# Equilibria and constants in CHEAQS: selection criteria, sources and assumptions
# Version 11 (November 2014)

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## Contents

## Introduction

This document accompanies the speciation program CHEAQS Next (a program for calculating CHemical Equilibria in AQuatic Systems), version Pro 2015.1 and higher. It gives information about the selection process for the equilibria and equilibrium constants for CHEAQS' database. Selecting equilibrium constants is an *important* step in equilibrium modelling. However, reported values in the literature may vary considerably (Zuehlke & Byrne, 1984), even up to a factor of 100 to 1000 (Giesy & Alberts, 1989). Selecting equilibrium constants is therefore a *critical* step as well. To ensure that the database of CHEAQS contains a consistent set of correct constants, values were taken from the NIST database 46 (version 8) where available (NIST database 46, 2004). This database has been compiled by the ultimate experts in this field, A.E. Martell and R.M. Smith, and is the electronic follow-up of their printed compilations (Martell & Smith, 1974, 1977, 1982; Smith & Martell, 1975, 1976, 1989).
A few other sources were used as well, but only after it was confirmed that for matching constants comparable values were given as in the NIST database.
For the inclusion of constants in the NIST database, fairly critical criteria were applied. However, if a constant has not been selected for the NIST database, it does not necessarily mean that the value is not correct; possibly the information to check the correctness is just incomplete. Therefore, it can be assumed that the values taken from the NIST database are most likely correct (within certain uncertainty limits) according to most recent insights, but this does not mean that the database is complete!

If you feel you are an expert in a certain field, do not hesitate to make changes to the database.

An important difference between this version 11 and previous versions is the way molecular weights are calculated. See page 113 for details.

## Selection criteria

The following selection criteria were applied.

1. If values were available from the NIST database 46, those constants were selected.
   1.1. If constants were available for ionic strength (I) of 0 and temperature of 25°C, those data were used. Skip 1.2 and 1.3.
   1.2. If only data were available for ionic strength (I) different from 0 and temperature of 25°C, those data were extrapolated to I=0 using the Davies-equation (see on-line help, item "Activity correction"). Skip 1.3.
   1.3. If only data were available for temperatures different from 25°C, those data were used. Extrapolation to I=0 was done as described under 1.2. No temperature correction was performed (see on-line help, item "Temperature correction").
   1.4. Values between brackets (classified by Martell & Smith as being "of questionable value") were *in*cluded.
   1.5. Several constants had to be converted to a different format before they could be entered. If this required other constants, already selected constants were used (if necessary after conversion to the appropriate I).
   1.6. If, for solids with the same stoichiometry, two solubility constants were available for different crystalline forms, the highest solubility constant was selected (i.e. the least soluble form).
2. If additional constants were available from other sources, those constants were selected if the data appeared sufficiently compatible with the NIST-data (see the Appendix).

For organic complexation, please refer to section II.6 Organic complexation, page 109.

## How to read this document

In part I of this document you will find the equilibria and constants selected from the NIST database. The first and second column contain the formulation of the equilibrium and the constant taken from the NIST database without any conversion (except for a few cases where an inversion of both the equilibrium and the constant took place). The third and fourth column contain the ionic strength (unit M) and temperature (unit °C) if different from the default values of 0 and 25°C resp. No data in these columns means default values. The last column (Conversion or remarks) contains the author's conversions, calculations and assumptions.
Complexes are first mentioned, followed by the solids and gases (if applicable). Part II basically uses the same setup. Part III contains the data of the molecular weights. The appendix demonstrates the compatibility of the different sources. Charges are omitted for readability, except for redox equilibria. Also, water is often not included in the formulation of the equilibria.

## Part I: NIST database 46 version 8

In part I you will find all the constants taken from the NIST database 46 version 8 (2004). The ligands are included in the order in which they are given in the CHEAQS database; the cations are given in the order in which they appear in the NIST database. All calculations were done using five decimals.

## Hydroxide ($OH^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 13.997 | | | |
| Li + L ⇆ LiL | 0.36 | | | |
| Na + L ⇆ NaL | 0.1 | | | |
| K + L ⇆ KL | 0.0 | 0.15 | 37 | I=0: 0.23787 |
| Be + L ⇆ BeL | 8.18 | 3.0 | | I=0: 7.63954 |
| Be + 2 L ⇆ $BeL_2$ | 16.22 | 0.1 | | I=0: 16.86073 |
| 2 Be + L ⇆ $Be_2L$ | 10.82 | 0.1 | | I=0: 10.82 |
| 3 Be + 3 L ⇆ $Be_3L_3$ | 33.1 | | | |
| 5 Be + 6 L ⇆ $Be_5L_6$ | 63.83 | 0.5 | | I=0: 65.17194 |
| 5 Be + 7 L ⇆ $Be_5L_7$ | 70.68 | 1.0 | | I=0: 72.50844 |
| 6 Be + 8 L ⇆ $Be_6L_8$ | 84.8 | | | |
| Mg + L ⇆ MgL | 2.58 | | | |
| 4 Mg + 4 L ⇆ $Mg_4L_4$ | 16.1<br>18.1 | 3.0 | | 16.1 using NaCl as background electrolyte; 18.1 using $NaClO_4$; used: average of 17.1<br>I=0: 16.55954 |
| Ca + L ⇆ CaL | 1.30 | | | |
| Sr + L ⇆ SrL | 0.82 | | | |
| Ba + L ⇆ BaL | 0.64 | | | |
| Sc + L ⇆ ScL | 9.7 | | | |
| Sc + 2 L ⇆ $ScL_2$ | 18.3 | | | |
| Sc + 3 L ⇆ $ScL_3$ | 23.9 | | | |
| Sc + 4 L ⇆ $ScL_4$ | 30 | | | |
| 2 Sc + 2 L ⇆ $Sc_2L_2$ | 22.0 | | | |
| 3 Sc + 5 L ⇆ $Sc_3L_5$ | 53.8 | | | |
| Y + L ⇆ YL | 6.3 | | | |
| 2 Y + 2 L ⇆ $Y_2L_2$ | 13.8 | | | |
| 3 Y + 5 L ⇆ $Y_3L_5$ | 38.4 | | | |
| La + L ⇆ LaL | 5.5 | | | |
| 2 La + 2 L ⇆ $La_2L_2$ | 10.5 | 2.0 | | I=0: 10.47112 |
| Ce + L ⇆ CeL | 5.7 | | | |
| 2 Ce + 2 L ⇆ $Ce_2L_2$ | 11.7 | 3.0 | | I=0: 11.15954 |
| Pr + L ⇆ PrL | 5.2 | 0.5 | | I=0: 6.00516 |
| 2 Pr + 2 L ⇆ $Pr_2L_2$ | 11.9 | 2.0 | | I=0: 11.87112 |
| Nd + L ⇆ NdL | 6.0 | | | |
| Nd + 4 L ⇆ $NdL_4$ | 18.6 | | | |
| 2 Nd + 2 L ⇆ $Nd_2L_2$ | 14.1 | | | |
| Sm + L ⇆ SmL | 6.1 | | | |
| 2 Sm + 2 L ⇆ $Sm_2L_2$ | 13.5 | 2.0 | | I=0: 13.47112 |
| Eu + L ⇆ EuL | 5.4 | 0.5 | | I=0: 6.20516 |
| 2 Eu + 2 L ⇆ $Eu_2L_2$ | 13.2 | 2.0 | | I=0: 13.17112 |
| Gd + L ⇆ GdL | 5.4 | 0.5 | | I=0: 6.20516 |
| 2 Gd + 2 L ⇆ $Gd_2L_2$ | 13.1 | 2.0 | | I=0: 13.07112 |
| Tb + L ⇆ TbL | 6.1 | | | |
| Dy + L ⇆ DyL | 5.6 | 0.5 | | I=0: 6.40516 |
| 2 Dy + 2 L ⇆ $Dy_2L_2$ | 14.0 | 2.0 | | I=0: 13.97112 |
| Ho + L ⇆ HoL | 5.7 | 0.5 | | I=0: 6.50516 |
| Er + L ⇆ ErL | 5.7 | 0.5 | | I=0: 6.50516 |
| 2 Er + 2 L ⇆ $Er_2L_2$ | 14.5 | 2.0 | | I=0: 14.47112 |
| Tm + L ⇆ TmL | 5.8 | 0.5 | | I=0: 6.60516 |
| Yb + L ⇆ YbL | 5.8 | 0.5 | | I=0: 6.60516 |
| 2 Yb + 2 L ⇆ $Yb_2L_2$ | 14.7 | 2.0 | | I=0: 14.67112 |
| Lu + L ⇆ LuL | 5.8 | 0.5 | | I=0: 6.60516 |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 8.1 | | | |
| 2 $(UO_2)$ + 2 L ⇆ $(UO_2)_2L_2$ | 22.42 | | | |
| 3 $(UO_2)$ + 5 L ⇆ $(UO_2)_3L_5$ | 54.4 | | | |
| Mn(II) + L ⇆ Mn(II)L | 3.4 | | | |
| Mn(II) + 4 L ⇆ $Mn(II)L_4$ | 7.7 | | | |
| 2 Mn(II) + L ⇆ $Mn(II)_2L$ | 3.4 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Mn(II) + 3 L ⇆ $Mn(II)_2L_3$ | 18.1 | | | |
| Fe(II) + L ⇆ Fe(II)L | 4.6 | | | |
| Fe(II) + 2 L ⇆ $Fe(II)L_2$ | 7.4 | | | |
| Fe(II) + 3 L ⇆ $Fe(II)L_3$ | 11 | | | |
| Co(II) + L ⇆ Co(II)L | 4.3 | | | |
| Co(II) + 2 L ⇆ $Co(II)L_2$ | 9.2 | | | |
| Co(II) + 3 L ⇆ $Co(II)L_3$ | 10.5 | | | |
| 4 Co(II) + 4 L ⇆ $Co(II)_4L_4$ | 25.5 | | | |
| Ni + L ⇆ NiL | 4.1 | | | |
| Ni + 2 L ⇆ $NiL_2$ | 9 | | | |
| Ni + 3 L ⇆ $NiL_3$ | 12 | | | |
| 4 Ni + 4 L ⇆ $Ni_4L_4$ | 28.3 | | | |
| Cu(II) + L ⇆ Cu(II)L | 6.5 | | | |
| 2 Cu(II) + L ⇆ $Cu(II)_2L$ | 7.7<br>8.4 | 3.0 | | 7.7 is for LiClO4 as background electrolyte; 8.4 for $NaClO_4$. Used: average 8.05<br>I=0: 8.05 |
| 2 Cu(II) + 2 L ⇆ $Cu(II)_2L_2$ | 17.5 | | | |
| 3 Cu(II) + 4 L ⇆ $Cu(II)_3L_4$ | 35.2 | | | |
| Cr(III) + L ⇆ Cr(III)L | 10.30 | | | |
| Cr(III) + 2 L ⇆ $Cr(III)L_2$ | 18.3 | | | |
| 2 Cr(III) + 2 L ⇆ $Cr(III)_2L_2$ | 24.0 | 1.0 | | I=0: 24.40632 |
| 3 Cr(III) + 4 L ⇆ $Cr(III)_3L_4$ | 37.0 | 1.0 | | I=0: 37.60948 |
| 4 Cr(III) + 6 L ⇆ $Cr(III)_4L_6$ | 80.2 | 1.0 | | I=0: 80.80948 |
| Fe(III) + L ⇆ Fe(III)L | 11.81 | | | |
| Fe(III) + 2 L ⇆ $Fe(III)L_2$ | 22.4 | | | |
| Fe(III) + 3 L ⇆ $Fe(III)L_3$ | 30.2 | | | |
| Fe(III) + 4 L ⇆ $Fe(III)L_4$ | 34.4 | | | |
| 2 Fe(III) + 2 L ⇆ $Fe(III)_2L_2$ | 25.10 | | | |
| 3 Fe(III) + 4 L ⇆ $Fe(III)_3L_4$ | 49.7 | | | |
| Co(III) + L ⇆ Co(III)L | 13.54 | 3.0 | | I=0: 12.72931 |
| Zr + L ⇆ ZrL | 14.3 | | | |
| Zr + 4 L ⇆ $ZrL_4$ | 47.6 | 1.0 | 20 | I=0: 49.63160 |
| Zr + 5 L ⇆ $ZrL_5$ | 54.0 | | | |
| 3 Zr + 4 L ⇆ $Zr_3L_4$ | 55.4 | | | |
| 4 Zr + 8 L ⇆ $Zr_4L_8$ | 106.0 | | | |
| Hf + L ⇆ HfL | 13.8 | | | |
| Hf + 5 L ⇆ $HfL_5$ | 52.8 | | | |
| Ag + L ⇆ AgL | 2.0 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 3.99 | | | |
| Pd + L ⇆ PdL | 10.8 | 1.0 | | I=0: 11.20632 |
| Zn + L ⇆ ZnL | 5.0 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | 11.1 | | | |
| Zn + 3 L ⇆ $ZnL_3$ | 13.6 | | | |
| Zn + 4 L ⇆ $ZnL_4$ | 14.8 | | | |
| 2 Zn + L ⇆ $Zn_2L$ | 5.0 | | | |
| 4 Zn + 4 L ⇆ $Zn_4L_4$ | 27.9 | 3.0 | | I=0: 27.35954 |
| Cd + L ⇆ CdL | 3.9 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 7.7 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 10.3 | 3.0 | | I=0: 9.48931 |
| Cd + 4 L ⇆ $CdL_4$ | 8.7 | | | |
| 2 Cd + L ⇆ $Cd_2L$ | 4.6 | | | |
| 4 Cd + 4 L ⇆ $Cd_4L_4$ | 23.2 | | | |
| Hg(II) + L ⇆ Hg(II)L | 10.60 | | | |
| Hg(II) + 2 L ⇆ $Hg(II)L_2$ | 21.83 | | | |
| 2 Hg(II) + L ⇆ $Hg(II)_2L$ | 10.7 | | | |
| 3 Hg(II) + 3 L ⇆ $Hg(II)_3L_3$ | 35.6 | | | |
| Sn(II) + L ⇆ Sn(II)L | 10.6 | | | |
| Sn(II) + 2 L ⇆ $Sn(II)_2L$ | 20.9 | | | |
| Sn(II) + 3 L ⇆ $Sn(II)_3L$ | 25.4 | | | |
| 2 Sn(II) + 2 L ⇆ $Sn(II)_2L_2$ | 23.2 | | | |
| 3 Sn(II) + 4 L ⇆ $Sn(II)_3L_4$ | 49.12 | | | |
| Pb(II) + L ⇆ Pb(II)L | 6.4 | | | |
| Pb(II) + 2 L ⇆ $Pb(II)L_2$ | 10.9 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pb(II) + 3 L ⇆ Pb(II)$L_3$ | 13.9 | | | |
| 2 Pb(II) + L ⇆ $Pb(II)_2L$ | 7.6 | | | |
| 3 Pb(II) + 4 L ⇆ $Pb(II)_3L_4$ | 32.1 | | | |
| 4 Pb(II) + 4 L ⇆ $Pb(II)_4L_4$ | 35.1 | | | |
| 6 Pb(II) + 8 L ⇆ $Pb(II)_6L_8$ | 68.4 | | | |
| Al + L ⇆ AlL | 9.00 | | | |
| Al + 2 L ⇆ $AlL_2$ | 17.7 | | | |
| Al + 3 L ⇆ $AlL_3$ | 25.3 | | | |
| Al + 4 L ⇆ $AlL_4$ | 33.3 | | | |
| 2 Al + 2 L ⇆ $Al_2L_2$ | 20.3 | | | |
| 3 Al + 4 L ⇆ $Al_3L_4$ | 42.1 | | | |
| 13 Al + 32 L ⇆ $Al_{13}O_4L_{24}$ | 349.3 | | | |
| Ga + L ⇆ GaL | 11.1 | | | |
| Ga + 2 L ⇆ $GaL_2$ | 21.3 | | | |
| Ga + 4 L ⇆ $GaL_4$ | 39.4 | | | |
| 2 Ga + 2 L ⇆ $Ga_2L_2$ | 25.8 | 0.5 | | I=0: 26.33678 |
| In + L ⇆ InL | 10.07 | | | |
| In + 2 L ⇆ $InL_2$ | 20.2 | | | |
| In + 3 L ⇆ $InL_3$ | 29.6 | | | |
| In + 4 L ⇆ $InL_4$ | 33.9 | | | |
| 2 In + 2 L ⇆ $In_2L_2$ | 23.2 | 3.0 | | I=0: 22.65954 |
| 4 In + 4 L ⇆ $In_4L_4$ | 47.8 | 0.1 | | I=0: 45.23710 |
| 4 In + 6 L ⇆ $In_4L_6$ | 43.1 | 3.0 | | I=0: 42.28931 |
| As(III) + L ⇆ As(III)L | 16.5 | | | not entered; As(III) only entered as anion/ligand |
| As(III) + 2 L ⇆ As(III)$L_2$ | 32.3 | | | |
| As(III) + 3 L ⇆ As(III)$L_3$ | 46.9 | | | |
| Bi + L ⇆ BiL | 12.9 | | | |
| Bi + 2 L ⇆ $BiL_2$ | 23.5 | 1.0 | | I=0: 24.51580 |
| Bi + 3 L ⇆ $BiL_3$ | 33.0 | | | (some poly(6 and 9)nuclear complexes of Bi skipped) |
| Bi + 4 L ⇆ $BiL_4$ | 34.8 | | | |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Be + L ⇆ BeL | 21.5 | | | |
| Mg + L ⇆ MgL | 11.1 | | | |
| Ca + 2 L ⇆ $CaL_2$ | 5.29 | | | |
| Ba + 2 L ⇆ $BaL_2(H_2O)_8$ | 3.6 | | | |
| Sc + 3 L ⇆ ScOL | 29.7 | | | |
| Y + 3 L ⇆ $YL_3$ | 25.9 | | | |
| La + 3 L ⇆ $LaL_3$ | 22.2 | | | |
| Ce + 3 L ⇆ $CeL_3$ | 23.9 | | | |
| Pr + 3 L ⇆ $PrL_3$ | 24.4 | | | |
| Nd + 3 L ⇆ $NdL_3$ | 26.0 | | | |
| Sm + 3 L ⇆ $SmL_3$ | 25.9 | | | |
| Eu + 3 L ⇆ $EuL_3$ | 26.5 | | | |
| Gd + 3 L ⇆ $GdL_3$ | 26.9 | | | |
| Tb + 3 L ⇆ $TbL_3$ | 26.3 | | | |
| Dy + 3 L ⇆ $DyL_3$ | 25.9 | | | |
| Ho + 3 L ⇆ $HoL_3$ | 26.6 | | | |
| Er + 3 L ⇆ $ErL_3$ | 26.6 | | | |
| Tm + 3 L ⇆ $TmL_3$ | 26.7 | | | |
| Yb + 3 L ⇆ $YbL_3$ | 26.6 | | | |
| Lu + 3 L ⇆ $LuL_3$ | 27.0 | | | |
| $(UO_2)$ + 2 L ⇆ $(UO_2)L_2(H_2O)$ | 22.0 | | | |
| Mn(II) + 2 L ⇆ Mn(II)$L_2$ | 12.8 | | | |
| Fe(II) + 2 L ⇆ Fe(II)$L_2$ | 15.1 | | | |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | 15.7 | | | |
| Ni + 2 L ⇆ $NiL_2$ | 17.2 | | | |
| Cu(II) + 2 L ⇆ Cu(II)O | 19.5 | | | |
| Cr(III) + 3 L ⇆ Cr(III)$L_3$ | 30.2 | | | |

