^{2-}$	$2Pb^{2+} + 2Cit^{3-} \leftrightarrow Pb_2(Cit)_2^{2-}$	12.94	Ekström and Olin (1978)
$Pb(Cit)_3^{7-}$	$Pb^{2+} + 3Cit^{3-} \leftrightarrow Pb(Cit)_3^{7-}$	4.74	Donda and Giuliana (1963)
$Pb_2(Cit)_3^{5-}$	$2Pb^{2+} + 3Cit^{3-} \leftrightarrow Pb_2(Cit)_3^{5-}$	13.29	Ekström and Olin (1978)
$PbHCit$	$Pb^{2+} + H^+ + Cit^{3-} \leftrightarrow PbHCit$	9.62	Section 5
$Pb_2H(Cit)_2^-$	$2Pb^{2+} + H^+ + 2Cit^{3-} \leftrightarrow Pb_2H(Cit)_2^-$	17.38	Ekström and Olin (1978)
PbH_2Cit^+	$Pb^{2+} + 2H^+ + Cit^{3-} \leftrightarrow PbH_2Cit^+$	12.38	Section 5
$PbH(Cit)_2^{3-}$	$Pb^{2+} + H^+ + 2Cit^{3-} \leftrightarrow PbH(Cit)_2^{3-}$	12.04	Ekström and Olin (1978)
$Pb(HCit)_2^{2-}$	$Pb^{2+} + 2H^+ + 2Cit^{3-} \leftrightarrow Pb(HCit)_2^{2-}$	16.88	Section 5
$PbH_3(Cit)_2^-$	$Pb^{2+} + 3H^+ + 2Cit^{3-} \leftrightarrow PbH_3(Cit)_2^-$	20.63	Ekström and Olin (1978)
$PbOHCit^{2-}$	$Pb^{2+} + H_2O + Cit^{3-} \leftrightarrow PbOHCit^{2-} + H^+$	-2.81	Ekström and Olin (1978)
$Pb_2OH(Cit)_2^{3-}$	$2Pb^{2+} + H_2O + 2Cit^{3-} \leftrightarrow Pb_2OH(Cit)_2^{3-} + H^+$	6.27	Ekström and Olin (1978)
$Pb_2(OH)_2(Cit)_2^{4-}$	$2Pb^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Pb_2(OH)_2(Cit)_2^{4-} + 2H^+$	-2.00	Ekström and Olin (1978)
$Pb_4OH(Cit)_3^{2-}$	$4Pb^{2+} + H_2O + 3Cit^{3-} \leftrightarrow Pb_4OH(Cit)_3^{2-} + H^+$	19.58	Ekström and Olin (1978)
$Pb_4(OH)_2(Cit)_3^{3-}$	$4Pb^{2+} + 2H_2O + 3Cit^{3-} \leftrightarrow Pb_4(OH)_2(Cit)_3^{3-} + 2H^+$	12.77	Ekström and Olin (1978)
$PbCitHPO_4^{3-}$	$Pb^{2+} + Cit^{3-} + H^+ + PO_4^{3-} \leftrightarrow PbCitHPO_4^{3-}$	23.16	Ramamoorthy and Manning (1975)
$PbMal$	$Pb^{2+} + Mal^{2-} \leftrightarrow PbMal$	3.88	Section 5

[A] Selected value was derived using the value of $Pb(Asp)_2^{2-}$ provided here, added to the original authors difference between $Pb(Asp)_2^{2-}$ and $Pb(Asp)_2CO_3^{4-}$

Table 17 (cont.). Selected stability constants for lead (Pb^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Pb(Mal)_2^{2-}$	$Pb^{2+} + 2Mal^{2-} \leftrightarrow Pb(Mal)_2^{2-}$	4.99	Section 5
$Pb(Mal)_3^{4-}$	$Pb^{2+} + 3Mal^{2-} \leftrightarrow Pb(Mal)_3^{4-}$	4.38	Section 5
$PbHMal^+$	$Pb^{2+} + H^+ + Mal^{2-} \leftrightarrow PbHMal^+$	7.01	Hammam *et al.* (1977)
$PbH(Mal)_2^-$	$Pb^{2+} + H^+ + 2Mal^{2-} \leftrightarrow PbH(Mal)_2^-$	9.50	Hammam *et al.* (1977)
$PbH(Mal)_3^{3-}$	$Pb^{2+} + H^+ + 3Mal^{2-} \leftrightarrow PbH(Mal)_3^{3-}$	9.84	Hammam *et al.* (1977)
$Pb(HMal)_2$	$Pb^{2+} + 2H^+ + 2Mal^{2-} \leftrightarrow Pb(HMal)_2$	12.97	Hammam *et al.* (1977)
$PbTri^-$	$Pb^{2+} + Tri^{3-} \leftrightarrow PbTri^-$	4.39	Ajayi *et al.* (1979)
$Pb(Tri)_2^{4-}$	$Pb^{2+} + 2Tri^{3-} \leftrightarrow Pb(Tri)_2^{4-}$	5.31	Ajayi *et al.* (1979)
$Pb_2(Tri)_2^{2-}$	$2Pb^{2+} + 2Tri^{3-} \leftrightarrow Pb_2(Tri)_2^{2-}$	10.92	Ajayi *et al.* (1979)
$PbHTri$	$Pb^{2+} + H^+ + Tri^{3-} \leftrightarrow PbHTri$	9.34	Ajayi *et al.* (1979)
PbH_2Tri^+	$Pb^{2+} + 2H^+ + Tri^{3-} \leftrightarrow PbH_2Tri^+$	13.02	Ajayi *et al.* (1979)
$PbH(Tri)_2^{3-}$	$Pb^{2+} + H^+ + 2Tri^{3-} \leftrightarrow PbH(Tri)_2^{3-}$	11.39	Ajayi *et al.* (1979)
$Pb(HTri)_2^{2-}$	$Pb^{2+} + 2H^+ + 2Tri^{3-} \leftrightarrow Pb(HTri)_2^{2-}$	16.74	Ajayi *et al.* (1979)
$PbH_3(Tri)_2^-$	$Pb^{2+} + 3H^+ + 2Tri^{3-} \leftrightarrow PbH_3(Tri)_2^-$	21.25	Ajayi *et al.* (1979)
$Pb_2H(Tri)_2^-$	$2Pb^{2+} + H^+ + 2Tri^{3-} \leftrightarrow Pb_2H(Tri)_2^-$	16.11	Ajayi *et al.* (1979)
Minerals			
$PbHPO_4$	$PbHPO_4 \leftrightarrow Pb^{2+} + HPO_4^{2-}$	-11.28	Brown *et al.* (1996b)

Table 18. Selected stability constants for zinc (Zn^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$ZnOH^+$	$Zn^{2+} + H_2O \leftrightarrow ZnOH^+ + H^+$	-8.92	Smith *et al.* (1998)
$Zn(OH)_2$	$Zn^{2+} + 2H_2O \leftrightarrow Zn(OH)_2 + 2H^+$	-17.80	Smith *et al.* (1998)
$Zn(OH)_3^-$	$Zn^{2+} + 3H_2O \leftrightarrow Zn(OH)_3^- + 3H^+$	-28.10	Smith *et al.* (1998)
$Zn(OH)_4^{2-}$	$Zn^{2+} + 4H_2O \leftrightarrow Zn(OH)_4^{2-} + 4H^+$	-40.50	Smith *et al.* (1998)
Zn_2OH^{3+}	$2Zn^{2+} + H_2O \leftrightarrow Zn_2OH^{3+} + H^+$	-8.50	Smith *et al.* (1998)
$Zn_2(OH)_6^{2-}$	$2Zn^{2+} + 6H_2O \leftrightarrow Zn_2(OH)_6^{2-} + 6H^+$	-57.80	Baes and Mesmer (1976)
$Zn_4(OH)_4^{4+}$	$4Zn^{2+} + 4H_2O \leftrightarrow Zn_4(OH)_4^{4+} + 4H^+$	-27.43	Smith *et al.* (1998)
$ZnCl^+$	$Zn^{2+} + Cl^- \leftrightarrow ZnCl^+$	0.20	Sverjensky *et al.* (1997)
$ZnCl_2$	$Zn^{2+} + 2Cl^- \leftrightarrow ZnCl_2$	0.25	Sverjensky *et al.* (1997)
$ZnOHCl$	$Zn^{2+} + H_2O + Cl^- \leftrightarrow ZnOHCl + H^+$	-7.48	Parkhurst (1990)
$ZnSO_4$	$Zn^{2+} + SO_4^{2-} \leftrightarrow ZnSO_4$	2.34	Smith *et al.* (1998)
$Zn(SO_4)_2^{2-}$	$Zn^{2+} + 2SO_4^{2-} \leftrightarrow Zn(SO_4)_2^{2-}$	3.63	Turner *et al.* (1981)
$Zn(SO_4)_3^{4-}$	$Zn^{2+} + 3SO_4^{2-} \leftrightarrow Zn(SO_4)_3^{4-}$	2.70	Turner *et al.* (1981)
$Zn(SO_4)_4^{6-}$	$Zn^{2+} + 4SO_4^{2-} \leftrightarrow Zn(SO_4)_4^{6-}$	-0.82	Turner *et al.* (1981)
$ZnNO_3^+$	$Zn^{2+} + CO_3^{2-} \leftrightarrow ZnNO_3^+$	0.32	Smith *et al.* (1998)
$Zn(NO_3)_2$	$Zn^{2+} + 2NO_3^- \leftrightarrow Zn(NO_3)_2$	-0.15	Smith *et al.* (1998)
$ZnCO_3$	$Zn^{2+} + CO_3^{2-} \leftrightarrow ZnCO_3$	5.10	Ferri *et al.* (1985)
$Zn(CO_3)_2^{2-}$	$Zn^{2+} + 2CO_3^{2-} \leftrightarrow Zn(CO_3)_2^{2-}$	7.25	Millero and Hawke (1992)
$ZnHCO_3^+$	$Zn^{2+} + H^+ + CO_3^{2-} \leftrightarrow ZnHCO_3^+$	11.52	Smith *et al.* (1998)
$Zn(OH)CO_3^-$	$Zn^{2+} + H_2O + CO_3^{2-} \leftrightarrow Zn(OH)CO_3^- + H^+$	-4.20	Bruno *et al.* (1990)

Table 18 (cont.). Selected stability constants for zinc (Zn^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$ZnHPO_4$	$Zn^{2+} + H^+ + PO_4^{3-} \leftrightarrow ZnHPO_4$	15.65	A
$Zn(HPO_4)_2^{2-}$	$Zn^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Zn(HPO_4)_2^{2-}$	31.80	Iuliano (1994)
$Zn_2(HPO_4)_2$	$2Zn^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Zn_2(HPO_4)_2$	34.94	Childs (1970)
$ZnH_2PO_4^+$	$Zn^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow ZnH_2PO_4^+$	20.46	Iuliano (1994)
$Zn(H_2PO_4)_2$	$Zn^{2+} + 4H^+ + 2PO_4^{3-} \leftrightarrow Zn(H_2PO_4)_2$	41.12	Iuliano (1994)
Organic complexes			
ZnAsp	$Zn^{2+} + Asp^{2-} \leftrightarrow ZnAsp$	6.67	Section 5
$Zn(Asp)_2^{2-}$	$Zn^{2+} + 2Asp^{2-} \leftrightarrow Zn(Asp)_2^{2-}$	10.91	Section 5
$Zn(Asp)_3^{4-}$	$Zn^{2+} + 3Asp^{2-} \leftrightarrow Zn(Asp)_3^{4-}$	12.38	Bottari *et al.* (1990)
$ZnHAsp^+$	$Zn^{2+} + H^+ + Asp^{2-} \leftrightarrow ZnHAsp^+$	12.03	Section 5
ZnH_2Asp^{2+}	$Zn^{2+} + 2H^+ + Asp^{2-} \leftrightarrow ZnH_2Asp^{2+}$	13.98	Bottari *et al.* (1990)
$ZnH(Asp)_2^-$	$Zn^{2+} + H^+ + 2Asp^{2-} \leftrightarrow ZnH(Asp)_2^-$	17.34	Bottari *et al.* (1990)
$ZnH(Asp)_3^{3-}$	$Zn^{2+} + H^+ + 3Asp^{2-} \leftrightarrow ZnH(Asp)_3^{3-}$	20.68	Bottari *et al.* (1990)
$Zn(HAsp)_2$	$Zn^{2+} + 2H^+ + 2Asp^{2-} \leftrightarrow Zn(HAsp)_2$	21.98	Bottari *et al.* (1990)
$ZnH_2(Asp)_3^{2-}$	$Zn^{2+} + 2H^+ + 3Asp^{2-} \leftrightarrow ZnH_2(Asp)_3^{2-}$	27.93	Bottari *et al.* (1990)
$Zn(OH)_2(Asp)_2^{4-}$	$Zn^{2+} + 2H_2O + 2Asp^{2-} \leftrightarrow Zn(OH)_2(Asp)_2^{4-} + 2H^+$	-11.14	Makar *et al.* (1976)
$Zn_2(OH)_2Asp$	$2Zn^{2+} + 2H_2O + Asp^{2-} \leftrightarrow Zn_2(OH)_2Asp + 2H^+$	-9.27	Berthon and Germonneau (1982)

A Mean selected value derived from Sigel *et al.* (1967), Childs (1970) and Ramamoorthy and Manning (1974b)

Table 18 (cont.). Selected stability constants for zinc (Zn^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$ZnCit^-$	$Zn^{2+} + Cit^{3-} \leftrightarrow ZnCit^-$	6.16	Section 5
$Zn(Cit)_2^{4-}$	$Zn^{2+} + 2Cit^{3-} \leftrightarrow Zn(Cit)_2^{4-}$	7.67	Section 5
$Zn(Cit)_3^{7-}$	$Zn^{2+} + 3Cit^{3-} \leftrightarrow Zn(Cit)_3^{7-}$	6.80	Section 5
$ZnHCit$	$Zn^{2+} + H^+ + Cit^{3-} \leftrightarrow ZnHCit$	10.18	Section 5
ZnH_2Cit^+	$Zn^{2+} + 2H^+ + Cit^{3-} \leftrightarrow ZnH_2Cit^+$	13.00	Section 5
$ZnH(Cit)_2^{3-}$	$Zn^{2+} + H^+ + 2Cit^{3-} \leftrightarrow ZnH(Cit)_2^{3-}$	13.73	Christie *et al.* (1991)
$ZnOHCit^{2-}$	$Zn^{2+} + H_2O + Cit^{3-} \leftrightarrow ZnOHCit^{2-} + H^+$	-1.81	Section 5
$Zn_2(OH)_2(Cit)_2^{4-}$	$2Zn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Zn_2(OH)_2(Cit)_2^{4-} + 2H^+$	-1.76	Section 5
$ZnCitHPO_4^{3-}$	$Zn^{2+} + Cit^{3-} + H^+ + PO_4^{3-} \leftrightarrow ZnCitHPO_4^{3-}$	23.93	Ramamoorthy and Manning (1975)
$ZnCu(OH)_2(Cit)_2^{4-}$	$Zn^{2+} + Cu^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow ZnCu(OH)_2(Cit)_2^{4-} + 2H^+$	2.30	Section 5
$CdZn(OH)_2(Cit)_2^{4-}$	$Cd^{2+} + Zn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CdZn(OH)_2(Cit)_2^{4-} + 2H^+$	-2.44	Amico *et al.* (1985)
$ZnMal$	$Zn^{2+} + Mal^{2-} \leftrightarrow ZnMal$	3.74	Section 5
$Zn(Mal)_2^{2-}$	$Zn^{2+} + 2Mal^{2-} \leftrightarrow Zn(Mal)_2^{2-}$	5.22	Powell and Johnson (1969)
$Zn(Mal)_3^{4-}$	$Zn^{2+} + 3Mal^{2-} \leftrightarrow Zn(Mal)_3^{4-}$	5.79	Makar *et al.* (1976)
$Zn_2(Mal)_2$	$2Zn^{2+} + 2Mal^{2-} \leftrightarrow Zn_2(Mal)_2$	9.25	Makar *et al.* (1976)
$Zn_2H(Mal)_2^+$	$2Zn^{2+} + H^+ + 2Mal^{2-} \leftrightarrow Zn_2H(Mal)_2^+$	12.36	Makar *et al.* (1976)
$ZnHMal^+$	$Zn^{2+} + H^+ + Mal^{2-} \leftrightarrow ZnHMal^+$	7.00	Section 5
$ZnH(Mal)_3^{3-}$	$Zn^{2+} + H^+ + 3Mal^{2-} \leftrightarrow ZnH(Mal)_3^{3-}$	11.59	Makar *et al.* (1976)
$ZnH_2(Mal)_3^{2-}$	$Zn^{2+} + H^+ + 3Mal^{2-} \leftrightarrow ZnH_2(Mal)_3^{2-}$	16.40	Makar *et al.* (1976)
$ZnOH(Mal)_3^{5-}$	$Zn^{2+} + H_2O + 3Mal^{2-} \leftrightarrow ZnOH(Mal)_3^{5-} + H^+$	-2.20	Makar *et al.* (1976)

Table 18 (cont.). Selected stability constants for zinc (Zn^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$ZnMalAsp^{2-}$	$Zn^{2+} + Mal^{2-} + Asp^{2-} \leftrightarrow ZnMalAsp^{2-}$	8.82	Ramanujam and Selvarajan (1981)
ZnSal	$Zn^{2+} + Sal^{2-} \leftrightarrow ZnSal$	7.83	Section 5
$Zn(Sal)_2^{2-}$	$Zn^{2+} + 2Sal^{2-} \leftrightarrow Zn(Sal)_2^{2-}$	11.84	Section 5
$ZnHSal^{+}$	$Zn^{2+} + H^{+} + Sal^{2-} \leftrightarrow ZnHSal^{+}$	15.62	Bai (1983)
$ZnTri^{-}$	$Zn^{2+} + Tri^{3-} \leftrightarrow ZnTri^{-}$	3.70	Campi *et al.* (1964)
ZnHTri	$Zn^{2+} + H^{+} + Tri^{3-} \leftrightarrow ZnHTri$	8.95	Campi *et al.* (1964)
ZnH_2Tri^{+}	$Zn^{2+} + 2H^{+} + Tri^{3-} \leftrightarrow ZnH_2Tri^{+}$	12.73	Campi *et al.* (1964)
Minerals			
$Zn(OH)_2$ [sweetite]	$Zn(OH)_2 + 2H^{+} \leftrightarrow Zn^{2+} + 2H_2O$	11.74	Smith *et al.* (1998)
$ZnCO_3$ [smithsonite]	$ZnCO_3 \leftrightarrow Zn^{2+} + CO_3^{2-}$	-9.84	Clever *et al.* (1992)
$ZnHPO_4$	$ZnHPO_4 \leftrightarrow Zn^{2+} + HPO_4^{2-}$	-6.74	Mel'nikov *et al.* (1981)

Table 19. Selected stability constants for copper (Cu^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$CuOH^+$	$Cu^{2+} + H_2O \leftrightarrow CuOH^+ + H^+$	-7.51	Smith *et al.* (1998)
$Cu(OH)_2$	$Cu^{2+} + 2H_2O \leftrightarrow Cu(OH)_2 + 2H^+$	-16.12	Smith *et al.* (1998)
$Cu(OH)_3^-$	$Cu^{2+} + 3H_2O \leftrightarrow Cu(OH)_3^- + 3H^+$	-26.89	Smith *et al.* (1998)
$Cu(OH)_4^{2-}$	$Cu^{2+} + 4H_2O \leftrightarrow Cu(OH)_4^{2-} + 4H^+$	-40.00	Smith *et al.* (1998)
Cu_2OH^{3+}	$2Cu^{2+} + H_2O \leftrightarrow Cu_2OH^{3+} + H^+$	-6.28	De Robertis *et al.* (1997)
$Cu_2(OH)_2^{2+}$	$2Cu^{2+} + 2H_2O \leftrightarrow Cu_2(OH)_2^{2+} + 2H^+$	-10.55	Smith *et al.* (1998)
$Cu_3(OH)_4^{2+}$	$3Cu^{2+} + 4H_2O \leftrightarrow Cu_3(OH)_4^{2+} + 4H^+$	-21.03	Smith *et al.* (1998)
$CuCl^+$	$Cu^{2+} + Cl^- \leftrightarrow CuCl^+$	0.64	Wang *et al.* (1997)
$CuCl_2$	$Cu^{2+} + 2Cl^- \leftrightarrow CuCl_2$	0.60	Wang *et al.* (1997)
$CuSO_4$	$Cu^{2+} + SO_4^{2-} \leftrightarrow CuSO_4$	2.34	Smith *et al.* (1998)
$CuNO_3^+$	$Cu^{2+} + CO_3^{2-} \leftrightarrow CuNO_3^+$	0.42	Smith *et al.* (1998)
$Cu(NO_3)_2$	$Cu^{2+} + 2NO_3^- \leftrightarrow Cu(NO_3)_2$	-0.12	Smith *et al.* (1998)
$CuCO_3$	$Cu^{2+} + CO_3^{2-} \leftrightarrow CuCO_3$	6.78	Smith *et al.* (1998)
$Cu(OH)CO_3^-$	$Cu^{2+} + H_2O + CO_3^{2-} \leftrightarrow Cu(OH)CO_3^- + H^+$	-2.66	Byrne and Miller (1985)
$CuHCO_3^+$	$Cu^{2+} + H^+ + CO_3^{2-} \leftrightarrow CuHCO_3^+$	12.13	Smith *et al.* (1998)
$CuPO_4^-$	$Cu^{2+} + PO_4^{3-} \leftrightarrow CuPO_4^-$	3.69	Falck (1992)
$Cu(PO_4)_2^{4-}$	$Cu^{2+} + 2PO_4^{3-} \leftrightarrow Cu(PO_4)_2^{4-}$	4.92	Falck (1992)
$CuHPO_4$	$Cu^{2+} + H^+ + PO_4^{3-} \leftrightarrow CuHPO_4$	15.65	A
$Cu(HPO_4)_2^{2-}$	$Cu^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Cu(HPO_4)_2^{2-}$	32.06	Ciavatta *et al.* (1993)

A Mean selected value derived from Ciavatta *et al.* (1993) and Zhao *et al.* (1996)

Table 19 (cont.). Selected stability constants for copper (Cu^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$CuH_2PO_4^+$	$Cu^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow CuH_2PO_4^+$	20.70	Ciavatta *et al.* (1993)
$Cu(H_2PO_4)_2$	$Cu^{2+} + 4H^+ + 2PO_4^{3-} \leftrightarrow Cu(H_2PO_4)_2$	41.06	Ciavatta *et al.* (1993)
$Cu_2(HPO_4)_2$	$2Cu^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Cu_2(HPO_4)_2$	35.44	Childs (1970)
Organic complexes			
CuAsp	$Cu^{2+} + Asp^{2-} \leftrightarrow CuAsp$	9.66	Section 5
Cu_2Asp^{2+}	$2Cu^{2+} + Asp^{2-} \leftrightarrow Cu_2Asp^{2+}$	11.20	Daniele *et al.* (1984a)
$Cu(Asp)_2^{2-}$	$Cu^{2+} + 2Asp^{2-} \leftrightarrow Cu(Asp)_2^{2-}$	16.62	Section 5
Cu_2Asp_2	$2Cu^{2+} + 2Asp^{2-} \leftrightarrow Cu_2Asp_2$	20.78	Daniele *et al.* (1984a)
$CuHAsp^+$	$Cu^{2+} + H^+ + Asp^{2-} \leftrightarrow CuHAsp^+$	13.41	Section 5
CuH_2Asp^{2+}	$Cu^{2+} + 2H^+ + Asp^{2-} \leftrightarrow CuH_2Asp^{2+}$	14.86	Bottari *et al.* (1989b)
$CuH(Asp)_2^-$	$Cu^{2+} + H^+ + 2Asp^{2-} \leftrightarrow CuH(Asp)_2^-$	21.60	Section 5
$Cu(HAsp)_2$	$Cu^{2+} + 2H^+ + 2Asp^{2-} \leftrightarrow Cu(HAsp)_2$	25.59	Section 5
$CuOHAsp^-$	$Cu^{2+} + H_2O + Asp^{2-} \leftrightarrow CuOHAsp^- + H^+$	-0.81	Lomozik *et al.* (1983)
$CuAspMal^{2-}$	$Cu^{2+} + Asp^{2-} + Mal^{2-} \leftrightarrow CuAspMal^{2-}$	13.22	Shah and Gupta (1980)
$CuAspSal^{2-}$	$Cu^{2+} + Asp^{2-} + Sal^{2-} \leftrightarrow CuAspSal^{2-}$	4.04	Diez-Cabellero *et al.* (1985b)
$CuCit^-$	$Cu^{2+} + Cit^{3-} \leftrightarrow CuCit^-$	7.35	Section 5
Cu_2Cit^+	$2Cu^{2+} + Cit^{3-} \leftrightarrow Cu_2Cit^+$	9.80	Campi *et al.* (1964)
$Cu(Cit)_2^{4-}$	$Cu^{2+} + 2Cit^{3-} \leftrightarrow Cu(Cit)_2^{4-}$	9.33	Section 5
$Cu_2(Cit)_2^{2-}$	$2Cu^{2+} + 2Cit^{3-} \leftrightarrow Cu_2(Cit)_2^{2-}$	16.95	Section 5