| | | | | |
|---|---|---|---|---|
| Fe(III) + 3 L $\leftrightarrows$ $(Fe(III)_2O_3)_{0.5}$ | 42.7 | | | Entered:<br>2 Fe(III) + 6 L $\leftrightarrows$ $Fe(III)_2O_3$<br>log(K)=2*42.7=85.4 |
| Co(III) + 3 L $\leftrightarrows$ $Co(III)L_3$ | 44.4 | | | |
| Zr + 4 L $\leftrightarrows$ $ZrO_2$ | 54.1 | | | |
| Hf + 4 L $\leftrightarrows$ $HfO_2$ | 54.8 | | | |
| Cu(I) + L $\leftrightarrows$ $(Cu(I)_2O)_{0.5}$ | 14.7 | | | Entered:<br>2 Cu(I) + 2 L $\leftrightarrows$ $Cu(I)_2O$<br>log(K)=2*14.7=29.4 |
| Ag + L $\leftrightarrows$ $(Ag_2O)_{0.5}$ | 7.71 | | | Entered:<br>2 Ag + 2 L $\leftrightarrows$ $Ag_2O$<br>log(K)=2*7.71=15.42 |
| Pd + 2 L $\leftrightarrows$ $Pd(OH)_2$ | 30.8 | 0.1 | | I=0: 31.44073 |
| Zn + 2 L $\leftrightarrows$ ZnO | 16.76 | | | |
| Cd + 2 L $\leftrightarrows$ $CdL_2$ | 14.35 | | | |
| Hg(II) + 2 L $\leftrightarrows$ Hg(II)O | 25.44 | | | |
| Sn(II) + 2 L $\leftrightarrows$ Sn(II)O | 26.2 | | | |
| Pb(II) + 2 L $\leftrightarrows$ Pb(II)O | 15.3 | | | |
| Al + 3 L $\leftrightarrows$ $AlL_3$ | 33.7 | | | |
| Ga + 3 L $\leftrightarrows$ $(Ga_2O_3)_{0.5}$ | 39.8 | | | Entered:<br>2 Ga + 6 L $\leftrightarrows$ $Ga_2O_3$<br>log(K)=2*39.8=79.6 |
| In + 3 L $\leftrightarrows$ $InL_3$ | 36.9 | | | |
| $BiL_3$ $\leftrightarrows$ $(Bi_2O_3)_{0.5}$ | 5.4 | | | Entered:<br>2 Bi + 6 L $\leftrightarrows$ $Bi_2O_3$<br>log(K)=2*5.4=10.8 |

## Borate ($H_2BO_3^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.236 | | | |
| HL + L ⇆ $HL_2$ | -0.07 | | | H+L ⇆ HL 9.236<br>HL+L ⇆ $HL_2$ -0.07<br>H + 2 L ⇆ $HL_2$ 9.166 |
| HL + $HL_2$ ⇆ $H_2L_3$ | 2.00 | | | H + L ⇆ HL 9.236<br>H + 2 L ⇆ $HL_2$ 9.166<br>HL + $HL_2$ ⇆ $H_2L_3$ 2.00<br>2 H +3 L ⇆ $H_2L_3$ 20.402 |
| $H_2L_3$ + L ⇆ $H_2L_4$ | 1.51 | | | $H_2L_3$ + L ⇆ $H_2L_4$ 1.51<br>2 H +3 L ⇆ $H_2L_3$ 20.402<br>2 H + 4 L ⇆ $H_2L_4$ 21.912 |
| Li + L ⇆ LiL | 0.34 | | | |
| Na + L ⇆ NaL | -0.15 | | | |
| Mg + L ⇆ MgL | 1.54 | | | |
| Ca + L ⇆ CaL | 1.76 | | | |
| Sr + L ⇆ SrL | 1.55 | | | |
| Ba + L ⇆ BaL | 1.49 | | | |
| Cu + L ⇆ CuL | 3.48 | 0.7 | | I=0: 3.97883 |
| Cu + 2 L ⇆ $CuL_2$ | 6.13 | 0.7 | | I=0: 6.87824 |
| Zn + L ⇆ ZnL | 0.9 | 0.7 | | I=0: 1.39883 |
| Zn + 2 L ⇆ $ZnL_2$ | 3.32 | 0.7 | | I=0: 4.06824 |
| Cd + L ⇆ CdL | 1.42 | 0.7 | | I=0: 1.91883 |
| Cd + 2 L ⇆ $CdL_2$ | 2.71 | 0.7 | | I=0: 3.45824 |
| Pb(II) + L ⇆ Pb(II)L | 2.2 | 0.7 | | I=0: 2.69883 |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 4.41 | 0.7 | | I=0: 5.15824 |
| Fe(III) + L ⇆ Fe(III)L | 6.58 | 0.7 | | I=0: 7.32824 |
| Ag + L ⇆ AgL | 0.45 | 3.0 | | I=0: 0.17977 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ag + 2 HL ⇆ H + $AgHL_2$ | -4.5 | 3.0 | | (H + L ⇆ HL)*2 19.01246 3.0<br>(9.50623*2)<br>Ag + 2 HL ⇆ H + $AgHL_2$ -4.5 3.0<br>Ag + H + 2 L ⇆ $AgHL_2$ 14.51246 3.0<br>I=0: 13.972 |