Table 19 (cont.). Selected stability constants for copper (Cu^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
CuHCit	$Cu^{2+} + H^+ + Cit^{3-} \leftrightarrow CuHCit$	10.86	Section 5
CuH_2Cit^+	$Cu^{2+} + 2H^+ + Cit^{3-} \leftrightarrow CuH_2Cit^+$	13.64	Section 5
$CuH(Cit)_2^{3-}$	$Cu^{2+} + H^+ + 2Cit^{3-} \leftrightarrow CuH(Cit)_2^{3-}$	14.26	Bottari (1975a)
$Cu(HCit)_2^{2-}$	$Cu^{2+} + 2H^+ + 2Cit^{3-} \leftrightarrow Cu(HCit)_2^{2-}$	19.56	Bottari (1975a)
$CuOHCit^{2-}$	$Cu^{2+} + H_2O + Cit^{3-} \leftrightarrow CuOHCit^{2-} + H^+$	2.77	Section 5
$Cu(OH)_2Cit^{3-}$	$Cu^{2+} + 2H_2O + Cit^{3-} \leftrightarrow Cu(OH)_2Cit^{3-} + 2H^+$	-9.71	Miloserdova *et al.* (1992)
$Cu(OH)_2(Cit)_2^{6-}$	$Cu^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Cu(OH)_2(Cit)_2^{6-} + 2H^+$	-8.00	Section 5
Cu_2OHCit	$2Cu^{2+} + H_2O + Cit^{3-} \leftrightarrow Cu_2OHCit + H^+$	6.75	Section 5
$Cu_2OH(Cit)_2^{3-}$	$2Cu^{2+} + H_2O + 2Cit^{3-} \leftrightarrow Cu_2OH(Cit)_2^{3-} + H^+$	12.09	Section 5
$Cu_2(OH)_2Cit^-$	$2Cu^{2+} + 2H_2O + Cit^{3-} \leftrightarrow Cu_2(OH)_2Cit^- + 2H^+$	4.47	Bottari (1975a)
$Cu_2(OH)_2(Cit)_2^{4-}$	$2Cu^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Cu_2(OH)_2(Cit)_2^{4-} + 2H^+$	6.58	Section 5
$Cu_2(OH)_3(Cit)_2^{5-}$	$2Cu^{2+} + 3H_2O + 2Cit^{3-} \leftrightarrow Cu_2(OH)_3(Cit)_2^{5-} + 3H^+$	-4.77	Sal'nikov and Zhuravleva (1986)
$CuMg(OH)_2(Cit)_2^{4-}$	$Cu^{2+} + Mg^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CuMg(OH)_2(Cit)_2^{4-} + 2H^+$	-0.24	Blomqvist and Still (1984)
$CuFe(Cit)_2^-$	$Cu^{2+} + Fe^{2+} + 2Cit^{3-} \leftrightarrow CuFe(Cit)_2^- + e^-$	11.66	Sal'nikov and Zhuravleva (1986)
$CuFe(OH)_2(Cit)_2^{3-}$	$Cu^{2+} + Fe^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CuFe(OH)_2(Cit)_2^{3-} + 2H^+ + e^-$	3.63	Sal'nikov and Zhuravleva (1986)
$CuFe(OH)_3(Cit)_2^{4-}$	$Cu^{2+} + Fe^{2+} + 3H_2O + 2Cit^{3-} \leftrightarrow CuFe(OH)_3(Cit)_2^{4-} + 3H^+ + e^-$	-4.17	Sal'nikov and Zhuravleva (1986)
$ZnCu(OH)_2(Cit)_2^{4-}$	$Zn^{2+} + Cu^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow ZnCu(OH)_2(Cit)_2^{4-} + 2H^+$	2.30	Section 5
CuMal	$Cu^{2+} + Mal^{2-} \leftrightarrow CuMal$	5.88	Section 5
$Cu(Mal)_2^{2-}$	$Cu^{2+} + 2Mal^{2-} \leftrightarrow Cu(Mal)_2^{2-}$	8.78	Section 5
$Cu(Mal)_3^{4-}$	$Cu^{2+} + 3Mal^{2-} \leftrightarrow Cu(Mal)_3^{4-}$	8.13	Section 5
$CuHMal^+$	$Cu^{2+} + H^+ + Mal^{2-} \leftrightarrow CuHMal^+$	8.14	Section 5

Table 19 (cont.). Selected stability constants for copper (Cu^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$Cu(HMal)_2$	$Cu^{2+} + 2H^+ + 2Mal^{2-} \leftrightarrow Cu(HMal)_2$	14.64	Tedesco and González-Quitana (1975)
$CuOHMal^-$	$Cu^{2+} + H_2O + Mal^{2-} \leftrightarrow CuOHMal^+ + H^+$	-0.34	A
$CuMalAsp^{2-}$	$Cu^{2+} + Mal^{2-} + Asp^{2-} \leftrightarrow CuMalAsp^{2-}$	13.17	Section 5
$CuMalSal^{2-}$	$Cu^{2+} + Mal^{2-} + Sal^{2-} \leftrightarrow CuMalSal^{2-}$	17.26	Venkatnarayana *et al.* (1988)
CuSal	$Cu^{2+} + Sal^{2-} \leftrightarrow CuSal$	11.25	Section 5
$Cu(Sal)_2{}^{2-}$	$Cu^{2+} + 2Sal^{2-} \leftrightarrow Cu(Sal)_2{}^{2-}$	19.24	Section 5
$CuHSal^+$	$Cu^{2+} + H^+ + Sal^{2-} \leftrightarrow CuHSal^+$	15.80	Section 5
$CuH(Sal)_2{}^-$	$Cu^{2+} + H^+ + 2Sal^{2-} \leftrightarrow CuH(Sal)_2{}^-$	26.07	Brumas *et al.* (1995)
$Cu(HSal)_2$	$Cu^{2+} + 2H^+ + 2Sal^{2-} \leftrightarrow Cu(HSal)_2$	31.55	Section 5
$CuTri^-$	$Cu^{2+} + Tri^{3-} \leftrightarrow CuTri^-$	4.72	Section 5
Cu_2Tri^+	$2Cu^{2+} + Tri^{3-} \leftrightarrow Cu_2Tri^+$	6.99	Campi *et al.* (1964)
CuHTri	$Cu^{2+} + H^+ + Tri^{3-} \leftrightarrow CuHTri$	9.91	Campi *et al.* (1964)
CuH_2Tri^+	$Cu^{2+} + 2H^+ + Tri^{3-} \leftrightarrow CuH_2Tri^+$	13.19	Campi *et al.* (1964)
$CuOHTri^{2-}$	$Cu^{2+} + H_2O + Tri^{3-} \leftrightarrow CuOHTri^{2-} + H^+$	-1.77	A

A Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

Table 19 (cont.). Selected stability constants for copper (Cu^{2+}) complexes

Species	Reaction	log K_o	Reference
Minerals			
$Cu(OH)_2$	$Cu(OH)_2 + 2H^+ \leftrightarrow Cu^{2+} + 2H_2O$	9.69	Hidmi and Edwards (1999)
$Cu_2(OH)_2CO_3$ [malachite]	$Cu_2(OH)_2CO_3 + 2H^+ \leftrightarrow 2Cu^{2+} + CO_3^{2-} + 2H_2O$	-5.30	Smith *et al.* (1998)
$Cu_3(OH)_2(CO_3)_2$ [azurite]	$Cu_3(OH)_2(CO_3)_2 + 2H^+ \leftrightarrow 3Cu^{2+} + 2CO_3^{2-} + 2H_2O$	-16.90	Smith *et al.* (1998)
$CuCO_3$	$CuCO_3 \leftrightarrow Cu^{2+} + CO_3^{2-}$	-11.45	Reiterer *et al.* (1981)

Table 20. Selected stability constants for cadmium (Cd^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes			
$CdOH^+$	$Cd^{2+} + H_2O \leftrightarrow CdOH^+ + H^+$	-10.10	Smith *et al.* (1998)
$Cd(OH)_2$	$Cd^{2+} + 2H_2O \leftrightarrow Cd(OH)_2 + 2H^+$	-20.30	Smith *et al.* (1998)
$Cd(OH)_3^-$	$Cd^{2+} + 3H_2O \leftrightarrow Cd(OH)_3^- + 3H^+$	-33.30	Smith *et al.* (1998)
$Cd(OH)_4^{2-}$	$Cd^{2+} + 4H_2O \leftrightarrow Cd(OH)_4^{2-} + 4H^+$	-47.30	Smith *et al.* (1998)
Cd_2OH^{3+}	$2Cd^{2+} + H_2O \leftrightarrow Cu_2OH^{3+} + H^+$	-9.40	Smith *et al.* (1998)
$Cd_4(OH)_4^{4+}$	$4Cd^{2+} + 4H_2O \leftrightarrow Cd_4(OH)_4^{4+} + 4H^+$	-32.80	Smith *et al.* (1998)
$CdCl^+$	$Cd^{2+} + Cl^- \leftrightarrow CdCl^+$	1.97	Sverjensky *et al.* (1997)
$CdCl_2$	$Cd^{2+} + 2Cl^- \leftrightarrow CdCl_2$	2.59	Sverjensky *et al.* (1997)
$CdCl_3^-$	$Cd^{2+} + 3Cl^- \leftrightarrow CdCl_3^-$	2.40	Sverjensky *et al.* (1997)
$CdOHCl$	$Cd^{2+} + H_2O + Cl^- \leftrightarrow CdOHCl + H^+$	-7.40	Parkhurst (1990)
$CdSO_4$	$Cd^{2+} + SO_4^{2-} \leftrightarrow CdSO_4$	2.46	Smith *et al.* (1998)
$Cd(SO_4)_2^{2-}$	$Cd^{2+} + 2SO_4^{2-} \leftrightarrow Cd(SO_4)_2^{2-}$	3.44	Turner *et al.* (1981)
$Cd(SO_4)_3^{4-}$	$Cd^{2+} + 3SO_4^{2-} \leftrightarrow Cd(SO_4)_3^{4-}$	3.09	Turner *et al.* (1981)
$Cd(SO_4)_4^{6-}$	$Cd^{2+} + 4SO_4^{2-} \leftrightarrow Cd(SO_4)_4^{6-}$	-0.72	Turner *et al.* (1981)
$CdNO_3^+$	$Cd^{2+} + CO_3^{2-} \leftrightarrow CdNO_3^+$	0.44	Smith *et al.* (1998)
$Cd(NO_3)_2$	$Cd^{2+} + 2NO_3^- \leftrightarrow Cd(NO_3)_2$	0.22	Smith *et al.* (1998)
$CdCO_3$	$Cd^{2+} + CO_3^{2-} \leftrightarrow CdCO_3$	4.42	A
$Cd(CO_3)_2^{2-}$	$Cd^{2+} + 2CO_3^{2-} \leftrightarrow Cd(CO_3)_2^{2-}$	6.86	B

A Mean selected value derived from Gardner (1974), Bilinski *et al.* (1976), Stella *et al.* (1984) and Rai *et al.* (1991)

B Mean selected value derived from Stella *et al.* (1984) and Rai *et al.* (1991)

Table 20 (cont.). Selected stability constants for cadmium (Cd^{2+}) complexes

Species	Reaction	log K_o	Reference
Inorganic complexes (cont.)			
$CdHCO_3^+$	$Cd^{2+} + H^+ + CO_3^{2-} \leftrightarrow CdHCO_3^+$	11.48	A
$CdHPO_4$	$Cd^{2+} + H^+ + PO_4^{3-} \leftrightarrow CdHPO_4$	16.17	B
$Cd(HPO_4)_2^{2-}$	$Cd^{2+} + 2H^+ + 2PO_4^{3-} \leftrightarrow Cd(HPO_4)_2^{2-}$	30.10	Iuliano and Porto (1994)
$CdH_2PO_4^+$	$Cd^{2+} + 2H^+ + PO_4^{3-} \leftrightarrow CdH_2PO_4^+$	20.76	Iuliano and Porto (1994)
$Cd(H_2PO_4)_2$	$Cd^{2+} + 4H^+ + 2PO_4^{3-} \leftrightarrow Cd(H_2PO_4)_2$	41.02	Iuliano and Porto (1994)
Organic complexes			
CdAsp	$Cd^{2+} + Asp^{2-} \leftrightarrow CdAsp$	5.40	Section 5
$Cd(Asp)_2^{2-}$	$Cd^{2+} + 2Asp^{2-} \leftrightarrow Cd(Asp)_2^{2-}$	8.84	Section 5
$Cd(Asp)_3^{4-}$	$Cd^{2+} + 3Asp^{2-} \leftrightarrow Cd(Asp)_3^{4-}$	10.61	Section 5
$CdHAsp^+$	$Cd^{2+} + H^+ + Asp^{2-} \leftrightarrow CdHAsp^+$	11.69	Bottari *et al.* (1989c)
CdH_2Asp^{2+}	$Cd^{2+} + 2H^+ + Asp^{2-} \leftrightarrow CdH_2Asp^{2+}$	14.31	Bottari *et al.* (1989c)
$CdH(Asp)_2^-$	$Cd^{2+} + H^+ + 2Asp^{2-} \leftrightarrow CdH(Asp)_2^-$	15.93	Bottari *et al.* (1989c)
$CdH(Asp)_3^{3-}$	$Cd^{2+} + H^+ + 3Asp^{2-} \leftrightarrow CdH(Asp)_3^{3-}$	18.85	Bottari *et al.* (1989c)
$Cd(HAsp)_2$	$Cd^{2+} + 2H^+ + 2Asp^{2-} \leftrightarrow Cd(HAsp)_2$	22.88	Bottari *et al.* (1989c)
$CdH_2(Asp)_3^{2-}$	$Cd^{2+} + 2H^+ + 3Asp^{2-} \leftrightarrow CdH_2(Asp)_3^{2-}$	26.58	Bottari *et al.* (1989c)
$CdOHAsp^-$	$Cd^{2+} + H_2O + Asp^{2-} \leftrightarrow CdOHAsp^- + H^+$	-4.39	Simões-Gonçalves and Dos-Santos (1985)

A Mean selected value derived from a recalculated value of Zirino and Yamamoto (1972; see Stipp *et al.*, 1993) and Néher-Neumann (1992)

B Mean selected value derived from Nozaki *et al.* (1973) and Ramamoorthy and Manning (1974b)

Table 20 (cont.). Selected stability constants for cadmium (Cd^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
$CdOH(Asp)_2^{2-}$	$Cd^{2+} + 2H_2O + 2Asp^{2-} \leftrightarrow CdOH(Asp)_2^{2-} + 2H^+$	-3.79	Rao and Subrahmanya (1964b)
$CdCit^-$	$Cd^{2+} + Cit^{3-} \leftrightarrow CdCit^-$	4.87	Section 5
$Cd(Cit)_2^{4-}$	$Cd^{2+} + 2Cit^{3-} \leftrightarrow Cd(Cit)_2^{4-}$	5.19	Section 5
$Cd(Cit)_3^{7-}$	$Cd^{2+} + 3Cit^{3-} \leftrightarrow Cd(Cit)_3^{7-}$	2.70	Section 5
CdHCit	$Cd^{2+} + H^+ + Cit^{3-} \leftrightarrow CdHCit$	9.46	Section 5
$CdH(Cit)_2^{3-}$	$Cd^{2+} + H^+ + 2Cit^{3-} \leftrightarrow CdH(Cit)_2^{3-}$	12.64	Section 5
$Cd(HCit)_2^{2-}$	$Cd^{2+} + 2H^+ + 2Cit^{3-} \leftrightarrow Cd(HCit)_2^{2-}$	15.68	Bottari (1975b)
$CdOHCit^{2-}$	$Cd^{2+} + H_2O + Cit^{3-} \leftrightarrow CdOHCit^{2-} + H^+$	-3.07	Section 5
$Cd_2(OH)_2(Cit)_2^{4-}$	$2Cd^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow Cd_2(OH)_2(Cit)_2^{4-} + 2H^+$	-4.54	Section 5
$CdCitHPO_4^{3-}$	$Cd^{2+} + Cit^{3-} + H^+ + PO_4^{3-} \leftrightarrow CdCitHPO_4^{3-}$	22.77	Ramamoorthy and Manning (1975)
$CdMn(OH)_2(Cit)_2^{4-}$	$Cd^{2+} + Mn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CdMn(OH)_2(Cit)_2^{4-} + 2H^+$	-4.89	Amico *et al.* (1985)
$CdZn(OH)_2(Cit)_2^{4-}$	$Cd^{2+} + Zn^{2+} + 2H_2O + 2Cit^{3-} \leftrightarrow CdZn(OH)_2(Cit)_2^{4-} + 2H^+$	-2.44	Amico *et al.* (1985)
CdMal	$Cd^{2+} + Mal^{2-} \leftrightarrow CdMal$	3.04	Section 5
$Cd(Mal)_2^{2-}$	$Cd^{2+} + 2Mal^{2-} \leftrightarrow Cd(Mal)_2^{2-}$	3.54	Section 5
$Cd(Mal)_3^{4-}$	$Cd^{2+} + 3Mal^{2-} \leftrightarrow Cd(Mal)_3^{4-}$	3.49	Section 5
$CdHMal^+$	$Cd^{2+} + H^+ + Mal^{2-} \leftrightarrow CdHMal^+$	7.23	Section 5
$CdH(Mal)_2^-$	$Cd^{2+} + H^+ + 3Mal^{2-} \leftrightarrow CdH(Mal)_2^-$	8.46	Schwarzenbach and Szilard (1962)
$Cd(HMal)_2$	$Cd^{2+} + 2H^+ + 2Mal^{2-} \leftrightarrow Cd(HMal)_2$	13.16	Schwarzenbach and Szilard (1962)
$CdOHMal^-$	$Cd^{2+} + H_2O + Mal^{2-} \leftrightarrow CdOHMal^+ + H^+$	-4.86	A

A Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

Table 20 (cont.). Selected stability constants for cadmium (Cd^{2+}) complexes

Species	Reaction	log K_o	Reference
Organic complexes (cont.)			
CdSal	$Cd^{2+} + Sal^{2-} \leftrightarrow CdSal$	6.45	Perrin (1958)
$CdHSal^+$	$Cd^{2+} + H^+ + Sal^{2-} \leftrightarrow CdHSal^+$	14.83	Section 5
$Cd(HSal)_2$	$Cd^{2+} + 2H^+ + 2Sal^{2-} \leftrightarrow Cd(HSal)_2$	28.76	Section 5
$CdTri^-$	$Cd^{2+} + Tri^{3-} \leftrightarrow CdTri^-$	3.44	A
CdHTri	$Cd^{2+} + H^+ + Tri^{3-} \leftrightarrow CdHTri$	8.72	B
$CdOHTri^{2-}$	$Cd^{2+} + H_2O + Tri^{3-} \leftrightarrow CdOHTri^{2-} + H^+$	-4.16	C
Minerals			
$Cd(OH)_2$	$Cd(OH)_2 + 2H^+ \leftrightarrow Cd^{2+} + 2H_2O$	13.65	Smith *et al.* (1998)
$CdCO_3$ [otavite]	$CdCO_3 \leftrightarrow Cd^{2+} + CO_3^{2-}$	-12.10	D
$CdHPO_4$	$CdHPO_4 \leftrightarrow Cd^{2+} + HPO_4^{2-}$	-8.56	Brown *et al.* (1996b)

A Selected value was derived from two independent methods: (i) the LFER between 1:1 Zn di- and tri-carboxylate complexes (ZnL) and their corresponding uranyl (CdL) complexes and (ii) the UTMIC, whereby available 1:1 metal tricarballylate (MTri) complexes are regressed against a corresponding value of $g_1(z_M/r_M^2 + g_2)$

B Selected value was derived from two independent methods: (i) the LFER between 1:1 metal tricarballylate complexes (ML) and 1:1:1 metal hydrogen tricarballylate (MHL) complexes and (ii) the unified theory of metal complexation (UTMIC), whereby available 1:1:1 metal hydrogen tricarballylate complexes are regressed against a corresponding value of $g_1(z_M/r_M^2 + g_2)$

C Selected value was derived using linear free energy relationship (LFER) between 1:1 metal di- and tri-carboxylate complexes (ML) and 1:1:1 metal hydroxy di- and tri-carboxylate complexes (MOHL)

D Mean selected value derived from Rai *et al.* (1991), Stipp *et al.* (1993) and Gamsjäger *et al.* (1999)

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5 Appendix

Stability constants for H, Na, Ca, Mg, Mn, Fe, Al, U, Pb, Zn, Cu and Cd complexes with aspartic, citric, malonic, salicylic and tricarballylic acids (that comprise the model FA) are given in **Tables A1–A5**, respectively. Only those data are listed where more than one datum for a particular stability constant was obtained from the literature. Mean values for each metal complex are given in Section 3.6 (**Tables 6–20**). If only a single datum was found in the literature, the referenced value is also given in Section 3.6.

Table A1. Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
CaAsp	2.46	Lumb and Martell (1953)
	2.53	Hardell (1966)
	2.07	Blaquiere and Berthon (1987)
	2.99	Maeda *et al.* (1990)
	2.52	De Stefano *et al.* (1995)
$CaHAsp^+$	11.58	Blaquiere and Berthon (1987)
	11.54	Maeda *et al.* (1990)
	11.44	De Stefano *et al.* (1995)
CaH_2Asp^{2+}	14.86	Blaquiere and Berthon (1987)
	14.33	De Stefano *et al.* (1995)
MgAsp	3.29	Lumb and Martell (1953)
	3.01	Blaquiere and Berthon (1987)
	3.11	Benedikovic *et al.* (1991)
	3.08	De Stefano *et al.* (1995)
$MgHAsp^+$	11.47	Blaquiere and Berthon (1987)
	11.33	De Stefano *et al.* (1995)
MgH_2Asp^{2+}	14.80	Blaquiere and Berthon (1987)
	14.02	De Stefano *et al.* (1995)
FeAsp	5.15	Perrin (1958)
	5.62	Benedikovic *et al.* (1991)
$Fe(Asp)_2^{2-}$	8.86	Perrin (1958)
	8.82	Benedikovic *et al.* (1991)
MnAsp	4.35	Albert (1952)
	4.60	Kroll (1952)
	4.31	Gowda and Venkatappa (1981)
	4.66	Zhuo *et al.* (1983)
	4.60	Benedikovic *et al.* (1991)

Table A1 (cont.). Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
$AlAsp^+$	8.62	Charlet *et al.* (1984)
	9.23	Berthon and Daydé (1992)
$AlHAsp^{2+}$	13.04	Charlet *et al.* (1984)
	12.46	Berthon and Daydé (1992)
UO_2HAsp^+	3.84	Feldman and Koval (1963)
	4.16	Bismondo and Rizzo (1989)
$UO_2(HAsp)_2$	15.42	Bismondo and Rizzo (1989)
	15.50	Janarthanam *et al.* (1995)
PbAsp	6.70	Rao and Subrahmanya (1964a)
	7.10	Kodama and Takahashi (1971)
	6.83	Khayat *et al.* (1979)
	6.94	Diez-Cabellero *et al.* (1985b)
	6.86	Dos Santos and Gonçalves (1986)
	6.93	Patil and Nemade (1988)
	6.81	Bottari *et al.* (1989a)
	6.77	Lu *et al.* (1991)
	6.94	Ahmed *et al.* (1996)
$Pb(Asp)_2^{2-}$	9.37	Diez-Cabellero *et al.* (1985b)
	9.85	Dos Santos and Gonçalves (1986)
	9.11	Bottari *et al.* (1989a)
	10.14	Lu *et al.* (1991)
$PbHAsp^+$	12.09	Khayat *et al.* (1979)
	12.31	Bottari *et al.* (1989a)
ZnAsp	6.70	Chaberek and Martell (1952)
	6.25	Happe (1973)
	6.74	Gergely and Farkas (1975)
	6.86	Joshi and Bhattacharya (1975)
	6.98	Makar *et al.* (1976)
	6.73	Guevremont and Rabenstein (1979)
	6.71	Shelke and Jahagirdar (1979)
	6.63	Gowda and Venkatappa (1981)
	6.81	Ramanujam and Selvarajan (1981)
	6.90	Berthon and Germonneau (1982)
	6.75	Lomozik *et al.* (1983)
	6.62	Weng and Leussing (1983)
	6.62	Diez-Cabellero *et al.* (1985b)
	6.76	Philip *et al.* (1988)
	6.26	Rao *et al.* (1989)
	6.69	Reddy *et al.* (1989)
	6.45	Bottari *et al.* (1990)

Table A1 (cont.). Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
ZnAsp (cont.)	6.71	Benedikovic *et al.* (1991)
	6.68	Nair *et al.* (1993)
	6.75	Patel *et al.* (1993)
	6.87	Ahmed *et al.* (1996)
	6.82	Mukherjee and Ghosh (1996)
	6.54	Shoukry *et al.* (1997a)
	6.55	Mukherjee and Sahu (1998)
	6.48	Vajhallya and Khan (1999)
$Zn(Asp)_2^{2-}$	10.76	Albert (1952)
	10.95	Chaberek and Martell (1952)
	10.66	Perkins (1953)
	11.14	Ishizuka *et al.* (1973)
	11.11	Gergely and Farkas (1975)
	10.75	Joshi and Bhattacharya (1975)
	11.07	Makar *et al.* (1976)
	11.21	Guevremont and Rabenstein (1979)
	10.96	Shelke and Jahagirdar (1979)
	10.92	Ramanujam and Selvarajan (1981)
	11.14	Berthon and Germonneau (1982)
	11.02	Lomozik *et al.* (1983)
	11.04	Weng and Leussing (1983)
	10.95	Diez-Cabellero *et al.* (1985b)
	11.09	Patil and Nemade (1988)
	10.75	Philip *et al.* (1988)
	10.73	Rao *et al.* (1989)
	10.43	Bottari *et al.* (1990)
	11.10	Benedikovic *et al.* (1991)
	10.62	Nair *et al.* (1993)
	10.76	Patel *et al.* (1993)
	10.63	Mukherjee and Sahu (1998)
	11.11	Vajhallya and Khan (1999)
$ZnHAsp^+$	11.79	Happe (1973)
	11.94	Ishizuka *et al.* (1973)
	12.85	Makar *et al.* (1976)
	11.82	Berthon and Germonneau (1982)
	12.47	Satyanaranya and Reddy (1989)
	11.30	Bottari *et al.* (1990)
CuAsp	9.43	Chabarek and Martell (1952)
	9.26	Martell *et al.* (1957)
	9.52	Gergely *et al.* (1974)
	9.88	Nagypál *et al.* (1974)
	9.80	Ritsma (1975)
	9.94	Brookes and Pettit (1977)
	9.52	Borisova and Savich (1977)