# Carbonate ($CO_3^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 10.329 | | | |
| HL + H ⇆ $H_2L$ | 6.352 | | | HL + H ⇆ $H_2L$ 6.352<br>H + L ⇆ HL 10.329<br>2 H + L ⇆ $H_2L$ 16.681 |
| Na + L ⇆ NaL | 1.27 | | | |
| Na + HL ⇆ NaHL | -0.3 | | | Na + HL ⇆ NaHL -0.3<br>H + L ⇆ HL 10.329<br>Na + H + L ⇆ NaHL 10.029 |
| Cs + L ⇆ CsL | -0.7 | 1.0 | | I=0: -0.29368 |
| Be + L ⇆ BeL | 7.34 | 3.0 | | I=0: 6.25909 |
| BeL ⇆ BeOHL + H | -6.56 | 3.0 | | BeL ⇆ BeOHL + H -6.56 3.0<br>Be + L ⇆ BeL 7.34 3.0<br>H + OH ⇆ H2O 14.26723 3.0<br>Be + L + OH ⇆ BeOHL + $H_2O$<br>15.04723 3.0<br>I=0: 13.96632 |
| BeOHL ⇆ $Be(OH)_2L$ + H | -7.54 | 3.0 | | BeOHL ⇆ $Be(OH)_2L$ + H -7.54 3.0<br>Be + OH + L ⇆ BeOHL 15.04723 3.0<br>H + OH ⇆ $H_2O$ 14.26723 3.0<br>Be + L + 2 OH ⇆ $Be(OH)_2L$ + $H_2O$<br>21.85446 3.0<br>I=0: 21.04377 |
| 3 Be + 3 L ⇆ $Be_3(OH)_3L_3$ + 3 H | 6.9 | 3.0 | | 3 Be + 3 L ⇆ $Be_3(OH)_3L_3$ + 3 H<br>6.9 3.0<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.26723) 42.80169 3.0<br>3 Be + 3 OH + 3 L ⇆ $Be_3(OH)_3L_3$ + 3 $H_2O$<br>49.70169 3.0<br>I=0: 47.26963 |
| 3 Be + L ⇆ $Be_3(OH)_2L$ + 2 H | -1.01 | 3.0 | | 3 Be + L ⇆ $Be_3(OH)_2L$ + 2 H<br>-1.01 3.0<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.26723): 28.53446 3.0<br>3 Be + L + 2 OH ⇆ $Be_3(OH)_2L$ + 2 $H_2O$<br>27.52446 3.0<br>I=0: 25.63286 |
| 5 Be + L ⇆ $Be_5(OH)_4L$ + 4 H | 0.22 | 3.0 | | 5 Be + L ⇆ $Be_5(OH)_4L$ + 4 H<br>0.22 3.0<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.26723): 57.06892 3.0<br>5 Be + L + 4 OH ⇆ $Be_5(OH)_4L$ + 4 $H_2O$<br>57.28892 3.0<br>I=0: 55.66755 |
| 6 Be + 2 L ⇆ $Be_6(OH)_5L_2$ + 5 H | 5.46 | 3.0 | | 6 Be + 2 L ⇆ $Be_6(OH)_5L_2$ + 5 H<br>5.46 3.0<br>5 H + 5 OH ⇆ 5 $H_2O$<br>(5*14.26723): 71.33615 3.0<br>6 Be + 2 L + 5 OH ⇆ $Be_6(OH)_5L_2$ + 5 $H_2O$<br>76.79615 3.0<br>I=0: 73.01295 |
| Mg + L ⇆ MgL | 2.92 | | | |
| Mg + HL ⇆ MgHL | 1.01 | | | Mg + HL ⇆ MgHL 1.01<br>H + L ⇆ HL 10.329<br>Mg + H + L ⇆ MgHL 11.339 |
| Ca + L ⇆ CaL | 3.22 | | | |
| Ca + HL ⇆ CaHL | 1.20 | | | Ca + HL ⇆ CaHL 1.20<br>H + L ⇆ HL 10.329<br>Ca + H + L ⇆ CaHL 11.529 |
| Sr + L ⇆ SrL | 2.81 | | | |
| Sr + HL ⇆ SrHL | 1.21 | | | Sr + HL ⇆ SrHL 1.21<br>H + L ⇆ HL 10.329<br>Sr + H + L ⇆ SrHL 11.539 |
| Ba + L ⇆ BaL | 2.71 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ba + HL ⇆ BaHL | 0.98 | | | Ba + HL ⇆ BaHL 0.98<br>H + L ⇆ HL 10.329<br>Ba + H + L ⇆ BaHL 11.309 |
| Y + L ⇆ YL | 7.73 | | | |
| Y + 2 L ⇆ $YL_2$ | 11.86 | | | |
| Y + HL ⇆ YHL | 2.4 | | | Y + HL ⇆ YHL 2.4<br>H + L ⇆ HL 10.329<br>Y + H + L ⇆ YHL 12.729 |
| 2 Y + L ⇆ $Y_2L$ | 8.06 | | | |
| La + L ⇆ LaL | 6.98 | | | |
| La + 2 L ⇆ $LaL_2$ | 11.86 | | | |
| La + HL ⇆ LaHL | 1.41 | 3.0 | | La + HL ⇆ LaHL 1.41 3.0<br>H + L ⇆ HL 10.86946 3.0<br>La + H + L ⇆ LaHL 12.27946 3.0<br>I=0: 10.92832 |
| 2 La + L ⇆ $La_2L$ | 6.92 | 3.0 | | I=0: 6.10931 |
| Ce + L ⇆ CeL | 7.31 | | | |
| Ce + 2 L ⇆ $CeL_2$ | 12.32 | | | |
| Ce + HL ⇆ CeHL | 1.6 | 0.7 | | Ce + HL ⇆ CeHL 1.6 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Ce + H + L ⇆ CeHL 11.43017 0.7<br>I=0: 12.67723 |
| Pr + L ⇆ PrL | 7.48 | | | |
| Pr + 2 L ⇆ $PrL_2$ | 12.63 | | | |
| Nd + L ⇆ NdL | 7.53 | | | |
| Nd + 2 L ⇆ $NdL_2$ | 12.73 | | | |
| Sm + L ⇆ SmL | 7.71 | | | |
| Sm + 2 L ⇆ $SmL_2$ | 13.09 | | | |
| Eu + L ⇆ EuL | 7.73 | | | |
| Eu + 2 L ⇆ $EuL_2$ | 13.19 | | | |
| Eu + HL ⇆ EuHL | 1.5 | 0.7 | | Eu + HL ⇆ EuHL 1.5 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Eu + H + L ⇆ EuHL 11.33017 0.7<br>I=0: 12.57723 |
| Gd + L ⇆ GdL | 7.64 | | | |
| Gd + 2 L ⇆ $GdL_2$ | 13.04 | | | |
| Gd + HL ⇆ GdHL | 1.9 | 0.7 | | Gd + HL ⇆ GdHL 1.9 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Gd + H + L ⇆ GdHL 11.73017 0.7<br>I=0: 12.97723 |
| Tb + L ⇆ TbL | 7.71 | | | |
| Tb + 2 L ⇆ $TbL_2$ | 13.34 | | | |
| Tb + HL ⇆ TbHL | 1.8 | 0.7 | | Tb + HL ⇆ TbHL 1.8 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Tb + H + L ⇆ TbHL 11.63017 0.7<br>I=0: 12.87723 |
| Dy + L ⇆ DyL | 7.81 | | | |
| Dy + 2 L ⇆ $DyL_2$ | 13.47 | | | |
| Ho + L ⇆ HoL | 7.80 | | | |
| Ho + 2 L ⇆ $HoL_2$ | 13.56 | | | |
| Er + L ⇆ ErL | 7.86 | | | |
| Er + 2 L ⇆ $ErL_2$ | 13.68 | | | |
| Tm + L ⇆ TmL | 7.93 | | | |
| Tm + 2 L ⇆ $TmL_2$ | 13.83 | | | |
| Yb + L ⇆ YbL | 8.06 | | | |
| Yb + 2 L ⇆ $YbL_2$ | 13.86 | | | |
| Yb + HL ⇆ YbHL | 1.5 | 0.7 | | Yb + HL ⇆ YbHL 1.5 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Yb + H + L ⇆ YbHL 11.33017 0.7<br>I=0: 12.57723 |
| Lu + L ⇆ LuL | 8.00 | | | |
| Lu + 2 L ⇆ $LuL_2$ | 13.93 | | | |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 9.6 | | | |
| $(UO_2)$ + 2 L ⇆ $(UO_2)L_2$ | 16.9 | | | |
| $(UO_2)$ + 3 L ⇆ $(UO_2)L_3$ | 21.6 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
| --- | --- | --- | --- | --- |
| 3 $(UO_2)$ + 6 L ⇆ $(UO_2)_3L_6$ | 54.0 | | | |
| 2 $(UO_2)$ + L ⇆ $(UO_2)_2(OH)_3L$ + 3 H | -0.9 | | | 2 $(UO_2)$ + L ⇆ $(UO_2)2(OH)_3L$ + 3 H -0.9<br>(H + OH ⇆ $H_2O$)<br>(3* 13.997) 41.991<br>2 $(UO_2)$ + L + 3 OH ⇆ $(UO_2)_2(OH)_3L$+ 3 $H_2O$ 41.091 |
| 3 $(UO_2)$ + L ⇆ $(UO_2)_3(OH)_3L$ + 3 H | 0.7 | | | 3 $(UO_2)$ + L ⇆ $(UO_2)_3(OH)_3L$ + 3 H 0.7<br>(H + OH ⇆ $H_2O$)<br>(3*13.997) 41.991<br>3 $(UO_2)$ + L + 3 OH ⇆ $(UO_2)_3(OH)_3L$+ 3 $H_2O$ 42.691 |
| 11 $(UO_2)$ + 6 L ⇆ $(UO_2)_{11}(OH)_{12}L_6$ + 12 H | 34 | | | 11 $(UO_2)$ + 6 L ⇆ $(UO_2)_{11}(OH)_{12}L_6$ +12 H 34<br>(H + OH ⇆ $H_2O$)<br>(12*13.997) 167.964<br>11 $(UO_2)$ + 6 L + 12 OH ⇆ $(UO_2)_{11}(OH)_{12}L_6$ + 12 $H_2O$ 201.964 |
| Mn(II) + L ⇆ Mn(II)L | 4.7 | | | |
| Mn(II) + HL ⇆ Mn(II)HL | 1.30 | | | Mn(II) + HL ⇆ Mn(II)HL 1.30<br>H + L ⇆ HL 10.329<br>Mn(II) + H + L ⇆ Mn(II)HL 11.629 |
| Fe(II) + HL ⇆ Fe(II)HL | 1.10 | | | Fe(II) + HL ⇆ Fe(II)HL 1.10<br>H + L ⇆ HL 10.329<br>Fe(II) + H + L ⇆ Fe(II)HL 11.429 |
| Co(II) + L ⇆ Co(II)L | 3.15 | 0.5 | | I=0: 4.22355 |
| Co(II) + HL ⇆ Co(II)HL | 1.39 | 0.7 | | Co(II) + HL ⇆ Co(II)HL 1.39 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Co(II) + H + L ⇆ Co(II)HL 11.22017 0.7<br>I=0: 12.21782 |
| Ni(II) + L ⇆ Ni(II)L | 3.57 | 0.7 | | I=0: 4.56765 |
| Ni(II) + HL ⇆ Ni(II)HL | 1.59 | 0.7 | | Ni(II) + HL ⇆ Ni(II)HL 1.59 0.7<br>H + L ⇆ HL 9.83017 0.7<br>Ni(II) + H + L ⇆ Ni(II)HL 11.42017 0.7<br>I=0: 12.41782 |
| Cu(II) + L ⇆ Cu(II)L | 6.77 | | | |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | 10.2 | | | |
| Cu(II) + HL ⇆ Cu(II)HL | 1.8 | | | Cu(II) + HL ⇆ Cu(II)HL 1.8<br>H + L ⇆ HL 10.329<br>Cu(II) + H + L ⇆ Cu(II)HL 12.129 |
| Fe(III) + L ⇆ Fe(III)(OH)L + H | -3.8 | 0.2 | | Fe(III) + L ⇆ Fe(III)(OH)L + H -3.8 0.2<br>H + OH = $H_2O$ 13.74405 0.2<br>Fe(III) + L + OH = Fe(III)(OH)L 9.94405 0.2<br>I=0: 11.71471 |
| Fe(III) + 2 L ⇆ Fe(III)$L_2$ | 7.4 | 0.2 | | I=0: 9.42361 |
| Zn + L ⇆ ZnL | 4.76 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | 7.3 | | | |
| 2 Zn + L ⇆ $Zn_2L$ | 4.16 | 3.0 | | I=0: 3.07909 |
| Zn + HL ⇆ ZnHL | 1.5 | | | Zn + HL ⇆ ZnHL 1.5<br>H + L ⇆ HL 10.329<br>Zn + H + L ⇆ ZnHL 11.829 |
| Cd + L ⇆ CdL | 3.5 | 0.1 | | I=0: 4.35430 |
| Cd + 2 L ⇆ $CdL_2$ | 6.37 | 0.1 | 20 | I=0: 7.22430 |
| Cd + HL ⇆ CdHL | 0.9 | 3.0 | | Cd + HL ⇆ CdHL 0.9 3.0<br>H + L ⇆ HL 10.86946 3.0<br>Cd + H + L ⇆ CdHL 11.76946 3.0<br>I=0: 10.68855 |
| Hg(II) + L ⇆ Hg(II)L | 11.0 | 0.5 | | I=0: 12.07355 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 14.5 | 0.5 | | I=0: 15.57355 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Hg(II) + HL ⇆ Hg(II)HL | 5.48 | 0.5 | | Hg(II) + HL ⇆ Hg(II)HL 5.48 0.5<br>H + L ⇆ HL 9.79222 0.5<br>Hg(II) + H + L ⇆ Hg(II)HL<br>15.27222 0.5<br>I=0: 16.34577 |
| Hg(II)L ⇆ Hg(II)OHL + H | -6.6 | 0.5 | | Hg(II)L ⇆ Hg(II)OHL + H<br>-6.6 0.5<br>Hg(II) + L ⇆ Hg(II)L 11 0.5<br>H + OH ⇆ $H_2O$ 13.72861 0.5<br>Hg(II) + L + OH ⇆ Hg(II)OHL<br>18.12861 0.5<br>I=0: 19.20216 |
| Pb(II) + L ⇆ Pb(II)L | 5.40 | 0.5 | | I=0: 6.47355 |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 8.86 | 0.5 | | I=0: 9.93355 |
| Pb(II) + OH + L ⇆ Pb(II)OHL | 10.9 | 3.0 | | I=0: 9.81909 |
| Pb(II) + HL ⇆ Pb(II)HL | 1.91 | 3.0 | | Pb(II) + HL ⇆ Pb(II)HL 1.91 3.0<br>H + L ⇆ HL 10.86946 3.0<br>Pb(II) + H + L ⇆ Pb(II)HL<br>12.77946 3.0<br>I=0: 11.69855 |
| 2 Pb(II) + L ⇆ Pb(II)$_2$L | 7.1 | 3.0 | | I=0: 6.01909 |
| 3 Pb(II) + L ⇆ Pb(II)$_3$L | 8.43 | 3.0 | | I=0: 8.43 |
| 2 Al + HL ⇆ $Al_2(OH)_2L$ + 3 H | -7.3 | 0.1 | | 2 Al + HL ⇆ $Al_2(OH)_2L$ + 3 H<br>-7.3 0.1<br>H + L ⇆ HL 9.90185 0.1<br>(H + OH ⇆ H2O)<br>(2* 13.78342) 27.56684 0.1<br>2 Al + L + 2 OH ⇆ $Al_2(OH)_2L$<br>30.16869 0.1<br>I=0: 32.30444 |
| 3 Al + HL ⇆ $Al_3(OH)_4HL$ + 4 H | -9.4 | 0.1 | | 3 Al + HL ⇆ $Al_3(OH)_4HL$ + 4 H<br>-9.4 0.1<br>H + L ⇆ HL 9.90185 0.1<br>OH + H ⇆ $H_2O$<br>(4*13.78342) 55.13368 0.1<br>3 Al + 4 OH + H + L ⇆ $Al_3(OH)_4HL$<br>55.63553 0.1<br>I=0: 57.77128 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Mg + L ⇆ MgL | 7.46 | | | |
| Ca + L ⇆ CaL | 8.48 | | | calcite |
| Sr + L ⇆ SrL | 9.27 | | | |
| Ba + L ⇆ BaL | 8.57 | | | |
| 2 Y + 3 L ⇆ $Y_2L_3$ | 33.0 | | | |
| 2 La + 3 L ⇆ $La_2L_3$ | 34.4 | | | |
| 2 Ce + 3 L ⇆ $Ce_2L_3$ | 31.1 | 3.0 | | I=0: 27.04657 |
| Nd + OH + L ⇆ NdOHL | 19.9 | 0.1 | | I=0: 21.39503 |
| 2 Nd + 3 L ⇆ $Nd_2L_3$ | 33.0 | | | |
| 2 Sm + 3 L ⇆ $Sm_2L_3$ | 32.5 | | | |
| Eu + OH + L ⇆ EuOHL | 20.2 | 0.1 | | I=0: 21.69503 |
| 2 Eu + 3 L ⇆ $Eu_2L_3$ | 32.3 | | | |
| 2 Gd + 3 L ⇆ $Gd_2L_3$ | 32.2 | | | |
| 2 Dy + 3 L ⇆ $Dy_2L_3$ | 31.5 | | | |
| 2 Yb + 3 L ⇆ $Yb_2L_3$ | 31.1 | | | |
| ($UO_2$) + L ⇆ ($UO_2$)L | 14.5 | | | |
| Mn(II) + L ⇆ Mn(II)L | 11.0 | | | |
| Fe(II) + L ⇆ Fe(II)L | 10.8 | | | |
| Co(II) + L ⇆ Co(II)L | 11.2 | | | |
| Ni + L ⇆ NiL | 11.2 | | | |
| Cu(II) + L ⇆ Cu(II)L | 11.5 | | | |
| 2 Cu(II) + 2 OH + L ⇆ Cu(II)$_2(OH)_2$L | 33.3 | | | malachite |
| 3 Cu(II) + 2 OH + 2 L ⇆ Cu(II)$_3(OH)_2L_2$ | 44.9 | | | azurite |

| | | | | |
|---|---|---|---|---|
| 2 Ag + L ⇆ $Ag_2L$ | 11.09 | | | |
| Zn + L ⇆ ZnL | 10.8 | | | |
| Cd + L ⇆ CdL | 12.1 | | | otavite |
| 3 Hg(II) + L ⇆ $Hg(II)_3O_2L$ + 4 H | 11.1 | | | 3 Hg(II) + L ⇆ $Hg(II)_3(OH)_4L(s)$ + 4 H 11.1<br>(H + OH ⇆ $H_2O$)<br>(4*13.997) 55.988<br>3 Hg(II) + L + 4 OH ⇆ $Hg(II)_3(OH)_4L(s)$ + 4 $H_2O$ 67.088 |
| Pb(II) + L ⇆ Pb(II)L | 13.2 | | | |
| 3 Pb(II) + 2 OH + 2 L ⇆ $Pb(II)_3(OH)_2L_2$ | 43.8 | 0.5 | | I=0: 46.75227 |
| 10 Pb(II) + 6 L ⇆ $Pb(II)_{10}(OH)_6OL_6$ + 8 H | 8.76 | | | 10 Pb(II) + 6 L ⇆ $Pb(II)_{10}(OH)_6L_6O$+ 8 H 8.76<br>(H + OH ⇆ $H_2O$)<br>(8*13.997) 111.976<br>10 Pb(II) + 6 L + 8 OH ⇆ $Pb(II)_{10}(OH)_6L_6O$ + 8 $H_2O$ 120.736 |

Gases:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_2L$ ⇆ $CO_2$ (g) | 1.466 | | | $H_2L$ ⇆ $CO_2$ (g) 1.466<br>2 H + L ⇆ $H_2L$ 16.681<br>2 H + L ⇆ $CO_2$ (g) 18.147 |

## Ammonia ($NH_3$)

Note: since $NH_3$ is an uncharged ligand, the Davies-correction yields the same values for I=0 as for any other I.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.244 | | | |
| Li + L ⇆ LiL | -0.7 | | | |
| Mg + L ⇆ MgL | 0.24 | 2.0 | | |
| Mg + 2 L ⇆ $MgL_2$ | 0.2 | | | |
| Ca + L ⇆ CaL | 0.2 | | | |
| Sr + L ⇆ SrL | 0.0 | | | |
| Ba + L ⇆ BaL | -0.1 | | | |
| Mn(II) + L ⇆ Mn(II)L | 0.84 | | | |
| Mn(II) + 2 L ⇆ Mn(II)$L_2$ | 1.25 | | | |
| Mn(II) + 3 L ⇆ Mn(II)$L_3$ | 1.38 | | | |
| Mn(II) + 4 L ⇆ Mn(II)$L_4$ | 1.24 | | | |
| Fe(II) + L ⇆ Fe(II)L | 1.40 | | | |
| Fe(II) + 2 L ⇆ Fe(II)$L_2$ | 2.25 | | | |
| Fe(II) + 3 L ⇆ Fe(II)$L_3$ | 2.68 | | | |
| Fe(II) + 4 L ⇆ Fe(II)$L_4$ | 2.75 | | | |
| Co(II) + L ⇆ Co(II)L | 2.08 | 0.1 | | |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | 3.70 | 1.0 | | |
| Co(II) + 3 L ⇆ Co(II)$L_3$ | 4.80 | 1.0 | | |
| Co(II) + 4 L ⇆ Co(II)$L_4$ | 5.52 | 1.0 | | |
| Co(II) + 5 L ⇆ Co(II)$L_5$ | 5.72 | 1.0 | | |
| Ni + L ⇆ NiL | 2.72 | | | |
| Ni + 2 L ⇆ $NiL_2$ | 4.88 | | | |
| Ni + 3 L ⇆ $NiL_3$ | 6.54 | | | |
| Ni + 4 L ⇆ $NiL_4$ | 7.67 | | | |
| Ni + 5 L ⇆ $NiL_5$ | 8.33 | | | |
| Ni + 6 L ⇆ $NiL_6$ | 8.30 | | | |
| Cu(II) + L ⇆ Cu(II)L | 4.02 | | | |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | 7.40 | | | |
| Cu(II) + 3 L ⇆ Cu(II)$L_3$ | 10.2 | | | |
| Cu(II) + 4 L ⇆ Cu(II)$L_4$ | 12.3 | | | |
| Cr(III)L ⇆ Cr(III)OHL + H | -4.4 | 0.5 | 20 | This equilibrium and the three next ones have not been entered. |
| Cr(III)$L_2$ ⇆ Cr(III)(OH)$L_2$ + H | -4.11 | 0.5 | 20 | |
| Cr(III)(OH)$L_2$ ⇆ Cr(III)$(OH)_2L_2$ + H | -6.59 | 0.5 | 20 | |
| Cr(III)$(OH)_2L_2$ ⇆ Cr(III)$(OH)_3L_2$ + H | -9.17 | 0.5 | 20 | |
| Cr(III)$L_5$ ⇆ Cr(III)$L_4$ + L | -1.6 | 4.0 | | Cr(III)$L_5$ ⇆ Cr(III)$L_4$ + L -1.6 4.0<br>Cr(III) + 5 L ⇆ Cr(III)$L_5$ 11.5 4.0<br>Cr(III) + 4 L ⇆ Cr(III)$L_4$ 9.9 4.0 |
| Cr(III)$L_6$ ⇆ Cr(III)$L_5$ + L | -1.5 | 4.0 | | Cr(III)$L_6$ ⇆ Cr(III)$L_5$ + L -1.5 4.0<br>Cr(III) + 6 L ⇆ Cr(III)$L_6$ 13 4.0<br>Cr(III) + 5 L ⇆ Cr(III)$L_5$ 11.5 4.0 |
| Cr(III) + 6 L ⇆ Cr(III)$L_6$ | 13 | 4.0 | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cr(III)$L_4$ ⇆ Cr(III)(OH)$L_4$ (cis) + H | -4.96 | 1 | | Cr(III)$L_4$ ⇆ Cr(III)(OH)$L_4$ (cis) + H -4.96 1<br>Cr(III) + 4 L ⇆ Cr(III)$L_4$ 9.9 1<br>H + OH ⇆ $H_2O$ 13.79384 1<br>Cr(III) + 4 L + OH ⇆ Cr(III)(OH)$L_4$ (cis) 18.73384 1<br>I=0: 19.34332 |
| Cr(III)OH$L_4$ ⇆ Cr(III)$(OH)_2L_4$ (cis) + H | -7.53 | 1 | | Cr(III)OH$L_4$ ⇆ Cr(III)$(OH)_2L_4$ (cis) + H -7.53 1<br>Cr(III) + 4 L + OH ⇆ Cr(III)(OH)$L_4$ (cis?)[1] 18.73384 1<br>H + OH ⇆ $H_2O$ 13.79384 1<br>Cr(III) + 4 L + 2 OH ⇆ Cr(III)(OH)$L_4$ (cis) 24.99768 1<br>I=0: 26.01348 |
| Cr(III)$L_4$ ⇆ Cr(III)(OH)$L_4$ (trans) + H | -4.38 | 1 | | Cr(III)$L_4$ ⇆ Cr(III)(OH)$L_4$ (trans) + H -4.38 1<br>Cr(III) + 4 L ⇆ Cr(III)$L_4$ 9.9 1<br>H + OH ⇆ $H_2O$ 13.79384 1<br>Cr(III) + 4 L + OH ⇆ Cr(III)(OH)$L_4$ (trans) 19.31384 1<br>I=0: 19.92332 |
| Cr(III)OH$L_4$ ⇆ Cr(III)$(OH)_2L_4$ (trans) + H | -7.78 | 1 | | Cr(III)OH$L_4$ ⇆ Cr(III)$(OH)_2L_4$ (trans) + H -7.78 1<br>Cr(III) + 4 L + OH ⇆ Cr(III)(OH)$L_4$ (trans?)[2] 19.31384 1<br>H + OH ⇆ $H_2O$ 13.79384 1<br>Cr(III) + 4 L + 2 OH ⇆ Cr(III)(OH)$L_4$ (trans) 25.32768 1<br>I=0: 26.34348 |
| Cr(III)(OH)$L_5$ + H ⇆ Cr(III)$L_5$ | 4.99 | 0.1 | | Cr(III)$L_5$ ⇆ Cr(III)(OH)$L_5$ + H -4.99 0.1<br>Cr(III) + 5 L ⇆ Cr(III)$L_5$ 11.5 0.1<br>H + OH ⇆ $H_2O$ 13.78342 0.1<br>Cr(III) + 5 L + OH ⇆ Cr(III)(OH)$L_5$ 20.29342 0.1<br>I=0: 20.93415 |
| Co(III)(OH)$L_3$ (fac) + H ⇆ Co(III)$L_3$ | 5.33 | 0.1 | 20 | Note: this equilibrium and the next one have not been entered |
| Co(III)$(OH)_2L_3$ (fac) + H ⇆ Co(III)(OH)$L_3$ | 7.6 | 0.1 | 20 | |
| Co(III)(OH)$L_4$ (cis) + H ⇆ Co(III)$L_4$ | 5.69 | 0.1 | 20 | Co(III)$L_4$ ⇆ Co(III)(OH)$L_4$ (cis) + H -5.69 0.1<br>Co(III) + 4 L ⇆ Co(III)$L_4$ 24.96 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Co(III) + OH + 4 L ⇆ Co(III)OH$L_4$ 33.05342 0.1<br>I=0: 33.69415 |
| Co(III)$(OH)_2L_4$ (cis) + H ⇆ Co(III)(OH)$L_4$ | 7.99 | 0.1 | 20 | Co(III)(OH)$L_4$ ⇆ Co(III)$(OH)_2L_4$ (cis) + H -7.99 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Co(III) + 2 OH + 4 L ⇆ Co(III)$(OH)_2L_4$ (cis) 5.79342 0.1<br>I=0: 6.86130 |

[1] It is not clear whether the cis or trans-version of Cr(III)(OH)$(NH_3)_4$ is meant. In this calculation, it is assumed that the cis-version reacts to form the cis-version of Cr(III)$(OH)_2(NH_3)_4$.This may be not correct.

[2] It is not clear whether the cis or trans-version of Cr(III)(OH)$(NH_3)_4$ is meant. In this calculation, it is assumed that the trans-version reacts to form the trans-version of Cr(III)$(OH)_2(NH_3)_4$.This may be not correct.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Co(III)$L_5$ ⇆ Co(III)$L_4$ + L | -5.07 | 2.0 | | Co(III)$L_5$ ⇆ Co(III)$L_4$ + L<br>-5.07 2<br>Co(III) + 5 L ⇆ Co(III)$L_5$<br>30.03 2<br>Co(III) + 4 L ⇆ Co(III)$L_4$<br>24.96 2 |
| Co(III)(OH)$L_5$ + H ⇆ Co(III)$L_5$ | 6.2 | 0.1 | | Co(III)$L_5$ ⇆ Co(III)(OH)$L_5$ + H<br>-6.2 0.1<br>Co(III) + 5 L ⇆ Co(III)$L_5$<br>30.03 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Co(III) + 5 L + OH ⇆ Co(III)OHL5<br>37.61342 0.1<br>I=0: 38.25415 |
| Co(III)$L_6$ ⇆ Co(III)$L_5$ + L | -4.33 | 1.0 | | Co(III)$L_6$ ⇆ Co(III)$L_5$ + L<br>-4.33 1<br>Co(III) + 6 L ⇆ Co(III)$L_6$<br>34.36 1<br>Co(III) + 5 L ⇆ Co(III)$L_5$<br>30.03 1 |
| Co(III) + 6 L ⇆ Co(III)$L_6$ | 34.36 | 1.0 | 30 | |
| Cu(I) + L ⇆ Cu(I)L | 5.74 | 2.0 | | |
| Cu(I) + 2 L ⇆ Cu(I)$L_2$ | 9.9 | 0.5 | | |
| Ag + L ⇆ AgL | 3.31 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 7.22 | | | |
| Pd + L ⇆ PdL | 9.6 | 1.0 | | |
| Pd + 2 L ⇆ $PdL_2$ | 18.5 | 1.0 | | |
| Pd + 3 L ⇆ $PdL_3$ | 26.0 | 1.0 | | |
| Pd + 4 L ⇆ $PdL_4$ | 32.8 | 1.0 | | |
| Zn + L ⇆ ZnL | 2.21 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | 4.50 | | | |
| Zn + 3 L ⇆ $ZnL_3$ | 6.86 | | | |
| Zn + 4 L ⇆ $ZnL_4$ | 8.89 | | | |
| Cd + L ⇆ CdL | 2.55 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 4.56 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 5.90 | | | |
| Cd + 4 L ⇆ $CdL_4$ | 6.72 | | | |
| Hg(II) + L ⇆ Hg(II)L | 8.75 | 2.0 | | |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 17.8 | 1.0 | | |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 18.2 | 2.0 | | |
| Hg(II) + 4 L ⇆ Hg(II)$L_4$ | 19.3 | 0.1 | | |
| Pb(II) + L ⇆ Pb(II)L | 1.55 | 5.0 | | |

## Nitrite ($NO_2^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 3.15 | | | |
| Mn(II) + L ⇆ Mn(II)L | 0.45 | 1.0 | | I=0: 0.85632 |
| Co(II) + L ⇆ Co(II)L | 0.44 | 1.0 | | I=0: 0.84632 |
| Ni + L ⇆ NiL | 0.77 | 1.0 | | I=0: 1.07632 |
| Ni + 2 L ⇆ $NiL_2$ | 1.08 | 1.0 | | I=0: 1.68948 |
| Cu(II) + L ⇆ Cu(II)L | 2.02 | | | |
| Cu(II) + 2 L ⇆ $Cu(II)L_2$ | 3.03 | | | |
| Fe(III) + L ⇆ Fe(III)L | 2.59 | 1.0 | | I=0: 3.19948 |
| Fe(III) + 2 L ⇆ $Fe(III)L_2$ | 3.70 | 1.0 | | I=0: 4.71580 |
| Fe(III) + L ⇆ $Fe(III)L_3$ | 5.45 | 1.0 | | I=0: 6.66896 |
| Ag + L ⇆ AgL | 2.32 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 2.51 | | | |
| Pd + 4 L ⇆ $PdL_4$ | 20.3 | 0.5 | | I=0: 20.83678 |
| Zn + L ⇆ ZnL | 0.37 | 1.0 | | I=0: 0.77632 |
| Zn + 2 L ⇆ $ZnL_2$ | 0.49 | 1.0 | | I=0: 1.09948 |
| Cd + L ⇆ CdL | 1.54 | 1.0 | | I=0: 1.94632 |
| Cd + 2 L ⇆ $CdL_2$ | 2.83 | 1.0 | | I=0: 3.43948 |
| Cd + 3 L ⇆ $CdL_3$ | 3.81 | 3.0 | | I=0: 2.99931 |
| Hg(II) + L ⇆ Hg(II)L | 5.94 | 1.0 | | I=0: 6.34632 |
| Hg(II) + 2 L ⇆ $Hg(II)L_2$ | 9.91 | 1.0 | | I=0: 10.51948 |
| Hg(II) + 3 L ⇆ $Hg(II)L_3$ | 11.45 | 1.0 | | I=0: 12.05948 |
| Hg(II) + 4 L ⇆ $Hg(II)L_4$ | 11.86 | 1.0 | | I=0: 12.26632 |
| Pb(II) + L ⇆ Pb(II)L | 2.51 | | | |
| Pb(II) + 2 L ⇆ $Pb(II)L_2$ | 2.7 | 2.0 | | I=0: 2.65669 |
| Pb(II) + 3 L ⇆ $Pb(II)L_3$ | 3.0 | 2.0 | | I=0: 2.95669 |
| $B(OH)_3$ + L ⇆ $B(OH)_3L$ | -0.49 | | | $H_2BO_3$ + H ⇆ $H_3BO_3$ 9.236<br>$B(OH)_3$ + L ⇆ $B(OH)_3L$ -0.49<br>$H_2BO_3$ + H + L ⇆ $B(OH)_3L$ 8.746<br>Note: $H_3BO_3$ is $B(OH)_3$ |
| Ga + L ⇆ GaL | 2.11 | 1.0 | | I=0: 2.71948 |
| In + L ⇆ InL | 2.6 | 1.0 | | I=0: 3.20948 |
| In + 2 L ⇆ $InL_2$ | 4.0 | 1.0 | | I=0: 5.01580 |
| In + 3 L ⇆ $InL_3$ | 4.9 | 1.0 | | I=0: 6.11896 |

## Solid:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ag + L ⇆ AgL (s) | 4.13 | | | |

## Nitrate ($NO_3^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Na + L ⇆ NaL | -0.55 | | | |
| K + L ⇆ KL | -0.19 | | | |
| Rb + L ⇆ RbL | -0.08 | | | |
| Cs + L ⇆ CsL | 0.02 | | | |
| Be + L ⇆ BeL | -0.9 | 1.0 | | I=0: -0.49368 |
| Ca + L ⇆ CaL | 0.5 | | | |
| Sr + L ⇆ SrL | 0.6 | | | |
| Ba + L ⇆ BaL | 0.7 | | | |
| Sc + L ⇆ ScL | 0.28 | 4.0 | | I=0: -1.34528 |
| Sc + 2 L ⇆ $ScL_2$ | -0.3 | 4.0 | | I=0: -3.00880 |
| La + L ⇆ LaL | 0.1 | 1.0 | | I=0: 0.70948 |
| Ce + L ⇆ CeL | 0.2 | 1.0 | | I=0: 0.80948 |
| Pr + L ⇆ PrL | 0.2 | 1.0 | | I=0: 0.80948 |
| Nd + L ⇆ NdL | 0.3 | 1.0 | | I=0: 0.90948 |
| Pm + L ⇆ PmL | 0.4 | 1.0 | | I=0: 1.00948 |
| Sm + L ⇆ SmL | 0.3 | 1.0 | | I=0: 0.90948 |
| Eu + L ⇆ EuL | 1.22 | | | |
| Gd + L ⇆ GdL | 0.0 | 1.0 | | I=0: 0.60948 |
| Tb + L ⇆ TbL | 0.88 | | | |
| Dy + L ⇆ DyL | -0.3 | 1.0 | | I=0: 0.30948 |
| Ho + L ⇆ HoL | -0.2 | 1.0 | | I=0: 0.40948 |
| Er + L ⇆ ErL | -0.3 | 1.0 | | I=0: 0.30948 |
| Tm + L ⇆ TmL | -0.25 | 1.0 | | I=0: 0.35948 |
| Yb + L ⇆ YbL | -0.2 | 1.0 | | I=0: 0.40948 |
| Lu + L ⇆ LuL | -0.2 | 1.0 | | I=0: 0.40948 |
| (U(VI)$O_2$) + L ⇆ (U(VI)$O_2$)L | 0.3 | | | |
| Mn(II) + L ⇆ Mn(II)L | 0.2 | | | |
| Mn(II) + 2 L ⇆ Mn(II)$L_2$ | 0.6 | | | |
| Co(II) + L ⇆ Co(II)L | 0.2 | | | |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | -0.3 | 0.5 | | I=0: 0.50516 |
| Ni + L ⇆ NiL | 0.4 | | | |
| Ni + 2 L ⇆ $NiL_2$ | -0.5 | 2.0 | | I=0: -0.54331 |
| Cu(II) + L ⇆ Cu(II)L | 0.5 | | | |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | -0.4 | | | |
| Fe(III) + L ⇆ Fe(III)L | 1.00 | | | |
| Zr + L ⇆ ZrL | 0.3 | 2.0 | | I=0: 0.24225 |
| Zr + 2 L ⇆ $ZrL_2$ | 0.1 | 4.0 | 20 | I=0: -3.69232 |
| Zr + 3 L ⇆ $ZrL_3$ | -0.3 | 4.0 | 20 | I=0: -5.17584 |
| Zr + 4 L ⇆ $ZrL_4$ | -0.8 | 4.0 | 20 | I=0: -6.21760 |
| Hf + L ⇆ HfL | 0.34 | 2.0 | | I=0: 0.28225 |
| Hf + 2 L ⇆ $HfL_2$ | 0.0 | 2.0 | | I=0: -0.10107 |
| Hf + 3 L ⇆ $HfL_3$ | -0.7 | 2.0 | | I=0: -0.82994 |
| Ag + L ⇆ AgL | -0.1 | | | |
| Zn + L ⇆ ZnL | 0.4 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | -0.3 | | | |
| Cd + L ⇆ CdL | 0.5 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 0.2 | | | |
| Hg(II) + L ⇆ Hg(II)L | 0.11 | 3.0 | | I=0: -0.43046 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 0.0 | 3.0 | | I=0: -0.81069 |
| Sn(II) + L ⇆ Sn(II)L | 0.44 | 1.0 | | I=0: 0.84632 |
| Pb(II) + L ⇆ Pb(II)L | 1.17 | | | |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 1.4 | | | |
| Pb(II) + 3 L ⇆ Pb(II)$L_3$ | 0.1 | 2.0 | | I=0: 0.05669 |
| Pb(II) + 4 L ⇆ Pb(II)$L_4$ | -0.3 | 3.0 | | I=0: -0.84046 |
| In + L ⇆ InL | 0.18 | 0.7 | 20 | I=0: 0.92824 |
| In + 2 L ⇆ $InL_2$ | -0.3 | 0.7 | 20 | I=0: 0.94706 |
| Bi + L ⇆ BiL | 1.7 | | | |

| | | | | |
|---|---|---|---|---|
| Bi + 2 L ⇆ $BiL_2$ | 2.5 | | | |
| Bi + 3 L ⇆ $BiL_3$ | 0.7 | 1.0 | | I=0: 1.91896 |
| Bi + 4 L ⇆ $BiL_4$ | 0.6 | 2.0 | | I=0: 0.51337 |