Table A1 (cont.). Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
CuAsp (cont.)	9.83	Sakurai *et al.* (1978)
	9.85	Mohan *et al.* (1979)
	9.26	Arbad *et al.* (1980)
	9.70	Claridge *et al.* (1980)
	9.42	Shah and Gupta (1980)
	9.47	Gowda and Venkapatta (1981)
	9.84	Ramanjum and Selvarajan (1981)
	9.86	Gergely and Farkas (1982)
	9.99	Lomozik *et al.* (1983)
	9.69	Daniele *et al.* (1984a)
	9.82	Liang and Olin (1984)
	9.26	Diez-Cabellero *et al.* (1986b)
	9.83	Lehtonen (1987)
	9.41	Prasad *et al.* (1987)
	9.21	Bottari *et al.* (1989b)
	9.52	Forresti and Nyholm (1989)
	9.81	Kiss *et al.* (1989)
	9.50	Satyanarayana and Reddy (1989)
	9.21	Killa *et al.* (1991a)
	9.67	Benedikovic *et al.* (1991)
	9.76	Pandeya and Patel (1991)
	9.81	Abd-El-Gabor *et al.* (1992)
	9.82	Boraei and Abd-Alla (1992)
	9.86	Abd-Alla and Mahmoud (1993)
	9.58	Patel *et al.* (1993)
	9.71	Ahmed *et al.* (1996)
	9.60	Esina *et al.* (1996)
	9.78	Mukherjee and Ghosh (1996)
	9.71	Kholeif and Anderegg (1997)
	9.70	Shoukry *et al.* (1997b)
	9.80	Mukherjee and Sahu (1998)
	9.69	Boraei *et al.* (1999)
	9.71	Khalil and Attia (1999)
$Cu(Asp)_2^{2-}$	16.43	Chabarek and Martell (1952)
	16.53	Gergely *et al.* (1974)
	16.61	Nagypál *et al.* (1974)
	16.75	Ritsma (1975)
	17.11	Brookes and Pettit (1977)
	16.69	Sakurai *et al.* (1978)
	16.63	Mohan *et al.* (1979)
	16.40	Arbad *et al.* (1980)
	16.05	Claridge *et al.* (1980)
	16.32	Shah and Gupta (1980)
	16.54	Ramanjum and Selvarajan (1981)
	16.84	Gergely and Farkas (1982)
	17.02	Lomozik *et al.* (1983)

Table A1 (cont.). Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
$Cu(Asp)_2^{2-}$ (cont.)	16.79	Daniele *et al.* (1984a)
	16.56	Liang and Olin (1984)
	16.79	Lehtonen (1987)
	16.25	Prasad *et al.* (1987)
	16.76	Patil and Nemade (1988)
	16.71	Bottari *et al.* (1989b)
	16.45	Forresti and Nyholm (1989)
	16.91	Kiss *et al.* (1989)
	16.52	Benedikovic *et al.* (1991)
	16.46	Killa *et al.* (1991a)
	16.62	Patel *et al.* (1993)
	16.76	Shoukry *et al.* (1997b)
$CuHAsp^+$	13.32	Nagypál *et al.* (1974)
	13.45	Ritsma (1975)
	13.66	Brookes and Pettit (1977)
	13.57	Sakurai *et al.* (1978)
	13.56	Claridge *et al.* (1980)
	13.47	Gergely and Farkas (1982)
	13.28	Lomozik *et al.* (1983)
	13.38	Daniele *et al.* (1984a)
	13.34	Liang and Olin (1984)
	13.48	Lehtonen (1987)
	13.21	Bottari *et al.* (1989b)
	13.19	Forresti and Nyholm (1989)
	13.49	Kiss *et al.* (1989)
	13.37	Benedikovic *et al.* (1991)
	13.35	Kholeif and Anderegg (1997)
$CuH(Asp)_2^-$	22.49	Brookes and Pettit (1977)
	21.08	Daniele *et al.* (1984a)
	21.45	Liang and Olin (1984)
	21.37	Bottari *et al.* (1989b)
	21.61	Forresti and Nyholm (1989)
$Cu(HAsp)_2$	26.65	Brookes and Pettit (1977)
	25.50	Daniele *et al.* (1984a)
	25.38	Liang and Olin (1984)
	25.51	Bottari *et al.* (1989b)
	24.91	Forresti and Nyholm (1989)
CdAsp	5.23	Chaberek and Martell (1952)
	5.25	Lumb and Martell (1953)
	5.16	Munze *et al.* (1969)
	5.66	Heijne and van Linden (1975)
	5.56	Joshi and Bhattacharya (1975)

Table A1 (cont.). Stability constant data for metal-aspartate complexes

Species	log K_o	Reference
CdAsp (cont.)	5.48	Gowda and Venkatappa (1981)
	5.31	Mundra *et al.* (1984)
	5.30	Valenta *et al.* (1984)
	5.54	Simões-Gonçalves and Dos-Santos (1985)
	5.55	Philip *et al.* (1988)
	5.35	Bottari *et al.* (1989c)
	5.34	Rao *et al.* (1989)
	5.54	Barnard *et al.* (1990)
	5.18	Dodke and Khan (1993)
	5.54	Patel *et al.* (1993)
	5.48	Ahmed *et al.* (1996)
$Cd(Asp)_2^{2-}$	8.96	Albert (1950)
	8.46	Chaberek and Martell (1952)
	9.06	Perkins (1953)
	8.63	Munze *et al.* (1969)
	9.06	Hansen and Ruzicka (1973)
	8.88	Joshi and Bhattacharya (1975)
	9.10	Valenta *et al.* (1984)
	9.18	Simões-Gonçalves and Dos-Santos (1985)
	8.88	Philip *et al.* (1988)
	8.66	Bottari *et al.* (1989c)
	8.64	Rao *et al.* (1989)
	8.93	Barnard *et al.* (1990)
	8.39	Dodke and Khan (1993)
	8.89	Patel *et al.* (1993)
$Cd(Asp)_3^{4-}$	10.31	Mundra *et al.* (1984)
	10.90	Simões-Gonçalves and Dos-Santos (1985)
	11.00	Bottari *et al.* (1989c)
	10.24	Dodke and Khan (1993)