Solid:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cu(II) + 1.5 OH + 0.5 L ⇆ Cu(II)$(OH)_{1.5}L_{0.5}$ | 16.37 | | | Cu(II) + 1.5 OH + 0.5 L ⇆ Cu(II)$(OH)_{1.5}L_{0.5}$ 16.37<br>(multiply by 2):<br>2 Cu(II) + 3 OH + L ⇆ $Cu(II)_2(OH)_3L$ 32.74 |
| Bi + L ⇆ BiOL + 2 H | 2.55 | | | Bi + L ⇆ BiOL + 2 H 2.55<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*13.997) 27.994<br>Bi + 2 OH + L ⇆ BiOL 30.544 |

# Fluoride ($F^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 3.18 | | | |
| HL + L ⇆ $HL_2$ | 0.6 | | | HL + L ⇆ $HL_2$ 0.6<br>H + L ⇆ HL 3.18<br>H + 2 L ⇆ $HL_2$ 3.78 |
| Li + L ⇆ LiL | 0.31 | | | |
| Na + L ⇆ NaL | 0.02 | | | |
| K + L ⇆ KL | -0.34 | | | |
| Rb + L ⇆ RbL | -0.22 | | | |
| Cs + L ⇆ CsL | -0.36 | | | |
| Be + L ⇆ BeL | 4.71 | 0.5 | | I=0: 5.24678 |
| Be + 2 L ⇆ $BeL_2$ | 8.32 | 0.5 | | I=0: 9.12516 |
| Be + 3 L ⇆ $BeL_4$ | 11.12 | 0.5 | | I=0: 11.92516 |
| Be + 4 L ⇆ $BeL_4$ | 13.39 | 0.5 | | I=0: 13.92678 |
| 3 Be + L ⇆ $Be_3(OH)_3L$ + 3 H | -4.18 | 3.0 | | 3 Be + L ⇆ $Be_3(OH)_3L$ + 3 H<br>-4.18 3.0<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.26723) 42.80169 3.0<br>3 Be + 3 OH + L ⇆ $Be_3(OH)_3L$<br>38.62169 3.0<br>I=0: 37.00032 |
| 3 Be + 2 L ⇆ $Be_3(OH)_3L_2$ + 3 H | -0.7 | 3.0 | | 3 Be + 2 L ⇆ $Be_3(OH)_3L_2$ + 3 H<br>-0.7 3.0<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.26723) 42.80169 3.0<br>3 Be + 3 OH + 2 L ⇆ $Be_3(OH)_3L_2$<br>42.10169 3.0<br>I=0: 39.93986 |
| Mg + L ⇆ MgL | 1.9 | | | |
| Ca + L ⇆ CaL | 0.6 | 0.5 | | I=0: 1.13678 |
| Sr + L ⇆ SrL | 0.15 | 1.0 | | I=0: 0.55632 |
| Ba + L ⇆ BaL | -0.2 | 1.0 | | I=0: 0.20632 |
| Sc + L ⇆ ScL | 7.08 | | | |
| Sc + 2 L ⇆ $ScL_2$ | 12.89 | | | |
| Sc + 3 L ⇆ $ScL_3$ | 17.4 | | | |
| Sc + 4 L ⇆ $ScL_4$ | 20.2 | | | |
| 2 Sc + 3 L ⇆ $Sc_2L_3$ | 19.0 | 0.5 | | I=0: 20.61033 |
| Y + L ⇆ YL | 4.81 | | | |
| Y + 2 L ⇆ $YL_2$ | 8.54 | | | |
| Y + 3 L ⇆ $YL_3$ | 12.14 | | | |
| La + L ⇆ LaL | 3.62 | | | |
| La + 2 L ⇆ $LaL_2$ | 5.08 | 0.5 | | I=0: 6.42194 |
| Ce + L ⇆ CeL | 3.90 | | | |
| Pr + L ⇆ PrL | 4.05 | | | |
| Nd + L ⇆ NdL | 4.17 | | | |
| Pm + L ⇆ PmL | 3.56 | 0.1 | | I=0: 4.20073 |
| Pm + 2 L ⇆ $PmL_2$ | 5.60 | 1.0 | | I=0: 6.61580 |
| Sm + L ⇆ SmL | 4.19 | | | |
| Eu + L ⇆ EuL | 4.27 | | | |
| Eu + 2 L ⇆ $EuL_2$ | 5.90 | 1.0 | | I=0: 6.9158 |
| Gd + L ⇆ GdL | 4.32 | | | |
| Tb + L ⇆ TbL | 4.43 | | | |
| Dy + L ⇆ DyL | 4.46 | | | |
| Ho + L ⇆ HoL | 4.57 | | | |
| Er + L ⇆ ErL | 4.59 | | | |
| Tm + L ⇆ TmL | 4.61 | | | |
| Yb + L ⇆ YbL | 4.63 | | | |
| Lu + L ⇆ LuL | 4.66 | | | |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 5.14 | | | |
| $(UO_2)$ + 2 L ⇆ $(UO_2)L_2$ | 8.60 | | | |
| $(UO_2)$ + 3 L ⇆ $(UO_2)L_3$ | 11.0 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $(UO_2)$ + 4 L ⇆ $(UO_2)L_4$ | 11.9 | | | |
| Mn(II) + L ⇆ Mn(II)L | 1.5 | | | |
| Fe(II) + L ⇆ Fe(II)L | 0.8 | 1.0 | | I=0: 1.20632 |
| Co(II) + L ⇆ Co(II)L | 1.4 | | | |
| Ni + L ⇆ NiL | 1.3 | | | |
| Cu(II) + L ⇆ Cu(II)L | 1.7 | | | |
| Cr(III) + L ⇆ Cr(III)L | 5.2 | | | |
| Cr(III) + 2 L ⇆ Cr(III)$L_2$ | 7.7 | 0.5 | | I=0: 9.04194 |
| Cr(III) + 3 L ⇆ Cr(III)$L_3$ | 10.1 | 0.5 | | I=0: 11.71033 |
| Fe(III) + L ⇆ Fe(III)L | 6.03 | | | |
| Fe(III) + 2 L ⇆ Fe(III)$L_2$ | 10.66 | | | |
| Fe(III) + 3 L ⇆ Fe(III)$L_3$ | 13.7 | | | |
| Zr + L ⇆ ZrL | 9.8 | | | |
| Zr + 2 L ⇆ $ZrL_2$ | 16.36 | 2.0 | | I=0: 16.25893 |
| Zr + 3 L ⇆ $ZrL_3$ | 22.31 | 2.0 | | I=0: 22.18006 |
| Zr + 4 L ⇆ $ZrL_4$ | 29.59 | 4.0 | | I=0: 24.17240 |
| Hf + L ⇆ HfL | 9.04 | 4.0 | | I=0: 6.87296 |
| Hf + 2 L ⇆ $HfL_2$ | 16.60 | 4.0 | | I=0: 12.80768 |
| Hf + 3 L ⇆ $HfL_3$ | 23.15 | 4.0 | | I=0: 18.27416 |
| Hf + 4 L ⇆ $HfL_4$ | 28.81 | 4.0 | | I=0: 23.39240 |
| Ag + L ⇆ AgL | 0.4 | | | |
| Zn + L ⇆ ZnL | 1.3 | | | |
| Cd + L ⇆ CdL | 1.2 | | | |
| Hg(II)+ L ⇆ Hg(II)L | 1.6 | | | |
| Sn(II) + L ⇆ Sn(II)L | 4.08 | 1.0 | | I=0: 4.48632 |
| Sn(II) + 2 L ⇆ Sn(II)$L_2$ | 6.68 | 1.0 | | I=0: 7.28948 |
| Sn(II) + 3 L ⇆ Sn(II)$L_3$ | 9.46 | 1.0 | | I=0: 10.06948 |
| Pb(II) + L ⇆ Pb(II)L | 1.72 | 0.1 | | I=0: 2.14715 |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 2.53 | 1.0 | | I=0: 3.13948 |
| $B(OH)_3$ | | | | (four complexes for $B(OH)_3$ not entered; not likely to be of environmental significance) |
| Al + L ⇆ AlL | 7.01 | | | |
| Al + 2 L ⇆ $AlL_2$ | 12.63 | | | |
| Al + 3 L ⇆ $AlL_3$ | 16.7 | | | |
| Al + 4 L ⇆ $AlL_4$ | 19.4 | | | |
| Ga + L ⇆ GaL | 4.47 | 0.5 | | I=0: 5.27516 |
| Ga + 2 L ⇆ $GaL_2$ | 8.00 | 0.5 | | I=0: 9.34194 |
| Ga + 3 L ⇆ $GaL_3$ | 10.47 | 0.5 | | I=0: 12.08033 |
| In + L ⇆ InL | 4.65 | | | |
| In + 2 L ⇆ $InL_2$ | 8.0 | | | |
| In + 3 L ⇆ $InL_3$ | 10.3 | | | |
| In + 4 L ⇆ $InL_4$ | 11.4 | | | |
| $As(OH)_3$ | | | | (a complex for $As(OH)_3$ not entered; not likely to be of environmental significance) |
| Bi + L ⇆ BiL | 4.48 | 2.0 | 30 | I=0: 4.43669 |
| $Si(OH)_4$ | | | | (two complexes for $Si(OH)_4$ not entered; not likely to be of environmental significance) |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Li + L ⇆ LiL | 2.77 | | | |
| Na + L ⇆ NaL | 0.49 | | | |
| Mg + L ⇆ MgL | 8.11 | | | |
| Ca + 2 L ⇆ $CaL_2$ | 10.50 | | | |
| Sr + 2 L ⇆ $SrL_2$ | 8.58 | | | |
| Ba + 2 L ⇆ $BaL_2$ | 5.82 | | | |
| Y + 3 L ⇆ $YL_3$ | 18.3 | | | |
| La + 3 L ⇆ $LaL_3$ | 18.7 | | | |
| Ce + 3 L ⇆ $CeL_3$ | 19.1 | | | |
| Pr + 3 L ⇆ $PrL_3$ | 18.9 | 0.1 | | I=0: 20.18145 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
| --- | --- | --- | --- | --- |
| Nd + 3 L ⇆ $NdL_3$ | 20.3 | | | |
| Sm + 3 L ⇆ $SmL_3$ | 17.9 | 0.1 | | I=0: 19.18145 |
| Eu + 3 L ⇆ $EuL_3$ | 21.9 | | | |
| Gd + 3 L ⇆ $GdL_3$ | 16.8 | 0.1 | | I=0: 18.08145 |
| Tb + 3 L ⇆ $TbL_3$ | 16.7 | 0.1 | | I=0: 17.98145 |
| Dy + 3 L ⇆ $DyL_3$ | 16.3 | 0.1 | | I=0: 17.58145 |
| Ho + 3 L ⇆ $HoL_3$ | 15.8 | 0.1 | | I=0: 17.08145 |
| Er + 3 L ⇆ $ErL_3$ | 18.0 | | | |
| Tm + 3 L ⇆ $TmL_3$ | 15.8 | 0.1 | | I=0: 17.08145 |
| Yb + 3 L ⇆ $YbL_3$ | 15.0 | 0.1 | | I=0: 16.28145 |
| Lu + 3 L ⇆ $LuL_3$ | 15.0 | 0.1 | | I=0: 16.28145 |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 7.44 | | | |
| Al(OH) + 2 L ⇆ $AlL_2$(OH) | 13.59 | | | Al(OH) + 2 L ⇆ $AlL_2$(OH) 13.59<br>Al + OH ⇆ Al(OH) 9.00<br>Al + OH + 2 L ⇆ $AlL_2$(OH) 22.59 |

## Silicate ($H_2SiO_4^{2-}$)

Note: in many equilibria water is produced. This is not always mentioned here (see page 7).