Table A2. Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$NaCit^{2-}$	1.43	Walser (1961)
	1.34	Rechnitz and Zamochnick (1964)
	1.41	Cucinotta *et al.* (1981)
	1.47	Daniele *et al.* (1985a)
	1.67	Daniele *et al.* (1990)
	1.54	De Robertis *et al.* (1995)
	1.54	De Stefano *et al.* (1999)
Na_2Cit^-	2.55	Daniele *et al.* (1990)
	2.48	De Robertis *et al.* (1995)
	2.38	De Stefano *et al.* (1999)
$NaHCit^-$	7.72	Arena *et al.* (1980)
	6.96	Cucinotta *et al.* (1981)
	7.18	Daniele *et al.* (1985a)
	7.50	Daniele *et al.* (1990)
	7.33	De Stefano *et al.* (1999)
NaH_2Cit	11.76	Arena *et al.* (1980)
	11.4	De Stefano *et al.* (1999)
$KCit^{2-}$	1.10	Bates and Pinching (1949)
	1.16	Walser (1961)
	1.23	Rechnitz and Zamochnick (1964)
	1.29	Daniele *et al.* (1980)
	1.36	Daniele *et al.* (1984c)
	1.54	Daniele *et al.* (1990)
	1.51	De Robertis *et al.* (1995)
	1.42	De Stefano *et al.* (1999)
K_2Cit^-	2.10	Daniele *et al.* (1990)
	2.13	De Robertis *et al.* (1995)
	1.93	De Stefano *et al.* (1999)
$KHCit^-$	6.56	Daniele *et al.* (1980)
	7.01	Daniele *et al.* (1984c)
	7.30	Daniele *et al.* (1990)
	7.13	De Stefano *et al.* (1999)
KH_2Cit	11.13	Daniele *et al.* (1984c)
	11.3	De Stefano *et al.* (1999)
$CaCit^-$	4.85	Bjerrum and Unmack (1929)
	4.67	Hastings *et al.* (1934)
	4.60	Joseph (1946)
	4.84	Heinz (1951)
	4.90	Davies and Hoyle (1953)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$CaCit^-$ (cont.)	4.60	Schubert (1954)
	4.68	Davies and Hoyle (1955)
	4.64	Lefebvre (1957)
	5.00	Pattnaik and Pani (1961)
	4.60	Walser (1961)
	4.61	Matushima (1963)
	4.82	Campi *et al.* (1964)
	4.95	Rechnitz and Hseu (1969)
	4.67	Rumbaut (1971)
	4.78	Field *et al.* (1975)
	4.82	Ramamoorthy and Manning (1975)
	4.76	May *et al.* (1977)
	4.70	Craggs *et al.* (1978)
	4.92	Pearce (1980)
	4.87	Amico *et al.* (1982)
	4.85	Hirokawa and Kiso (1982)
	4.71	Rizkalla *et al.* (1985)
	4.82	Blaquiere and Berthon (1987)
	4.84	Singh *et al.* (1991)
	4.77	Glab *et al.* (1992)
	4.63	Glab *et al.* (1993)
	4.80	Mironov *et al.* (1996)
	4.91	De Stefano *et al.* (1999)
$Ca(Cit)_2^{4-}$	5.70	Blaquiere and Berthon (1987)
	5.88	Ashby and Sleet (1992)
CaHCit	9.66	Heinz (1951)
	9.42	Davies and Hoyle (1953)
	9.46	Davies and Hoyle (1955)
	9.32	Campi *et al.* (1964)
	9.18	Meyer (1974)
	9.55	Field *et al.* (1975)
	9.26	Pearce (1980)
	9.30	Amico *et al.* (1982)
	9.16	Hirokawa and Kiso (1982)
	9.78	Rizkalla *et al.* (1985)
	9.31	Blaquiere and Berthon (1987)
	9.23	De Stefano *et al.* (1999)
CaH_2Cit^+	12.64	Campi *et al.* (1964)
	12.63	Pearce (1980)
	12.71	Blaquiere and Berthon (1987)
	12.57	Butina *et al.* (1992)
$Ca(HCit)_2^{2-}$	19.53	Heinz (1951)
	18.44	May *et al.* (1977)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$MgCit^-$	4.65	Hastings *et al.* (1934)
	4.89	Nördbo (1938)
	4.53	Li *et al.* (1959)
	5.00	Walser (1961)
	4.91	Watanabe *et al.* (1963)
	4.67	Campi *et al.* (1964)
	4.90	Pattnaik and Pani (1965)
	5.01	Tate *et al.* (1965)
	4.93	Blair (1969)
	5.13	Grzybowski *et al.* (1970)
	4.66	Field *et al.* (1975)
	4.75	May *et al.* (1977)
	4.85	Pearce (1980)
	4.87	Amico *et al.* (1982)
	4.92	Hirokawa and Kiso (1982)
	4.74	Rizkalla *et al.* (1985)
	4.79	Blaquiere and Berthon (1987)
	4.92	Ghandour *et al.* (1988a)
	4.70	Glab *et al.* (1993)
	4.71	De Stefano *et al.* (1999)
MgHCit	8.79	Li *et al.* (1959)
	9.07	Campi *et al.* (1964)
	9.07	Tate *et al.* (1965)
	9.14	Grzybowski *et al.* (1970)
	8.97	Meyer (1974)
	9.16	Field *et al.* (1975)
	9.00	Pearce (1980)
	8.88	Amico *et al.* (1982)
	9.11	Rizkalla *et al.* (1985)
	9.18	Blaquiere and Berthon (1987)
	8.84	De Stefano *et al.* (1999)
MgH_2Cit^+	12.43	Campi *et al.* (1964)
	12.19	Pearce (1980)
	12.71	Blaquiere and Berthon (1987)
	12.57	Butina *et al.* (1992)
$FeCit^-$	5.67	Timberlake (1964)
	5.67	Tate *et al.* (1965)
	6.08	Field *et al.* (1974)
	6.02	Amico *et al.* (1979)
FeHCit	9.73	Timberlake (1964)
	9.87	Tate *et al.* (1965)
	10.12	Field *et al.* (1974)
	10.00	May *et al.* (1977)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
FeHCit (cont.)	10.42	Amico *et al.* (1979)
	9.74	Glebov *et al.* (1990)
FeH_2Cit^+	12.83	Hamm *et al.* (1954)
	12.75	May *et al.* (1977)
	12.70	Amico *et al.* (1979)
	12.68	Glebov *et al.* (1990)
FeCit	0.61	Bertin-Batsch (1952)
	0.29	Warner and Weber (1953)
	0.66	Hamm *et al.* (1954)
	0.36	Timberlake (1964)
	0.12	Field *et al.* (1974)
	0.38	Trunova *et al.* (1993)
$Fe(Cit)_2^{3-}$	6.00	Ramamoorthy and Manning (1975)
	6.13	Ribas *et al.* (1989)
$FeHCit^+$	0.94	Lanford and Quinnan (1948)
	0.88	Hamm *et al.* (1954)
	1.39	Field *et al.* (1974)
	0.94	Kostromina *et al.* (1975)
	1.48	Vanura and Kuca (1978)
	1.28	May *et al.* (1977)
	1.37	Ribas *et al.* (1989)
	1.26	Trunova *et al.* (1993)
$Fe(HCit)_2^-$	13.39	May *et al.* (1977)
	13.31	Ribas *et al.* (1989)
$FeOHCit^-$	-2.17	Hamm *et al.* (1954)
	-2.60	Field *et al.* (1974)
	-2.07	May *et al.* (1977)
	-2.87	Manzurola *et al.* (1989)
	-3.02	Ribas *et al.* (1989)
	-2.27	Trunova *et al.* (1993)
$Fe(OH)_2Cit^{2-}$	-10.06	Hamm *et al.* (1954)
	-10.00	May *et al.* (1977)
$Fe_2(OH)_2(Cit)_2^{2-}$	-2.95	Timberlake (1964)
	-2.74	Sal'nikov and Zhuravleva (1986)
	-2.56	Glebov *et al.* (1990)
$Fe_2(OH)_3(Cit)_2^{3-}$	-8.47	Sal'nikov and Zhuravleva (1986)
	-7.03	Glebov *et al.* (1990)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$MnCit^-$	4.99	Li *et al.* (1957)
	5.15	Wiberg (1958)
	5.09	Li *et al.* (1959)
	5.43	Grzybowski *et al.* (1970)
	4.87	Kalinichenko (1970)
	5.26	May *et al.* (1977)
	5.29	Roos and Williams (1977)
	5.32	Amico *et al.* (1979)
	5.09	Amico *et al.* (1985)
	4.72	Grigor'eva *et al.* (1985)
$Mn(Cit)_2^{4-}$	6.68	Grzybowski *et al.* (1970)
	6.33	Sharma and Singh (1978)
MnHCit	9.33	Lefebvre (1957)
	9.42	Li *et al.* (1959)
	9.66	Pattnaik and Pani (1961)
	9.50	Grzybowski *et al.* (1970)
	9.30	Kalinichenko (1970)
	9.65	Amico *et al.* (1979)
MnH_2Cit^+	13.10	Besse *et al.* (1970)
	13.18	Amico *et al.* (1979)
$MnOHCit^{2-}$	-3.87	Pattnaik and Pani (1961)
	-2.66	Roos and Williams (1977)
AlCit	10.39	Pattnaik and Pani (1961)
	10.58	Ramamoorthy and Manning (1975)
	10.49	May *et al.* (1977)
	10.06	Jackson (1982)
	10.14	Öhman and Sjöberg (1983a)
	9.91	Motekaitis and Martell (1984)
	10.72	Lopez-Quintela *et al.* (1984)
	10.29	Gregor and Powell (1986)
	10.21	Jons *et al.* (1988)
	10.44	Venturini and Berthon (1989)
	9.72	Findlow *et al.* (1990)
$Al(Cit)_2^{3-}$	15.29	May *et al.* (1977)
	15.26	Öhman and Sjöberg (1983a)
	15.32	Gregor and Powell (1986)
	15.26	Venturini and Berthon (1989)
	14.98	Findlow *et al.* (1990)
$AlHCit^+$	12.69	May *et al.* (1977)
	12.31	Jackson (1982)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$AlHCit^+$ (cont.)	12.38	Öhman and Sjöberg (1983a)
	13.27	Motekaitis and Martell (1984)
	12.95	Lopez-Quintela *et al.* (1984)
	12.94	Gregor and Powell (1986)
	12.76	Jons *et al.* (1988)
	12.69	Venturini and Berthon (1989)
	12.04	Findlow *et al.* (1990)
AlH_2Cit^{2+}	13.79	Knoche and Lopez-Quintela (1983)
	14.07	Lopez-Quintela *et al.* (1984)
$AlOHCit^-$	6.56	Pattnaik and Pani (1961)
	6.59	Jackson (1982)
	6.81	Motekaitis and Martell (1984)
	6.43	Jons *et al.* (1988)
	6.33	Öhman (1988)
	6.66	Findlow *et al.* (1990)
$AlOH(Cit)_2^{4-}$	8.35	Gregor and Powell (1986)
	8.02	Venturini and Berthon (1989)
	8.49	Findlow *et al.* (1990)
$Al(OH)_2Cit^{2-}$	-0.75	Pattnaik and Pani (1961)
	-0.42	Öhman (1988)
	0.43	Findlow *et al.* (1990)
$Al(OH)_2(Cit)_2^{5-}$	-0.20	May *et al.* (1977)
	-0.12	Gregor and Powell (1986)
	-0.21	Venturini and Berthon (1989)
$Al_3(OH)_4(Cit)_3^{4-}$	21.09	Öhman and Sjöberg (1983a)
	19.24	Venturini and Berthon (1989)
UO_2Cit^-	0.89	Li *et al.* (1959)
	0.70	Feldman *et al.* (1960)
	-0.36	Rajan and Martell (1965)
	-0.48	Ohyoshi *et al.* (1975)
	-0.65	Vanura and Kuca (1980)
	0.61	Hamed *et al.* (1994)
	-0.03	Bronikowski *et al.* (1996)
$(UO_2)_2(Cit)_2^{2-}$	3.55	Feldman *et al.* (1960)
	3.14	Rajan and Martell (1965)
	1.76	Markovits *et al.* (1972)
	2.01	Sircar (1984)
UO_2HCit	2.36	Ohyoshi *et al.* (1975)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
UO_2HCit (cont.)	2.20	Vanura and Kuca (1980)
$UO_2H_2Cit^+$	5.31	Ohyoshi *et al.* (1975)
	3.82	Vanura and Kuca (1980)
$PbCit^-$	5.18	Donda and Giuliana (1963)
	5.36	Bottari and Vicedomini (1973)
	5.65	Ekström and Olin (1978)
	5.76	May *et al.* (1977)
	5.49	Diez-Caballero *et al.* (1985a)
	5.38	Janós (1993)
$Pb(Cit)_2^{4-}$	6.50	Donda and Giuliana (1963)
	6.70	Bottari and Vicedomini (1973)
	6.53	Ekström and Olin (1978)
	6.20	Diez-Caballero *et al.* (1985a)
PbHCit	9.65	Bottari and Vicedomini (1973)
	9.59	Ekström and Olin (1978)
PbH_2Cit^+	12.35	Bottari and Vicedomini (1973)
	12.40	Ekström and Olin (1978)
$Pb(HCit)_2^{2-}$	17.09	Bottari and Vicedomini (1973)
	16.67	Ekström and Olin (1978)
$ZnCit^-$	6.16	Schubert *et al.* (1958)
	6.31	Li *et al.* (1959)
	6.17	Okác and Kolarík (1959)
	5.85	Furlani and Cervone (1962)
	6.14	Matsushima (1963)
	6.25	Campi *et al.* (1964)
	6.14	Ramamoorthy and Manning (1974c)
	6.38	Field *et al.* (1975)
	6.10	Daniele and Ostacoli (1977)
	6.18	Berthon *et al.* (1978)
	6.11	Daniele *et al.* (1978)
	6.28	Rajan *et al.* (1978)
	6.06	Mali and Sen (1981)
	6.30	Capone *et al.* (1986)
	6.01	Christie *et al.* (1991)
$Zn(Cit)_2^{4-}$	7.76	Migal and Sychev (1958)
	8.14	Okác and Kolarík (1959)
	7.00	Furlani and Cervone (1962)
	8.09	Berthon *et al.* (1978)
	7.40	Capone *et al.* (1986)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$Zn(Cit)_2^{4-}$ (cont.)	7.60	Christie *et al.* (1991)
$Zn(Cit)_3^{7-}$	6.82	Happe (1973)
	6.78	Capone *et al.* (1986)
ZnHCit	10.28	Li *et al.* (1959)
	10.22	Okác and Kolarík (1959)
	10.54	Pattnaik and Pani (1961)
	9.63	Furlani and Cervone (1962)
	10.51	Matsushima (1963)
	10.20	Campi *et al.* (1964)
	9.88	Happe (1973)
	10.48	Field *et al.* (1975)
	10.14	Berthon *et al.* (1978)
	9.93	Daniele *et al.* (1978)
	10.21	Capone *et al.* (1986)
	10.11	Christie *et al.* (1991)
ZnH_2Cit^+	12.84	Campi *et al.* (1964)
	13.16	Besse *et al.* (1970)
$ZnOHCit^{2-}$	-2.33	Meites (1951)
	-1.90	Kovalenko and Vistyak (1959)
	-2.07	Pattnaik and Pani (1961)
	-0.95	Christie *et al.* (1991)
$Zn_2(OH)_2(Cit)_2^{4-}$	-1.24	Berthon *et al.* (1978)
	-2.04	Daniele *et al.* (1978)
	-1.99	Capone *et al.* (1986)
$ZnCu(OH)_2(Cit)_2^{4-}$	2.37	Amico *et al.* (1980)
	2.23	Blomqvist and Still (1984)
$CuCit^-$	7.29	Warner and Weber (1953)
	7.54	Das *et al.* (1960)
	7.18	Campi *et al.* (1964)
	7.31	Ramamoorthy *et al.* (1972)
	7.56	Petit-Ramel and Khalil (1974)
	7.49	Sal'nikov and Zhuravleva (1986)
	7.16	Ghandour *et al.* (1988b)
	7.28	Piispanen and Lajunen (1995)
$Cu(Cit)_2^{4-}$	9.01	Lefebvre (1957)
	8.90	Petit-Ramel and Khalil (1974)
	9.84	Sal'nikov and Zhuravleva (1986)
	9.58	Taneja *et al.* (1992)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$Cu_2(Cit)_2^{2-}$	17.07	Field *et al.* (1974)
	16.95	Daniele *et al.* (1975a)
	16.78	Daniele *et al.* (1984c)
	17.00	Sircar (1984)
CuHCit	10.99	Suzuki (1952)
	11.10	Das *et al.* (1960)
	10.64	Campi *et al.* (1964)
	10.69	Besse *et al.* (1970)
	10.56	Petit-Ramel and Khalil (1974)
	10.81	Field *et al.* (1974)
	10.97	Daniele *et al.* (1975a)
	11.05	Daniele *et al.* (1984c)
	10.90	Tripathi *et al.* (1992)
CuH_2Cit^+	13.50	Warner and Weber (1953)
	13.84	Campi *et al.* (1964)
	13.22	Petit-Ramel and Khalil (1974)
	13.39	Sal'nikov and Zhuravleva (1986)
	14.08	Tripathi *et al.* (1992)
	13.81	Piispanen and Lajunen (1995)
$CuOHCit^{2-}$	2.76	Warner and Weber (1953)
	2.56	Das *et al.* (1960)
	2.53	Campi *et al.* (1964)
	3.24	Petit-Ramel and Khalil (1974)
	2.47	Field *et al.* (1974)
	3.03	Rajan *et al.* (1978)
$Cu(OH)_2(Cit)_2^{6-}$	-8.70	Meites (1950)
	-7.30	Sal'nikov and Zhuravleva (1986)
Cu_2OHCit	6.83	Campi *et al.* (1964)
	6.78	Still and Wikberg (1980)
	6.63	Daniele *et al.* (1984c)
$Cu_2OH(Cit)_2^{3-}$	12.03	Daniele *et al.* (1975a)
	12.10	Still and Wikberg (1980)
	12.13	Daniele *et al.* (1984c)
$Cu_2(OH)_2(Cit)_2^{4-}$	6.61	Lefebvre (1957)
	6.16	Bottari (1975a)
	6.86	Daniele *et al.* (1975a)
	6.66	Still and Wikberg (1980)
	6.06	Olin and Wallén (1983)
	6.73	Daniele *et al.* (1984c)
	6.85	Sal'nikov and Zhuravleva (1986)