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 13.2 | | | |
| H + HL ⇆ $H_2L$ | 9.84 | | | H + HL ⇆ $H_2L$ 9.84<br>H + L ⇆ HL 13.2<br>2 H + L ⇆ $H_2L$ 23.04 |
| 2 $H_2L$ ⇆ $Si_2O_3(OH)_4$ + 2 H | -18.00 | 0.5 | | 2 $H_2L$ ⇆ $Si_2O_3(OH)_4$ + 2 H + $H_2O$<br>-18.00 0.5<br>4 H + 2 L ⇆ 2 $H_2L$<br>(2*22.23484) 44.46968 0.5<br>2 H + 2 L ⇆ $Si_2O_3(OH)_4$ + $H_2O$<br>26.46968 0.5<br>I=0: 27.27484 |
| $Si_2O_3(OH)_4$ + H ⇆ $Si_2O_2(OH)_5$ | 10.25 | 0.5 | | $Si_2O_3(OH)_4$ + H ⇆ $Si_2O_2(OH)_5$<br>10.25 0.5<br>2 H + 2 L ⇆ $Si_2O_3(OH)_4$ 26.46968 0.5<br>3 H + 2 L ⇆ $Si_2O_2(OH)_5$ 36.71968 0.5<br>I=0: 38.06162 |
| 2 $Si(OH)_4$ ⇆ $Si_2O(OH)_6$ | 1.2 | 0.5 | | 2 $Si(OH)_4$ ⇆ $Si_2O(OH)_6$ 1.2 0.5<br>4 H + 2 L ⇆ 2 $H_2L$<br>(2*22.23484) 44.46968 0.5<br>4 H + 2 L ⇆ $Si_2O(OH)_6$ 45.66968 0.5<br>I=0: 47.28001 |
| 3 $H_2L$ ⇆ 3 H + $Si_3O_6(OH)_3$ (cyclo) | -26.43 | 0.5 | | 3 $H_2L$ ⇆ 3 H + $Si_3O_6(OH)_3$ (cyclo) + 3 $H_2O$<br>-26.43 0.5<br>6 H + 3 L ⇆ 3 $H_2L$<br>(3*22.23484) 66.70452 0.5<br>3 H + 3 L ⇆ $Si_3O_6(OH)_3$ (cyclo) + $H_2O$<br>40.27452 0.5<br>I=0: 41.07968 |
| 3 $H_2L$ ⇆ 3 H + $Si_3O_5(OH)_5$ (linear) | -25.40 | 0.5 | | 3 $H_2L$ ⇆ 3 H + $Si_3O_5(OH)_5$ (linear) + 2 $H_2O$ -25.40 0.5<br>6 H + 3 L ⇆ 3 $H_2L$<br>(3*22.23484) 66.70452 0.5<br>3 H + 3 L ⇆ $Si_3O_5(OH)_5$ (linear) + 2 $H_2O$<br>41.30452 0.5<br>I=0: 42.10968 |
| 4 $H_2L$ ⇆ 3 H + $Si_4O_7(OH)_5$ (cyclo) | -23.42 | 0.5 | | 4 $H_2L$ ⇆ 3 H + $Si_4O_7(OH)_5$ (cyclo) + 4 $H_2O$<br>-23.42 0.5<br>8 H + 4 L ⇆ 4 $H_2L$<br>(4*22.23484) 88.93936 0.5<br>5 H + 4 L ⇆ $Si_4O_7(OH)_5$ (cyclo) + 4 $H_2O$<br>63.53936 0.5<br>I=0: 65.14969 |
| $Si_4O_7(OH)_5$ (cyclo) ⇆ $Si_4O_8(OH)_4$ + H | -9.39 | 0.5 | | $Si_4O_7(OH)_5$ (cyclo) ⇆ $Si_4O_8(OH)_4$ + H<br>-9.39 0.5<br>5 H + 4 L ⇆ $Si_4O_7(OH)_5$ (cyclo) + 4 $H_2O$<br>63.53936 0.5<br>4 H + 4 L ⇆ $Si_4O_8(OH)_4$ + 4 $H_2O$<br>54.14936 0.5<br>I=0: 54.68614 |
| Mg + $H_2L$ ⇆ MgHL + H | -8.8 | 1.0 | | Mg + $H_2L$ ⇆ MgHL + H -8.8 1.0<br>2 H + L ⇆ $H_2L$ 22.43052 1.0<br>Mg + H + L ⇆ MgHL 13.63052 1.0<br>I=0: 14.44316 |
| MgHL + $H_2L$ ⇆ $MgH_2L_2$ + H | -6.3 | 1.0 | | MgHL + $H_2L$ ⇆ $MgH_2L_2$ + H -6.3 1.0<br>Mg + H + L ⇆ MgHL 13.63052 1.0<br>2 H + L ⇆ $H_2L$ 22.43052 1.0<br>Mg + 2 H + 2 L ⇆ $MgH_2L_2$ 29.76104 1.0<br>I=0: 31.18316 |
| MgL + H ⇆ MgHL | 9.06 | 1.0 | | MgL + H ⇆ MgHL 9.06 1.0<br>invert:<br>MgHL ⇆ MgL + H -9.06 1.0<br>Mg + H + L ⇆ MgHL 13.63052 1.0<br>Mg + L ⇆ MgL 4.57052 1.0<br>I=0: 5.38316 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ca + $H_2L$ ⇆ CaHL + H | −9.1 | 1.0 | | Ca + $H_2L$ ⇆ CaHL + H -9.1 1.0<br>2 H + L ⇆ $H_2L$ 22.43052 1.0<br>Ca + H + L ⇆ CaHL 13.33052 1.0<br>I=0: 14.14316 |
| CaHL + $H_2L$ ⇆ $CaH_2L_2$ + H | -7.0 | 1.0 | | CaHL + $H_2L$ ⇆ $CaH_2L_2$ + H -7.0 1.0<br>Ca + H + L ⇆ CaHL 13.33052 1.0<br>2 H + L ⇆ $H_2L$ 22.43052 1.0<br>Ca + 2 H + 2 L ⇆ $CaH_2L_2$ 28.76104 1.0<br>I=0: 30.18316 |
| CaL + H ⇆ CaHL | 9.89 | 1.0 | | CaL + H ⇆ CaHL 9.89 1.0<br>invert:<br>CaHL ⇆ CaL + H -9.89 1.0<br>Ca + H + L ⇆ CaHL 13.33052 1.0<br>Ca + L ⇆ CaL 3.44052 1.0<br>I=0: 4.25316 |
| Eu + $H_2L$ ⇆ EuHL + H | -2.3 | 0.1 | | Eu + $H_2L$ ⇆ EuHL + H -2.3 0.1<br>2 H + L ⇆ $H_2L$ 22.39927 0.1<br>Eu + H + L ⇆ EuHL 20.09927 0.1<br>I=0: 21.16715 |
| EuHL + $H_2L$ ⇆ $EuH_2L_2$ + H | -5.2 | 0.1 | | EuHL + $H_2L$ ⇆ $EuH_2L_2$ + H -5.2 0.1<br>Eu + H + L ⇆ EuHL 20.09927 0.1<br>2 H + L ⇆ $H_2L$ 22.39927 0.1<br>Eu + 2 H + 2 L ⇆ $EuH_2L_2$ 37.29854 0.1<br>I=0: 39.22072 |
| $(UO_2)$ + $H_2L$ ⇆ $(UO_2)$HL + H | -1.8 | | | $(UO_2)$ + $H_2L$ ⇆ $(UO_2)$HL + H -1.8<br>2 H + L ⇆ $H_2L$ 23.04<br>$(UO_2)$ + H + L ⇆ $(UO_2)$HL 21.24 |
| Fe(III)+ $H_2L$ ⇆ Fe(III)HL + H | -0.6 | 0.1 | | Fe(III) + $H_2L$ ⇆ Fe(III)HL + H<br>-0.6 0.1<br>2 H + L ⇆ $H_2L$ 22.39927 0.1<br>Fe(III) + H + L ⇆ Fe(III)HL<br>21.79927 0.1<br>I=0: 22.86715 |
| Al + $H_2L$ ⇆ AlHL + H | -2.5 | 0.1 | | Al + $H_2L$ ⇆ Al HL + H -2.5 0.1<br>2 H + L ⇆ $H_2L$ 22.39927 0.1<br>Al + H + L ⇆ AlHL 19.89927 0.1<br>I=0: 20.96715 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_2L$ ⇆ $SiO_2$ | 4.0<br>(quartz) | | | $H_2L$ ⇆ $SiO_2$ 4.0<br>2 H + L ⇆ $H_2L$ 23.04<br>2 H + L ⇆ $SiO_2$ 27.04 |
| 2 Mg + 3 $H_4L$ + 4 OH ⇆<br>$Mg_2Si_3O_8(H_2O)_{3.5}$ + 4.5 $H_2O$ | 38.8 | | 50 | H-balance is not correct. Personal communication with Dr. Martell: should read:<br>2 Mg + 3 $H_2L$ + 4 OH ⇆ $Mg_2Si_3O_8(H_2O)_{3.5}$ +<br>4.5 $H_2O$ 38.8<br>2 H + L ⇆ $H_2L$<br>(3*23.04) 69.12<br>$H_2O$ ⇆ H + OH<br>(4*-13.997) -55.988<br>2 Mg + 2 H + 3 L ⇆ $Mg_2Si_3O_8(H_2O)_{3.5}$<br>51.932 |
| Ca + L ⇆ CaL | 7.2 | | | |
| 2 $(UO_2)$ + L ⇆ $(UO_2)_2L$ | 6.0 | 0.1 | | Not correct: charge of solid is not zero! Therefore solid NOT entered. |

## Phosphate ($PO_4^{3-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 12.375 | | | |
| HL + H ⇆ $H_2L$ | 7.198 | | | HL + H ⇆ $H_2L$ 7.198<br>H + L ⇆ HL 12.375<br>2 H + L ⇆ $H_2L$ 19.573 |
| $H_2L$ + H ⇆ $H_3L$ | 2.148 | | | $H_2L$ + H ⇆ $H_3L$ 2.148<br>2 H + L ⇆ $H_2L$ 19.573<br>3 H + L ⇆ $H_3L$ 21.721 |
| $H_3L$ + H ⇆ $H_4L$ | 0.0 | 3.0 | | $H_3L$ + H ⇆ $H_4L$ 0.0 3.0<br>3 H + L ⇆ $H_3L$ 23.34237 3.0<br>4 H + L ⇆ $H_4L$ 23.34237 3.0<br>I=0: 21.721 |
| Li + L ⇆ LiL | 0.95 | 0.15 | 37 | I=0: 1.66362 |
| Li + HL ⇆ LiHL | 0.73 | 0.1 | | Li + HL ⇆ LiHL 0.73 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Li + H + L ⇆ LiHL 12.46427 0.1<br>I=0: 13.53215 |
| Li + $H_2L$ ⇆ $LiH_2L$ | 0.2 | 0.5 | 37 | Li + $H_2L$ ⇆ $LiH_2L$ 0.2 0.5<br>2 H + L ⇆ $H_2L$ 18.23106 0.5<br>Li + 2 H + L ⇆ $LiH_2L$ 18.43106 0.5<br>I=0: 20.04139 |
| Na + L ⇆ NaL | 1.43 | | | |
| Na + HL ⇆ NaHL | 1.07 | | | Na + HL ⇆ NaHL 1.07<br>H + L ⇆ HL 12.375<br>Na + H + L ⇆ NaHL 13.445 |
| Na + $H_2L$ ⇆ $NaH_2L$ | 0.3 | | | Na + $H_2L$ ⇆ $NaH_2L$ 0.3<br>2 H + L ⇆ $H_2L$ 19.573<br>Na + 2 H + L ⇆ $NaH_2L$ 19.873 |
| NaL + Na ⇆ $Na_2L$ | 1.16 | | | |
| $Na_2L$ + H ⇆ $Na_2HL$ | 10.73 | | | $Na_2L$ + H ⇆ $Na_2HL$ 10.73<br>NaL + Na ⇆ $Na_2L$ 1.16<br>Na + L ⇆ NaL 1.43<br>2 Na + H + L ⇆ $Na_2HL$ 13.32 |
| K + L ⇆ KL | 1.43 | | | |
| K + HL ⇆ KHL | 0.88 | | | K + HL ⇆ KHL 0.88<br>H + L ⇆ HL 12.375<br>K + H + L ⇆ KHL 13.255 |
| K + $H_2L$ ⇆ $KH_2L$ | 0.3 | | | K + $H_2L$ ⇆ $KH_2L$ 0.3<br>2 H + L ⇆ $H_2L$ 19.573<br>K + 2 H + L ⇆$KH_2L$ 19.873 |
| KL + L ⇆ $K_2L$ | 0.83 | | | |
| $K_2L$ + H ⇆ $K_2HL$ | 11.24 | | | $K_2L$ + H ⇆ $K_2HL$ 11.24<br>KL + K ⇆ $K_2L$ 0.83<br>K + L ⇆ KL 1.37<br>2 K + H + L ⇆ $K_2HL$ 13.44 |
| $NH_4$ + HL ⇆ $NH_4HL$ | 0.8 | 0.15 | 37 | $NH_4$ + HL ⇆ $NH_4HL$ 0.8 0.15<br>$NH_3$ + H ⇆ $NH_4$ 9.244 0.15<br>H + L ⇆ HL 11.66138 0.15<br>$NH_3$ + 2 H + L ⇆ $NH_4HL$ 21.70538 0.15<br>I=0: 22.89475 |
| $NH_4$ + $H_2L$ ⇆ $NH_4H_2L$ | -0.1 | 0.15 | 37 | $NH_4$ + $H_2L$ ⇆ $NH_4H_2L$ -0.1 0.15<br>$NH_3$ + H ⇆ $NH_4$ 9.244 0.15<br>2 H + L ⇆$H_2L$ 18.38363 0.15<br>NH3 + 3 H + L ⇆ $NH_4H_2L$ 27.52763 0.15<br>I=0: 28.95488 |
| Be + $H_2L$ ⇆ $BeH_2L$ | 1.86 | 3.0 | | Be + $H_2L$ ⇆ $BeH_2L$ 1.86 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Be + 2 H + L ⇆ $BeH_2L$ 22.78414 3.0<br>I=0: 20.89254 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Be + 2\ H_2L \leftrightarrows Be(H_2L)_2$ | 4.31 | 3.0 | | $Be + 2\ H_2L \leftrightarrows Be(H_2L)_2$ 4.31 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Be + 4\ H + 2\ L \leftrightarrows Be(H_2L)_2$ 46.15828 3.0<br>I=0: 42.64531 |
| $2\ Be + 2\ H_3L \leftrightarrows Be_2H_5L_2 + H$ | -0.43 | 3.0 | | $2\ Be + 2\ H_3L \leftrightarrows Be_2H_5L_2 + H$ -0.43 3.0<br>$3\ H + L \leftrightarrows H_3L$ (*2)<br>(=2*23.34237) 46.68474 3.0<br>$2\ Be + 5\ H + 2\ L \leftrightarrows Be_2H_5L_2$ 46.25474 3.0<br>I=0: 43.28223 |
| $3\ Be + 6\ H_3L \leftrightarrows Be_3H_{17}L_6 + H$ | -12.12 | 3.0 | | $3\ Be + 6\ H_3L \leftrightarrows Be_3H_{17}L_6 + H$<br>-12.12 3.0<br>$3\ H + L \leftrightarrows H_3L$ (*6)<br>(=6*23.34237) 140.05422 3.0<br>$3\ Be + 17\ H + 6\ L \leftrightarrows Be_3H_{17}L_6$<br>127.93422 3.0<br>I=0: 120.09759 |
| $Be_3H_{15}L_6 + 2\ H \leftrightarrows Be_3H_{17}L_6$ | 10.06 | 3.0 | | $Be_3H_{15}L_6 + 2\ H \leftrightarrows Be_3H_{17}L_6$ 10.06 3.0<br>invert:<br>$Be_3H_{17}L_6 \leftrightarrows Be_3H_{15}L_6 + 2\ H$ -10.06 3.0<br>$3\ Be + 17\ H + 6\ L \leftrightarrows Be_3H_{17}L_6$<br>127.93422 3.0<br>$3\ Be + 15\ H + 6\ L \leftrightarrows Be_3H_{15}L_6$<br>117.87422 3.0<br>I=0: 108.14599 |
| $3\ Be + 8\ H_3L \leftrightarrows Be_3H_{18}L_8 + 6\ H$ | 1.57 | 3.0 | | $3\ Be + 8\ H_3L \leftrightarrows Be_3H_{18}L_8 + 6\ H$<br>1.57 3.0<br>$3\ H + L \leftrightarrows H_3L$ (*8)<br>(=8*23.34237) 186.73896 3.0<br>$3\ Be + 18\ H + 8\ L \leftrightarrows Be_3H_{18}L_8$<br>188.30896 3.0<br>I=0: 174.52730 |
| $Mg + HL \leftrightarrows MgHL$ | 2.80 | | | $Mg + HL \leftrightarrows MgHL$ 2.80<br>$H + L \leftrightarrows HL$ 12.375<br>$Mg + H + L \leftrightarrows MgHL$ 15.175 |
| $Mg + H_2L \leftrightarrows MgH_2L$ | 0.16 | 3.0 | | $Mg + H_2L \leftrightarrows MgH_2L$ 0.16 3.0<br>$2\ H + L \leftrightarrows H_2L$ 20.92414 3.0<br>$Mg + 2\ H + L \leftrightarrows MgH_2L$ 21.08414 3.0<br>I=0: 19.19254 |
| $Mg + 2\ H_2L \leftrightarrows Mg(H_2L)_2$ | 0.64 | 3.0 | | $Mg + 2\ H_2L \leftrightarrows Mg(H_2L)_2$ 0.64 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Mg + 4\ H + 2\ L \leftrightarrows Mg(H_2L)_2$ 42.48828 3.0<br>I=0: 38.97531 |
| $MgH_3L_2 + H \leftrightarrows Mg(H_2L)_2$ | 4.99 | 3.0 | | $MgH_3L_2 + H \leftrightarrows Mg(H_2L)_2$ 4.99 3.0<br>invert:<br>$Mg(H_2L)_2 \leftrightarrows MgH_3L_2 + H$ -4.99 3.0<br>$Mg + 4\ H + 2\ L \leftrightarrows Mg(H_2L)_2$ 42.48828 3.0<br>$Mg + 3\ H + 2\ L \leftrightarrows MgH_3L_2$ 37.49828 3.0<br>I=0: 34.25554 |
| $Ca + HL \leftrightarrows CaHL$ | 2.66 | | | $Ca + HL \leftrightarrows CaHL$ 2.66<br>$H + L \leftrightarrows HL$ 12.375<br>$Ca + H + L \leftrightarrows CaHL$ 15.035 |
| $Ca + H_2L \leftrightarrows CaH_2L$ | 1.35 | | | $Ca + H_2L \leftrightarrows CaH_2L$ 1.35<br>$2\ H + L \leftrightarrows H_2L$ 19.573<br>$Ca + 2\ H + L \leftrightarrows CaH_2L$ 20.923 |
| $Ca + 2\ H_2L \leftrightarrows Ca(H_2L)_2$ | 0.67 | 3.0 | | $Ca + 2\ H_2L \leftrightarrows Ca(H_2L)_2$ 0.67 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Ca + 4\ H + 2\ L \leftrightarrows Ca(H_2L)_2$ 42.51828 3.0<br>I=0: 39.00531 |
| $Sr + HL \leftrightarrows SrHL$ | 1.64<br>1.38 | 0.1 | | 1.64 is when using tetraalkyl ammonium salt as background electrolyte; 1.38 when using Na-salt as background electrolyte; used: average of 1.51<br>$Sr + HL \leftrightarrows SrHL$ 1.51 0.1<br>$H + L \leftrightarrows HL$ 11.73427 0.1<br>$Sr + H + L \leftrightarrows SrHL$ 13.24427 0.1<br>I=0: 14.73930 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Sr + $H_2L$ ⇆ $SrH_2L$ | 0.4 | 0.1 | 20 | Sr + $H_2L$ ⇆ $SrH_2L$ 0.4 0.1<br>2 H + L ⇆ $H_2L$ 18.50512 0.1<br>Sr + 2 H + L ⇆ $SrH_2L$ 18.90512 0.1<br>I=0: 20.40015 |
| Ba + HL ⇆ BaHL | 1.36 | 0.1 | | Ba + HL ⇆ BaHL 1.36 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Ba + H + L ⇆ BaHL 13.09427 0.1<br>I=0: 14.58930 |
| Ba + $H_2L$ ⇆ $Ba(H_2L)$ | 0.00 | 3.0 | | Ba + $H_2L$ ⇆ $Ba(H_2L)$ 0.00 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Ba + 2 H + L ⇆ $Ba(H_2L)$ 20.92414 3.0<br>I=0: 19.03254 |
| Ba + 2 $H_2L$ ⇆ $Ba(H_2L)_2$ | -0.01 | 3.0 | | Ba + 2 $H_2L$ ⇆ $Ba(H_2L)_2$ -0.01 3.0<br>2 H + L ⇆ $H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>Ba + 4 H + 2 L ⇆ $Ba(H_2L)_2$ 41.83828 3.0<br>I=0: 38.32531 |
| Y + $H_2L$ ⇆ $YH_2L$ | 2.65 | | | Y + $H_2L$ ⇆ $YH_2L$ 2.65<br>2 H + L ⇆ $H_2L$ 19.573<br>Y + 2 H + L ⇆ $YH_2L$ 22.223 |
| La + $H_2L$ ⇆ $LaH_2L$ | 1.61 | 0.5 | | La + $H_2L$ ⇆ $LaH_2L$ 1.61 0.5<br>2 H + L ⇆ $H_2L$ 18.23106 0.5<br>La + 2 H + L ⇆ $H_2L$ 19.84106 0.5<br>I=0: 21.98817 |
| Ce + L ⇆ CeL | 11.73 | | | |
| Ce + $H_2L$ ⇆ $CeH_2L$ | 2.33 | | | Ce + $H_2L$ ⇆ $CeH_2L$ 2.33<br>2 H + L ⇆ $H_2L$ 19.573<br>Ce + 2 H + L ⇆ $CeH_2L$ 21.903 |
| Pm + $H_2L$ ⇆ $PmH_2L$ | 2.51 | | | Pm + $H_2L$ ⇆ $PmH_2L$ 2.51<br>2 H + L ⇆ $H_2L$ 19.573<br>Pm + 2 H + L ⇆ $PmH_2L$ 22.083 |
| Gd + L ⇆ GdL | 12.19 | | | |
| Gd + HL ⇆ GdHL | 5.91 | | | Gd + HL ⇆ GdHL 5.91<br>H + L ⇆ HL 12.375<br>Gd + H + L ⇆ GdHL 18.285 |
| Gd + 2 HL ⇆ $GdH_2L_2$ | 9.97 | | | Gd + 2 HL ⇆ $GdH_2L_2$ 9.97<br>H + L ⇆ HL<br>(2*12.375) 24.750<br>Gd + 2 H + 2 L ⇆ $GdH_2L_2$ 34.720 |
| Gd + $H_2L$ ⇆ $GdH_2L$ | 2.74 | | | Gd + $H_2L$ ⇆ $GdH_2L$ 2.74<br>2 H + L ⇆ $H_2L$ 19.573<br>Gd + 2 H + L ⇆ $GdH_2L$ 22.313 |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 13.25 | | | |
| $(UO_2)$ + HL ⇆ $(UO_2)HL$ | 7.28 | | | $(UO_2)$ + HL ⇆ $(UO_2)HL$ 7.2<br>H + L ⇆ HL 12.375<br>$(UO_2)$ + H + L ⇆ $(UO_2)HL$ 19.575 |
| $(UO_2)$ + $H_2L$ ⇆ $(UO_2)H_2L$ | 3.26 | | | $(UO_2)$ + $H_2L$ ⇆ $(UO_2)H_2L$ 3.26<br>2 H + L ⇆ $H_2L$ 19.573<br>$(UO_2)$ + 2 H + L ⇆ $(UO_2)H_2L$<br>22.833 |
| $(UO_2)H_2L$ + H ⇆ $(UO_2)H_3L$ | 0.8 | | | $(UO_2)H_2L$ + H ⇆ $(UO_2)H_3L$ 0.8<br>$(UO_2)$ + 2 H + L ⇆ $(UO_2)H_2L$<br>22.833<br>$(UO_2)$ + 3 H + L ⇆ $(UO_2)H_3L$<br>23.633 |
| Mn(II) + HL ⇆ Mn(II)HL | 2.70<br>2.45 | 0.1 | | 2.70 is when using tetraalkyl ammonium salt as background electrolyte; 2.45 when using Na-salt as background electrolyte; used: average of 2.575<br>Mn(II) + HL ⇆ Mn(II)HL 2.575 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Mn(II) + H + L ⇆ Mn(II)HL<br>14.30927 0.1<br>I=0: 15.80430 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Fe(II) + HL ⇆ Fe(II)HL | 2.46 | 3.0 | | Fe(II) + HL ⇆ Fe(II)HL 2.46 3.0<br>H+ L ⇆ HL 13.18569 3.0<br>Fe(II) + H + L ⇆ Fe(II)HL<br>15.64569 3.0<br>I=0: 13.75409 |
| Fe(II) + $H_2L$ ⇆ Fe(II)$H_2L$ | 0.55 | 3.0 | | Fe(II) + $H_2L$ ⇆ Fe(II)$H_2L$ 0.55 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Fe(II) + 2 H + L ⇆ Fe(II)$H_2L$<br>21.47414 3.0<br>I=0: 19.58254 |
| Fe(II) + 2 $H_2L$ ⇆ Fe(II)$(H_2L)_2$ | 1.82 | 3.0 | | Fe(II) + 2 $H_2L$ ⇆ Fe(II)$(H_2L)_2$<br>1.82 3.0<br>2 H + L ⇆ $H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>Fe(II) + 4 H + 2 L ⇆ Fe(II)$(H_2L)_2$<br>43.66828 3.0<br>I=0: 40.15531 |
| Fe(II)$H_3L_2$ + H ⇆ Fe(II)$(H_2L)_2$ | 5.29 | 3.0 | | Fe(II)$H_3L_2$ + H ⇆ Fe(II)$(H_2L)_2$<br>5.29 3.0<br>invert:<br>Fe(II)$(H_2L)_2$ ⇆ Fe(II)$H_3L_2$ + H<br>-5.29 3.0<br>Fe(II) + 4 H + 2 L ⇆ Fe(II)$(H_2L)_2$<br>43.66828 3.0<br>Fe(II) + 3 H + 2 L ⇆ Fe(II)$H_3L_2$ 38.37828<br>3.0<br>I=0: 35.13554 |
| Co(II) + HL ⇆ Co(II)HL | 2.20 | 0.1 | | Co(II) + HL ⇆ Co(II)HL 2.20 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Co(II) + H + L ⇆ Co(II)HL<br>13.93427 0.1<br>I=0: 15.42930 |
| Co(II) + $H_2L$ ⇆ Co(II)$H_2L$ | 0.51 | 3.0 | | Co(II) + $H_2L$ ⇆ Co(II)$H_2L$ 0.51 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Co(II) + 2 H + L ⇆ Co(II)$H_2L$<br>21.43414 3.0<br>I=0: 19.54254 |
| Co(II) + 2 $H_2L$ ⇆ Co(II)$(H_2L)_2$ | 1.03 | 3.0 | | Co(II) + 2 $H_2L$ ⇆ Co(II)$(H_2L)_2$<br>1.03 3.0<br>2 H + L ⇆ $H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>Co(II) + 4 H + 2 L ⇆ Co(II)$(H_2L)_2$<br>42.87828 3.0<br>I=0: 39.36531 |
| Ni + HL ⇆ NiHL | 2.10 | 0.1 | | Ni + HL ⇆ NiHL 2.10 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Ni + H + L ⇆ NiHL 13.83427 0.1<br>I=0: 15.32930 |
| Ni + $H_2L$ ⇆ Ni$H_2L$ | 0.5 | 0.1 | | Ni + $H_2L$ ⇆ Ni$H_2L$ 0.5 0.1<br>2 H + L ⇆ $H_2L$ 18.50512 0.1<br>Ni + 2 H + L ⇆ Ni$H_2L$ 19.00512 0.1<br>I=0: 20.50015 |
| Cu(II) + HL ⇆ Cu(II)HL | 3.27 | 0.1 | | Cu(II) + HL ⇆ Cu(II)HL 3.27 0.1<br>H + L ⇆ HL 11.73427 0.1<br>Cu(II) + H + L ⇆ Cu(II)HL<br>15.00427 0.1<br>I=0: 16.49930 |
| Cu(II) + $H_2L$ ⇆ Cu(II)$H_2L$ | 0.64 | 3.0 | | Cu(II) + $H_2L$ ⇆ Cu(II)$H_2L$ 0.64 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Cu(II) + 2 H + L ⇆ Cu(II)$H_2L$<br>21.56414 3.0<br>I=0: 19.67254 |