Table A2 (cont.). Stability constant data for metal-citrate complexes

Species	log K_o	Reference
$Cu_2(OH)_2(Cit)_2^{4-}$ (cont.)	6.69	Piispanen and Lajunen (1995)
$CdCit^-$	4.67	Meites (1950)
	4.66	Migal and Sychev (1958)
	5.36	Treumann and Ferris (1958)
	5.41	Li *et al.* (1959)
	5.02	Campi *et al.* (1964)
	4.71	Furlani and Cervone (1962)
	5.03	Ramamoorthy and Manning (1975)
	4.56	May *et al.* (1977)
	4.93	Daniele *et al.* (1979)
	5.00	Krishna *et al.* (1984)
	4.99	Capone *et al.* (1986)
	4.33	Jaber (1986)
	5.21	Ghandour *et al.* (1988a)
	4.14	Killa *et al.* (1991b)
	5.40	Glab *et al.* (1992)
	4.50	Janós (1993)
$Cd(Cit)_2^{4-}$	5.39	Furlani and Cervone (1962)
	5.24	Bottari (1975b)
	5.13	May *et al.* (1977)
	5.10	Grenthe *et al.* (1984)
	5.99	Capone *et al.* (1986)
	4.69	Jaber (1986)
	4.81	Killa *et al.* (1991b)
$Cd(Cit)_3^{7-}$	2.57	Jaber (1986)
	2.82	Killa *et al.* (1991b)
CdHCit	9.88	Pattnaik and Pani (1957)
	9.60	Li *et al.* (1959)
	9.42	Campi *et al.* (1964)
	9.20	May *et al.* (1977)
	9.30	Daniele *et al.* (1979)
	9.35	Capone *et al.* (1986)
CdH_2Cit^+	12.55	Campi *et al.* (1964)
	12.72	Daniele *et al.* (1979)
$CdOHCit^{2-}$	-2.95	Daniele *et al.* (1979)
	-3.19	Capone *et al.* (1986)
$Cd_2(OH)_2(Cit)_2^{4-}$	-4.54	Grenthe *et al.* (1984)
	-4.54	Capone *et al.* (1986)

Table A3. Stability constant data for metal-malonate complexes

Species	log K_o	Reference
$NaMal^-$	0.74	Archer *et al.* (1965)
	0.82	Dygert *et al.* (1970)
	0.72	Kläning and Østerby (1976)
	0.81	Daniele *et al.* (1983)
	0.91	Daniele *et al.* (1985a)
	0.90	De Robertis *et al.* (1995)
$KMal^-$	0.85	Daniele *et al.* (1983)
	0.84	Daniele *et al.* (1984b)
	1.01	Daniele *et al.* (1985a)
CaMal	2.47	Cannan and Kilbrick (1938)
	2.35	Stock and Davies (1949)
	2.44	Schubert and Lindenbaum (1952)
	2.70	Campi (1963)
	2.37	Ostacoli *et al.* (1968)
	2.50	Ghosh and Nair (1970)
	2.34	Kereichuk and Mokhnatova (1976)
	2.50	Kläning and Østerby (1976)
	2.39	Craggs *et al.* (1979)
	2.51	Daniele *et al.* (1984b)
	2.39	Daniele *et al.* (1985a)
	2.64	De Robertis *et al.* (1995)
	2.40	Fein *et al.* (1995)
$CaHMal^+$	6.66	Cannan and Kilbrick (1938)
	6.91	Campi (1963)
	6.64	Daniele *et al.* (1984b)
	6.59	Daniele *et al.* (1985a)
MgMal	2.83	Simms (1928)
	2.80	Money and Davies (1932)
	2.92	Cannan and Kilbrick (1938)
	2.85	Stock and Davies (1949)
	2.84	Evans and Monk (1952)
	2.80	Campi (1963)
	2.97	Ostacoli *et al.* (1968)
	2.84	Parthasarthy and Ambujavalli (1972)
	2.86	Kläning and Østerby (1976)
	2.86	Burger *et al.* (1988)
	2.92	Ren and Kratochvil (1995)
$MgHMal^+$	6.66	Cannan and Kilbrick (1938)
	6.94	Campi (1963)
	7.07	Ostacoli *et al.* (1968)
FeMal	2.98	Dellien (1977)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
FeMal (cont.)	3.05	Micskei (1987)
$Fe(Mal)_2^{2-}$	3.30	Schaap *et al.* (1954)
	3.19	Cape *et al.* (1974)
$FeMal^+$	-3.95	Deneux *et al.* (1968)
	-3.84	Cavasino and Di-Dio (1971)
	-3.70	Ramamoorthy and Manning (1973)
	-3.89	Salvadó *et al.* (1989)
$Fe(Mal)_2^-$	1.99	Ramamoorthy and Manning (1973)
	2.46	Dutt *et al.* (1976)
	2.42	Salvadó *et al.* (1989)
$Fe(Mal)_3^{3-}$	6.34	Dutt *et al.* (1976)
	5.52	Salvadó *et al.* (1989)
MnMal	3.27	Li et al. (1957)
	3.27	Nair and Nancollas (1961)
	3.39	Nozaki *et al.* (1970)
	3.58	Sigel *et al.* (1977)
$AlMal^+$	7.72	Jackson and Cosgrove (1982)
	7.99	Powell and Town (1993)
	7.75	Kiss *et al.* (1994)
	7.49	Ridley *et al.* (1998)
$Al(Mal)_2^-$	13.16	Jackson and Cosgrove (1982)
	13.07	Powell and Town (1993)
	12.95	Kiss *et al.* (1994)
	12.62	Ridley *et al.* (1998)
$Al(Mal)_3^{3-}$	14.76	Jackson and Cosgrove (1982)
	15.21	Powell and Town (1993)
	14.91	Kiss *et al.* (1994)
UO_2Mal	-3.10	Athavale *et al.* (1967)
	-2.52	Rajan and Martell (1967)
	-2.90	Ramamoorthy and Santappa (1969)
	-2.53	Vanni *et al.* (1969)
	-2.56	Portanova *et al.* (1973)
	-2.81	Di Bernardo *et al.* (1977)
	-2.98	Selvaraj and Santappa (1977)
	-2.62	Kumari and Chaturvedi (1979)
	-2.90	Shelke and Jahagirdar (1981)
	-2.62	Arbad (1985)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
$UO_2(Mal)_2^{2-}$	1.02	Athavale *et al.* (1967)
	1.47	Rajan and Martell (1967)
	1.11	Ramamoorthy and Santappa (1969)
	1.35	Vanni *et al.* (1969)
	1.43	Portanova *et al.* (1973)
	1.25	Di Bernardo *et al.* (1977)
	1.04	Selvaraj and Santappa (1977)
	1.07	Shelke and Jahagirdar (1981)
	1.24	Bandiwadekar and Chavar (1988)
PbMal	3.96	Yasuda *et al.* (1960)
	4.01	Gaur and Palrecha (1969)
	3.99	Nozaki *et al.* (1970)
	4.01	Maheswari *et al.* (1974)
	3.60	Hammam *et al.* (1977)
	3.80	Garg *et al.* (1984a)
	3.71	Ruiz-Cabrera *et al.* (1985)
	3.94	Liu *et al.* (1991)
$Pb(Mal)_2^{2-}$	5.03	Gaur and Palrecha (1969)
	5.09	Nozaki *et al.* (1970)
	5.06	Maheswari *et al.* (1974)
	5.01	Hammam *et al.* (1977)
	4.60	Garg *et al.* (1984a)
	4.83	Ruiz-Cabrera *et al.* (1985)
	4.71	Shivare and Singh (1985)
	5.60	Liu *et al.* (1991)
$Pb(Mal)_3^{4-}$	4.32	Gaur and Palrecha (1969)
	4.43	Maheswari *et al.* (1974)
	4.16	Hammam *et al.* (1977)
	4.27	Garg *et al.* (1984a)
	4.58	Ruiz-Cabrera *et al.* (1985)
	4.50	Shivare and Singh (1985)
ZnMal	3.62	Riley and Fisher (1929)
	3.68	Money and Davies (1932)
	3.79	Cannan and Kilbrick (1938)
	3.75	James (1951)
	3.56	Yasuda *et al.* (1960)
	3.83	Campi (1963)
	3.82	Nair (1965)
	3.85	Rowlands and Monk (1966)
	3.81	Ostacoli *et al.* (1968)
	3.83	Powell and Johnson (1969)
	3.80	Evans and Monk (1970)
	3.71	Daniele *et al.* (1975b)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
ZnMal (cont.)	3.61	Makar *et al.* (1976)
	3.82	Pushparaja and Suderanan (1980)
	3.83	Mali and Sen (1981)
	3.71	Ramanujam and Selvarajan (1981)
	3.46	Fuentes *et al.* (1989)
	3.82	Nepal and Dubby (1989)
	3.69	Padmarathi and Satyanarayana (1997)
$ZnHMal^+$	7.03	Cannan and Kilbrick (1938)
	7.35	Campi (1963)
	7.10	Ostacoli *et al.* (1968)
	6.68	Tedesco and González-Quintana (1974)
	6.82	Makar *et al.* (1976)
CuMal	5.65	Ives and Riley (1931)
	5.60	Money and Davies (1932)
	6.34	Britton and Jarret (1935)
	5.55	Stock and Davies (1949)
	5.84	Peacock and James (1951)
	5.60	Bobtelsky and Bar-Gadda (1953)
	5.70	Gelles and Nancollas (1956)
	5.86	Yasuda *et al.* (1960)
	5.80	Jones and Stock (1962)
	6.40	Campi (1963)
	5.43	Athavale *et al.* (1967)
	5.49	Bonnet and Mihailova (1968)
	5.90	Ostacoli *et al.* (1968)
	5.44	Mihailova and Bonnet (1969)
	5.88	Powell and Johnson (1969)
	5.95	Ghosh and Nair (1970)
	5.96	Griesser and Sigel (1970)
	6.39	Nozaki *et al.* (1970)
	5.83	Ostacoli *et al.* (1973)
	6.19	Gordienko and Mikhailyuk (1974)
	5.70	Khurana *et al.* (1975)
	5.90	Bonomo *et al.* (1976)
	5.91	Arena *et al.* (1978a)
	6.15	El-Ezaby *et al.* (1979)
	5.82	Mohan *et al.* (1979)
	5.99	Shelke and Jahagirdar (1979)
	5.92	Grasso *et al.* (1980)
	5.97	Mali and Pethe (1980)
	5.72	Narasimhulu and Seshaiah (1980)
	5.82	Shah and Gupta (1980)
	5.99	Placeres *et al.* (1981)
	5.99	Ramanujam and Selvarajan (1981)
	6.16	Ramanujam and Krishnan (1981)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
CuMal (cont.)	6.11	Daniele *et al.* (1982)
	6.11	Garg *et al.* (1984b)
	6.12	Zhou *et al.* (1984)
	5.96	Arbad (1985)
	5.32	Reddy *et al.* (1987)
	5.69	Venkatnarayana *et al.* (1988)
	5.80	Coetzee (1989)
	6.14	Ullah and Bhattacharya (1990)
	5.61	Das and Manwal (1994)
	6.13	Gomes *et al.* (1997)
	5.92	Padmarathi and Satyanarayana (1997)
	5.68	Khalil and Radalla (1998)
$Cu(Mal)_2^{2-}$	8.56	Riley (1930)
	8.44	Money and Davies (1932)
	8.42	Gelles and Nancollas (1956)
	8.67	Athavale *et al.* (1967)
	8.87	Bonnet and Mihailova (1968)
	8.43	Ostacoli *et al.* (1968)
	8.47	Mihailova and Bonnet (1969)
	8.81	Powell and Johnson (1969)
	8.79	Nozaki *et al.* (1970)
	8.59	Ostacoli *et al.* (1973)
	7.96	Khurana *et al.* (1975)
	8.43	Bonomo *et al.* (1976)
	8.74	Arena *et al.* (1978a)
	9.60	El-Ezaby *et al.* (1979)
	8.55	Mohan *et al.* (1979)
	9.26	Shelke and Jahagirdar (1979)
	8.71	Grasso *et al.* (1980)
	9.27	Mali and Pethe (1980)
	9.15	Narasimhulu and Seshaiah (1980)
	8.17	Shah and Gupta (1980)
	8.30	Placeres *et al.* (1981)
	8.67	Ramanujam and Selvarajan (1981)
	8.71	Ramanujam and Krishnan (1981)
	9.08	Daniele *et al.* (1982)
	8.03	Garg *et al.* (1984b)
	8.67	Zhou *et al.* (1984)
	9.26	Arbad (1985)
	8.26	Diez-Caballero *et al.* (1986a)
	8.71	Reddy *et al.* (1987)
	8.97	Venkatnarayana *et al.* (1988)
	9.57	Ullah and Bhattacharya (1990)
	8.93	Foti *et al.* (1994)
	9.05	Khalil and Radalla (1998)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
$Cu(Mal)_3^{4-}$	8.50	Nozaki *et al.* (1970)
	7.77	Placeres *et al.* (1981)
$CuHMal^+$	8.26	Ostacoli *et al.* (1968)
	8.03	Tedesco and González-Quintana (1974)
	8.05	Arena *et al.* (1978a)
	8.15	Grasso *et al.* (1980)
	8.20	Daniele *et al.* (1982)
$CuMalAsp^{2-}$	13.22	Shah and Gupta (1980)
	13.12	Ramanujam and Selvarajan (1981)
CdMal	2.98	Riley and Fisher (1929)
	3.29	Money and Davies (1932)
	3.55	Ferrell *et al.* (1934)
	3.25	Stock and Davies (1949)
	3.15	Yasuda *et al.* (1960)
	3.18	Jones and Stock (1962)
	2.73	Schwarzenbach and Szilard (1962)
	3.36	Campi (1963)
	3.49	Ostacoli *et al.* (1968)
	3.49	Nozaki *et al.* (1970)
	3.04	Sharma and Gaur (1978)
	2.86	Kelkar and Nemade (1979)
	3.04	Kharitonov *et al.* (1981)
	2.52	Sachan *et al.* (1982)
	2.56	Kulshrestha *et al.* (1987)
	2.70	Nema and Khan (1987)
	2.81	Placeres *et al.* (1988)
	2.66	Killa (1989)
	3.40	Jain *et al.* (1992)
	2.74	Hassanein *et al.* (1993)
	2.66	Al-Ahmadi and Katib (1997)
	3.45	Ridley *et al.* (1998)
$Cd(Mal)_2^{2-}$	3.64	Schwarzenbach and Szilard (1962)
	3.22	Khurana and Gupta (1972)
	3.17	Sharma and Gaur (1978)
	3.64	Kelkar and Nemade (1979)
	3.46	Shivhare *et al.* (1981)
	3.57	Kulshrestha *et al.* (1987)
	3.80	Nema and Khan (1987)
	3.16	Placeres *et al.* (1988)
	3.92	Killa (1989)
	3.57	Ismail (1992)
	3.65	Jain *et al.* (1992)
	3.62	Hassanein *et al.* (1993)

Table A3 (cont.). Stability constant data for metal-malonate complexes

Species	log K_o	Reference
$Cd(Mal)_2^{2-}$ (cont.)	3.57	Al-Ahmadi and Katib (1997)
$Cd(Mal)_3^{4-}$	3.40	Khurana and Gupta (1972)
	3.25	Sharma and Gaur (1978)
	3.15	Jadhav *et al.* (1978)
	3.43	Kelkar and Nemade (1979)
	3.60	Shivhare *et al.* (1981)
	3.48	Sachan *et al.* (1982)
	3.48	Kulshrestha *et al.* (1987)
	3.74	Placeres *et al.* (1988)
	3.65	Killa (1989)
	3.58	Ismail (1992)
	3.52	Jain *et al.* (1992)
	3.65	Al-Ahmadi and Katib (1997)
$CdHMal^+$	6.94	Schwarzenbach and Szilard (1962)
	7.16	Campi (1963)
	7.60	Ostacoli *et al.* (1968)

Table A4. Stability constant data for metal-salicylate complexes

Species	log K_o	Reference
CaSal	5.26	Arena *et al.* (1978b)
	3.59	Petho (1989)
	4.14	Dahlund and Olin (1990)
$CaHSal^+$	14.34	Davies (1938)
	14.41	Joseph (1946)
	14.16	Bell and Waind (1951)
	14.42	Schubert (1954)
	14.95	Daniele *et al.* (1985a)
	13.75	Dahlund and Olin (1990)
MgSal	6.07	May *et al.* (1977)
	6.13	Arena *et al.* (1978b)
	5.76	Petho (1989)
	5.85	Dahlund and Olin (1990)
$Mg(Sal)_2^{2-}$	10.45	May *et al.* (1977)
	8.46	Petho (1989)
FeSal	7.40	Perrin (1958)
	7.62	Petho (1989)
$Fe(Sal)_2^{2-}$	12.10	Perrin (1958)
	12.32	Petho (1989)
$FeSal^+$	4.66	Babko (1945)
	4.41	Vareille (1955)
	4.75	Perrin (1958)
	4.69	Shchigol (1961)
	4.69	Ching *et al.* (1961)
	4.42	Ernst and Menashi (1963)
	4.54	Park (1966)
	4.57	McBryde *et al.* (1970)
	4.31	Saini and Mentasti (1970)
	4.69	Pal and Lahiri (1973)
	4.62	Ramamoorthy and Manning (1973)
	4.55	Vasil'eva *et al.* (1973)
	4.43	Chattopadhyaya and Singh (1974)
	4.44	May et al. (1977)
	4.29	David and David (1979)
	4.63	Chattopadhyaya *et al.* (1982a)
	4.79	Dash and Mohanty (1989)
	4.89	Petho (1989)
$Fe(Sal)_2^-$	16.91	Perrin (1958)
	16.75	Colleter (1960)
	17.46	Pecci and Foye (1960)

Table A4 (cont.). Stability constant data for metal-salicylate complexes

Species	log K_o	Reference
$Fe(Sal)_2^-$ (cont.)	16.75	Shchigol (1961)
	15.55	Ogawa and Tobe (1966)
$Fe(Sal)_3^{3-}$	22.76	Babko (1945)
	24.00	Vareille (1955)
	24.82	Colleter (1960)
	24.27	Ogawa and Tobe (1966)
	25.39	Park (1966)
	23.93	Petho (1989)
MnSal	6.80	Perrin (1958)
	6.97	Krisnamoorthy *et al.* (1985)
$AlSal^+$	14.71	Secco and Venturini (1975)
	15.02	Rajan *et al.* (1975)
	14.56	Öhman and Sjöberg (1983b)
	14.68	Kiss *et al.* (1993)
$Al(Sal)_2^-$	25.58	Joshi (1974)
	25.75	Öhman and Sjöberg (1983b)
	25.67	Kiss *et al.* (1993)
$Al(Sal)_3^{3-}$	35.89	Rajan *et al.* (1975)
	34.00	Kiss *et al.* (1993)
$AlOH(Sal)_2^{2-}$	17.68	Öhman and Sjöberg (1983b)
	18.12	Kiss *et al.* (1993)
UO_2Sal	4.05	Hök-Berkström (1956)
	3.89	Bartusek (1967)
	4.01	Jagagirdar and Khanolkar (1973)
	3.86	Simões-Gonçalves and Mota (1987)
	4.08	Yousif and Imarah (1989)
$UO_2(Sal)_2^{2-}$	12.64	Bartusek (1967)
	14.45	Jagagirdar and Khanolkar (1973)
	13.89	Simões-Gonçalves and Mota (1987)
	13.77	Singh and Saxena (1991)
UO_2HSal^+	7.37	Hök-Berkström (1956)
	6.47	Simões-Gonçalves and Mota (1987)
ZnSal	7.85	Perrin (1958)
	7.97	Krisnamoorthy *et al.* (1985)
	7.66	Das (1989)

Table A4 (cont.). Stability constant data for metal-salicylate complexes

Species	log K_o	Reference
$Zn(Sal)_2^{2-}$	11.47	May *et al.* (1977)
	12.21	Das *et al.* (1989)
CuSal	11.49	Babko (1947)
	11.50	Perrin (1958)
	11.28	Pecci and Foye (1960)
	11.68	Das and Aditya (1965)
	11.51	Hsiu-Chin (1966)
	11.50	L'Heureux and Martell (1966)
	11.10	Perrin *et al.* (1967)
	11.66	Condike and Martell (1969)
	10.94	Habashy (1969)
	11.20	Brun and Schrøder (1975)
	11.41	Jagagirdar and Khanolkar (1975)
	11.18	Abbasi *et al.* (1978)
	11.02	Arena *et al.* (1978a)
	11.61	El-Ezaby and El-Khalafawy (1981)
	11.00	Chattopadhyaya *et al.* (1982b)
	11.56	Dhat and Jahagirdar (1982)
	10.67	Gupta *et al.* (1982)
	11.74	Lajunen *et al.* (1983)
	10.62	Cassasas and Tauler (1984)
	11.69	Venkatnarayana *et al.* (1984)
	10.71	Krisnamoorthy *et al.* (1985)
	11.71	Diaz-Cabellero *et al.* (1986a)
	11.18	Cazorla *et al.* (1988)
	11.28	Dahlund and Olin (1988)
	10.59	Anjaneyulu and Rao (1989)
	11.21	Das (1989)
	11.29	Petho (1989)
	10.67	Cassasas *et al.* (1990)
	10.91	Ventry *et al.* (1991)
	11.17	Brumas *et al.* (1995)
	11.48	Khalil and Radalla (1998)
$Cu(Sal)_2^{2-}$	19.60	Vasil'ev and Gorokhovski (1953)
	19.40	Perrin (1958)
	19.96	Heitner-Wirguin (1960)
	19.16	Pecci and Foye (1960)
	19.17	Perrin *et al.* (1967)
	19.82	Habashy (1969)
	19.87	Brun and Schrøder (1975)
	19.28	Jagagirdar and Khanolkar (1975)
	19.23	Abbasi *et al.* (1978)
	19.05	Dhat and Jahagirdar (1982)
	18.37	Cassasas and Tauler (1984)
	19.30	Venkatnarayana *et al.* (1984)
	19.18	Dahlund and Olin (1988)

Table A4 (cont.). Stability constant data for metal-salicylate complexes

Species	log K_o	Reference
$Cu(Sal)_2^{2-}$ (cont.)	18.97	Anjaneyulu and Rao (1989)
	18.71	Das (1989)
	19.16	Petho (1989)
	18.31	Cassasas *et al.* (1990)
	19.00	Brumas *et al.* (1995)
	19.94	Khalil and Radalla (1998)
$CuHSal^+$	15.85	Vasil'ev and Gorokhovski (1953)
	15.88	Habashy (1969)
	16.10	Brun and Schrøder (1975)
	16.11	Maheshwari *et al.* (1975)
	15.16	Dahlund and Olin (1988)
	15.71	Brumas *et al.* (1995)
$Cu(HSal)_2$	31.69	Vasil'ev and Gorokhovski (1953)
	31.68	Habashy (1969)
	32.73	Brun and Schrøder (1975)
	30.09	Maheshwari *et al.* (1975)
$CdHSal^+$	15.16	Zolotukhin and Galenets (1963)
	14.80	Gaur *et al.* (1966)
	14.61	Dhuley *et al.* (1975)
	14.75	Hassanein *et al.* (1993)
$Cd(HSal)_2$	28.72	Gaur *et al.* (1966)
	28.24	Dhuley *et al.* (1975)
	29.31	Hassanein *et al.* (1993)

Table A5. Stability constant data for metal-tricarballyate complexes

Species	log K_o	Reference
$HTri^{2-}$	6.63	Li *et al.* (1959)
	6.53	Campi *et al.* (1964)
	6.67	A
	6.44	Barnes and Bristow (1969)
	6.38	Purdie *et al.* (1972)
	6.46	Jackson (1982)
	6.49	De Stefano *et al.* (1994)
	6.30	Sutheimer *et al.* (1995)
H_2Tri^-	11.54	Li *et al.* (1959)
	11.39	Campi *et al.* (1964)
	11.32	A
	11.33	Barnes and Bristow (1969)
	11.25	Purdie *et al.* (1972)
	11.38	Jackson (1982)
	11.40	De Stefano *et al.* (1994)
	11.32	Sutheimer *et al.* (1995)
H_3Tri	15.05	Li *et al.* (1959)
	15.00	Campi *et al.* (1964)
	14.95	A
	14.92	Purdie *et al.* (1972)
	14.99	Jackson (1982)
	15.08	De Stefano *et al.* (1994)
	15.03	Sutheimer *et al.* (1995)
$CaTri^-$	3.27	Schubert and Lindenbaum (1952)
	3.44	Campi *et al.* (1964)
	3.28	De Stefano *et al.* (1994)
CaHTri	8.80	Campi *et al.* (1964)
	8.67	De Stefano *et al.* (1994)
CaH_2Tri^+	12.68	Campi *et al.* (1964)
	12.45	De Stefano *et al.* (1994)
$MgTri^-$	3.43	Li *et al.* (1959)
	3.33	Campi *et al.* (1964)
	3.26	De Stefano *et al.* (1994)
MgHTri	8.35	Li *et al.* (1959)
	8.54	Campi *et al.* (1964)
	8.61	De Stefano *et al.* (1994)

A Selected value was derived from unpublished work by Laramy and Leussing, as cited by Barnes and Bristow (1969).

Table A5 (cont.). Stability constant data for metal-tricarballyate complexes

Species	log K_o	Reference
MgH_2Tri^+	12.56	Campi *et al.* (1964)
	12.39	De Stefano *et al.* (1994)
$CuTri^-$	4.98	Campi *et al.* (1964)
	4.45	Brown *et al.* (1999)