| Cu(II) + 2 $H_2L$ ⇆ Cu(II)$(H_2L)_2$ | 1.03 | 3.0 | | Cu(II) + 2 $H_2L$ ⇆ Cu(II)$(H_2L)_2$<br>1.03 3.0<br>2 H + L ⇆ $H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>Cu(II) + 4 H + 2 L ⇆ Cu(II)$(H_2L)_2$<br>42.87828 3.0<br>I=0: 39.36531 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Cu(II)H_3L_2 + H \leftrightarrows Cu(II)(H_2L)_2$ | 3.80 | 3.0 | | $Cu(II)H_3L_2 + H \leftrightarrows Cu(II)(H_2L)_2$<br>3.80 3.0<br>invert:<br>$Cu(II)(H_2L)_2 \leftrightarrows Cu(II)H_3L_2 + H$<br>-3.80 3.0<br>$Cu(II) + 4\ H + 2\ L \leftrightarrows Cu(II)(H_2L)_2$<br>42.87828 3.0<br>$Cu(II) + 3\ H + 2\ L \leftrightarrows Cu(II)H_3L_2$<br>39.07828 3.0<br>I=0: 35.83554 |
| $Cu(II)H_2L_2 + H \leftrightarrows Cu(II)H_3L_2$ | 4.8 | 3.0 | | $Cu(II)H_2L_2 + H \leftrightarrows Cu(II)H_3L_2$ 4.8 3.0<br>invert:<br>$Cu(II)H_3L_2 \leftrightarrows Cu(II)H_2L_2 + H$<br>-4.8 3.0<br>$Cu(II) + 3\ H + 2\ L \leftrightarrows Cu(II)H_3L_2$<br>39.07828 3.0<br>$Cu(II) + 2\ H + 2\ L \leftrightarrows Cu(II)H_2L_2$<br>34.27828 3.0<br>I=0: 31.57599 |
| $Cr(III) + HL \leftrightarrows Cr(III)HL$ | 2.56 | 0.1 | | $Cr(III) + HL \leftrightarrows Cr(III)HL$ 2.56 0.1<br>$H + L \leftrightarrows HL$ 11.73427 0.1<br>$Cr(III) + H + L \leftrightarrows Cr(III)HL$<br>14.29427 0.1<br>I=0: 16.21645 |
| $Fe(III) + HL \leftrightarrows Fe(III)HL$ | 8.30 | 0.5 | | $Fe(III) + HL \leftrightarrows Fe(III)HL$ 8.30 0.5<br>$H + L \leftrightarrows HL$ 11.56984 0.5<br>$Fe(III) + H + L \leftrightarrows Fe(III)HL$<br>19.86984 0.5<br>I=0: 22.28533 |
| $Fe(III) + H_2L \leftrightarrows Fe(III)H_2L$ | 3.47 | 0.5 | | $Fe(III) + H_2L \leftrightarrows Fe(III)H_2L$<br>3.47 0.5<br>$2\ H + L \leftrightarrows H_2L$ 18.23106 0.5<br>$Fe(III) + 2\ H + L \leftrightarrows Fe(III)H_2L$<br>21.70106 0.5<br>I=0: 23.84817 |
| $Fe(III) + 2\ H_2L \leftrightarrows Fe(III)(H_2L)_2$ | 6.03 | 3.0 | | $Fe(III) + 2\ H_2L \leftrightarrows Fe(III)(H_2L)_2$<br>6.03 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Fe(III) + 4\ H + 2\ L \leftrightarrows Fe(III)(H_2L)_2$<br>47.87828 3.0<br>I=0: 43.82485 |
| $Fe(III) + 3\ H_2L \leftrightarrows Fe(III)(H_2L)_3$ | 8.1 | 3.0 | | $Fe(III) + 3\ H_2L \leftrightarrows Fe(III)(H_2L)_3$<br>8.1 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*3)<br>(=3*20.92414) 62.77242 3.0<br>$Fe(III) + 6\ H + 3\ L \leftrightarrows Fe(III)(H_2L)_3$<br>70.87242 3.0<br>I=0: 65.19762 |
| $Fe(III)H_2L + H \leftrightarrows Fe(III)H_3L$ | 0.6 | 3.0 | | $Fe(III)H_2L + H \leftrightarrows Fe(III)H_3L$<br>0.6 3.0<br>$Fe(III) + 2\ H + L \leftrightarrows Fe(III)H_2L$<br>26.01 3.0<br>$Fe(III) + 3\ H + L \leftrightarrows Fe(III)H_3L$<br>26.61 3.0<br>I=0: 24.98863 |
| $Cu(I) + H_2L \leftrightarrows Cu(I)H_2L$ | 0.5 | 3.0 | | $Cu(I) + H_2L \leftrightarrows Cu(I)H_2L$ 0.5 3.0<br>$2\ H + L \leftrightarrows H_2L$ 20.92414 3.0<br>$Cu(I) + 2\ H + L \leftrightarrows Cu(I)H_2L$<br>21.42414 3.0<br>I=0: 19.80277 |
| $Cu(I) + 2\ H_2L \leftrightarrows Cu(I)(H_2L)_2$ | 1.48 | 3.0 | | $Cu(I) + 2\ H_2L \leftrightarrows Cu(I)(H_2L)_2$<br>1.48 3.0<br>$2\ H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Cu(I) + 4\ H + 2\ L \leftrightarrows Cu(I)(H_2L)_2$<br>43.32828 3.0<br>I=0: 40.35577 |
| $Cu(I)H_2L_2 + H \leftrightarrows Cu(I)H_3L_2$ | 4.3 | 3.0 | | Can not be related to components; not entered |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Ag + H_2L \leftrightarrows AgH_2L$ | -0.17 | 3.0 | | $Ag + H_2L \leftrightarrows AgH_2L$ -0.17 3.0<br>$2 H + L \leftrightarrows H_2L$ 20.92414 3.0<br>$Ag + 2 H + L \leftrightarrows AgH_2L$ 20.75414 3.0<br>I=0: 19.13277 |
| $Ag + 2 H_2L \leftrightarrows Ag(H_2L)_2$ | -0.1 | 3.0 | | $Ag + 2 H_2L \leftrightarrows Ag(H_2L)_2$ -0.1 3.0<br>$2 H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Ag + 4 H + 2 L \leftrightarrows Ag(H_2L)_2$<br>41.74828 3.0<br>I=0: 38.77577 |
| $AgHL + H \leftrightarrows AgH_2L$ | 5.39 | 3.0 | | $AgHL + H \leftrightarrows AgH_2L$ 5.39 3.0<br>invert:<br>$AgH_2L \leftrightarrows AgHL + H$ -5.39 3.0<br>$Ag + 2 H + L \leftrightarrows AgH_2L$ 20.75414 3.0<br>$Ag + H + L \leftrightarrows AgHL$ 15.36414 3.0<br>I=0: 14.01300 |
| $AgH_2L_2 + H \leftrightarrows AgH_3L_2$ | 4.45 | 3.0 | | Can not be related to components; not entered |
| $Zn + HL \leftrightarrows ZnHL$ | 2.46 | 0.1 | | $Zn + HL \leftrightarrows ZnHL$ 2.46 0.1<br>$H + L \leftrightarrows HL$ 11.73427 0.1<br>$Zn + H + L \leftrightarrows ZnHL$ 14.19427 0.1<br>I=0: 15.68930 |
| $Zn + H_2L \leftrightarrows ZnH_2L$ | 0.37 | 3.0 | | $Zn + H_2L \leftrightarrows ZnH_2L$ 0.37 3.0<br>$2 H + L \leftrightarrows H_2L$ 20.92414 3.0<br>$Zn + 2 H + L \leftrightarrows ZnH_2L$ 21.29414 3.0<br>I=0: 19.40254 |
| $Zn + 2 H_2L \leftrightarrows Zn(H_2L)_2$ | 1.10 | 3.0 | | $Zn + 2 H_2L \leftrightarrows Zn(H_2L)_2$ 1.10 3.0<br>$2 H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Zn + 4 H + 2 L \leftrightarrows Zn(H_2L)_2$ 42.94828 3.0<br>I=0: 39.43531 |
| $ZnH_3L_2 + H \leftrightarrows Zn(H_2L)_2$ | 4.9 | 3.0 | | $ZnH_3L_2 + H \leftrightarrows Zn(H_2L)_2$ 4.9 3.0<br>invert:<br>$Zn(H_2L)_2 \leftrightarrows ZnH_3L_2 + H$ -4.9 3.0<br>$Zn + 4 H + 2 L \leftrightarrows Zn(H_2L)_2$ 42.94828 3.0<br>$Zn + 3 H + 2 L \leftrightarrows ZnH_3L_2$ 38.04828 3.0<br>I=0: 34.80554 |
| $ZnH_2L_2 + H \leftrightarrows ZnH_3L_2$ | 3.3 | 3.0 | | $ZnH_2L_2 + H \leftrightarrows ZnH_3L_2$ 3.3 3.0<br>invert:<br>$ZnH_3L_2 \leftrightarrows ZnH_2L_2 + H$ -3.3 3.0<br>$Zn + 3 H + 2 L \leftrightarrows ZnH_3L_2$ 38.04828 3.0<br>$Zn + 2 H + 2 L \leftrightarrows ZnH_2L_2$ 34.74828 3.0<br>I=0: 32.04599 |
| $ZnHL_2 + H \leftrightarrows ZnH_2L_2$ | 5.76 | 3.0 | | $ZnHL_2 + H \leftrightarrows ZnH_2L_2$ 5.76 3.0<br>invert:<br>$ZnH_2L_2 \leftrightarrows ZnHL_2 + H$ -5.76 3.0<br>$Zn + 2 H + 2 L \leftrightarrows ZnH_2L_2$ 34.74828 3.0<br>$Zn + H + 2 L \leftrightarrows ZnHL_2$ 28.98828 3.0<br>I=0: 27.09668 |
| $Cd + HL \leftrightarrows CdHL$ | 2.85 | 0.1 | | $Cd + HL \leftrightarrows CdHL$ 2.85 0.1<br>$H + L \leftrightarrows HL$ 11.73427 0.1<br>$Cd + H + L \leftrightarrows CdHL$ 14.58427 0.1<br>I=0: 16.07930 |
| $Cd + H_2L \leftrightarrows CdH_2L$ | 0.76 | 3.0 | | $Cd + H_2L \leftrightarrows CdH_2L$ 0.76 3.0<br>$2 H + L \leftrightarrows H_2L$ 20.92414 3.0<br>$Cd + 2 H + L \leftrightarrows CdH_2L$ 21.68414 3.0<br>I=0: 19.79254 |
| $Cd + 2 H_2L \leftrightarrows Cd(H_2L)_2$ | 1.01 | 3.0 | | $Cd + 2 H_2L \leftrightarrows Cd(H_2L)_2$ 1.01 3.0<br>$2 H + L \leftrightarrows H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>$Cd + 4 H + 2 L \leftrightarrows Cd(H_2L)_2$ 42.85828 3.0<br>I=0: 39.34531 |
| $CdH_3L_2 + H \leftrightarrows Cd(H_2L)_2$ | 4.03 | 3.0 | | $CdH_3L_2 + H \leftrightarrows Cd(H_2L)_2$ 4.03 3.0<br>invert:<br>$Cd(H_2L)_2 \leftrightarrows CdH_3L_2 + H$ -4.03 3.0<br>$Cd + 4 H + 2 L \leftrightarrows Cd(H_2L)_2$ 42.85828 3.0<br>$Cd + 3 H + 2 L \leftrightarrows CdH_3L_2$ 38.82828 3.0<br>I=0: 35.58554 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $CdH_2L_2$ + H ⇆ $CdH_3L_2$ | 5.67 | 3.0 | | $CdH_2L_2$ + H ⇆ $CdH_3L_2$ 5.67 3.0<br>invert:<br>$CdH_3L_2$ ⇆ $CdH_2L_2$ + H -5.67 3.0<br>Cd + 3 H + 2 L ⇆ $CdH_3L_2$ 38.82828 3.0<br>Zn + 2 H + 2 L ⇆ $ZnH_2L_2$ 33.15828 3.0<br>I=0: 30.45599 |
| Hg(II) + L ⇆ Hg(II)L | 14.0 | 3.0 | | I=0: 12.37863 |
| Hg(II) + HL ⇆ Hg(II)HL | 8.8 | 3.0 | | Hg(II) + HL ⇆ Hg(II)HL 8.8 3.0<br>H + L ⇆ HL 13.18569 3.0<br>Hg(II) + H + L ⇆ Hg(II)HL<br>21.98569 3.0<br>I=0: 20.09409 |
| Pb(II) + HL ⇆ Pb(II)HL | 3.1 | | | Pb(II) + HL ⇆ Pb(II)HL 3.1<br>H+ L ⇆ HL 12.375<br>Pb(II) + H + L ⇆ Pb(II)HL<br>15.475 |
| Pb(II) + $H_2L$ ⇆ Pb(II)$H_2L$ | 1.5 | | | Pb(II) + $H_2L$ ⇆ Pb(II)$H_2L$ 1.5<br>2 H + L ⇆ $H_2L$ 19.573<br>Pb(II) + 2 H + L ⇆ Pb(II)$H_2L$<br>21.073 |
| Al + L ⇆ AlL | 15.32 | 0.15 | 37 | I=0: 17.46087 |
| 2 Al + L ⇆ $Al_2L$ | 16.7 | 0.2 | | I=0: 18.97656 |
| Al + HL ⇆ AlHL | 6.12 | 0.2 | | Al + HL ⇆ AlHL 6.12 0.2<br>H + L ⇆ HL 11.61615 0.2<br>Al + H + L ⇆ AlHL 17.73615 0.2<br>I=0: 20.01271 |
| Al + $H_2L$ ⇆ $AlH_2L$ | 2.02 | 3.0 | | Al + $H_2L$ ⇆ $AlH_2L$ 2.02 3.0<br>2 H + L ⇆ $H_2L$ 20.92414 3.0<br>Al + 2 H + L ⇆ $AlH_2L$ 22.94414 3.0<br>I=0: 20.78231 |
| Al + 2 $H_2L$ ⇆ $Al(H_2L)_2$ | 4.82 | 3.0 | | Al + 2 $H_2L$ ⇆ $Al(H_2L)_2$ 4.82 3.0<br>2 H + L ⇆ $H_2L$ (*2)<br>(=2*20.92414) 41.84828 3.0<br>Al + 4 H + 2 L ⇆ $Al(H_2L)_2$ 46.66828 3.0<br>I=0: 42.61485 |
| $Al_2(OH)L$ + H ⇆ $Al_2L$ | 2.44 | 0.2 | | $Al_2(OH)L$ + H ⇆ $Al_2L$ 2.44 0.2<br>invert:<br>$Al_2L$ ⇆ $Al_2(OH)L$ + H -2.44 0.2<br>2 Al + L ⇆ $Al_2L$ 16.7 0.2<br>OH + H ⇆ $H_2O$ 13.74405 0.2<br>2 Al + OH + L ⇆ $Al_2(OH)L$ 28.00405 0.2<br>I=0: 31.03947 |
| $Al_2L$ ⇆ $Al_2(OH)_2L$ + 2 H | -6.79 | 0.2 | | $Al_2L$ ⇆ $Al_2(OH)_2L$ + 2 H -6.79 0.2<br>2 Al + L ⇆ $Al_2L$ 16.7 0.2<br>OH + H ⇆ $H_2O$<br>(2*13.74405) 27.48810 0.2<br>2 Al + 2 OH + L ⇆ $Al_2(OH)_2L$<br>37.39810 0.2<br>I=0: 40.93942 |
| Ga + HL ⇆ GaHL | 7.26 | 1.0 | | Ga + HL ⇆ GaHL 7.26 1.0<br>H + L ⇆ HL 11.67552 1.0<br>Ga + H + L ⇆ GaHL 18.93552 1.0<br>I=0: 20.76396 |
| Ga + $H_2L$ ⇆ $GaH_2L$ | 1.48 | 1.0 | | Ga + $H_2L$ ⇆ $GaH_2L$ 1.48 1.0<br>2 H + L ⇆ $H_2L$ 18.55720 1.0<br>Ga + 2 H + L ⇆ $GaH_2L$ 20.03720 1.0<br>I=0: 21.66248 |
| In + $H_2L$ ⇆ $InH_2L$ | 2.43 | 1.0 | 20 | In + $H_2L$ ⇆ $InH_2L$ 2.43 1.0<br>2 H + L ⇆ $H_2L$ 18.55720 1.0<br>In + 2 H + L ⇆ $InH_2L$ 20.98720 1.0<br>I=0: 22.61248 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Mg + HL ⇆ $MgHL(H_2O)_3$ | 5.80 | | | Mg + HL ⇆ $MgHL(H_2O)_3$ 5.80<br>H + L ⇆ HL 12.375<br>Mg + H + L ⇆ MgHL 18.175 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 3 Mg + 2 L ⇆ $Mg_3L_2$ | 23.28 | | | |
| Ca + HL ⇆ CaHL | 6.90 | | | Ca + HL ⇆ $CaHL(H_2O)_2$ 6.90<br>H + L ⇆ HL 12.375<br>Ca + H + L ⇆ CaHL 19.275 |
| 3 Ca + 2 L ⇆ $Ca_3L_2$ | 28.92 | | | |
| 4 Ca + H + 3 L ⇆ $Ca_4HL_3(H_2O)_3$ | 47.08 | | | |
| 5 Ca + OH + 3 L ⇆ $Ca_5(OH)L_3(H_2O)$ | 58.33 | | | |
| Sr + HL ⇆ SrHL | 6.92 | | 20 | Sr + HL ⇆ SrHL 6.92<br>H + L ⇆ HL 12.375<br>Sr + H + L ⇆ SrHL 19.295 |
| Ba + HL ⇆ BaHL | 7.40 | | 20 | Ba + HL ⇆ BaHL 7.4<br>H + L ⇆ HL 12.375<br>Ba + H + L ⇆ BaHL 19.775 |
| Y + L ⇆ YL | 25.02 | | | |
| La + L ⇆ LaL | 25.75 | | | |
| Ce + L ⇆ CeL | 26.3 | | | |
| Pr + L ⇆ PrL | 26.4 | | | |
| Nd + L ⇆ NdL | 26.20 | | | |
| Sm + L ⇆ SmL | 26.19 | | | |
| Eu + L ⇆ EuL | 25.96 | | | |
| Gd + L ⇆ GdL | 25.6 | | | |
| Tb + L ⇆ TbL | 25.39 | | | |
| Dy + L ⇆ DyL | 25.2 | | | |
| Ho + L ⇆ HoL | 25.1 | | | |
| Er + L ⇆ ErL | 25.1 | | | |
| Tm + L ⇆ TmL | 25.0 | | | |
| Yb + L ⇆ YbL | 24.9 | | | |
| Lu + L ⇆ LuL | 24.8 | | | |
| $(UO_2)$ + HL ⇆ $(UO_2)HL$ | 11.85 | | | $(UO_2)$ + HL ⇆ $(UO_2)HL$ 11.85<br>H + L ⇆ HL 12.375<br>$(UO_2)$ + H + L ⇆ $(UO_2)HL$ 24.225 |
| 3 $(UO_2)$ + 2 L ⇆ $(UO_2)_3L_2$ | 49.4 | | | |
| 3 Fe(II) + 2 L ⇆ $Fe(II)_3L_2(H_2O)_8$ | 37.76 | | | |
| Fe(III) + L ⇆ $Fe(III)L(H_2O)_2$ | 26.4 | | | |
| 3 Ag + L ⇆ $Ag_3L$ | 17.59 | | | |
| 3 Zn + 2 L ⇆ $Zn_3L_2(H_2O)_4$ | 35.42 | | | |
| 5 Cd + 4 HL ⇆ 2 H + $Cd_5H_2L_4(H_2O)_4$ | 25.4 | 3.0 | | 5 Cd + 4 HL ⇆ 2 H + $Cd_5H_2L_4(H_2O)_4$ 25.4 3.0<br>4 H + 4 L ⇆ 4 HL (4*13.18569) 52.74276 3.0<br>5 Cd + 2 H + 4 L ⇆ $Cd_5H_2L_4(H_2O)_4$ 78.14276 3.0<br>I=0: 70.30613 |
| Hg(II) + HL ⇆ Hg(II)HL | 13.1 | 3.0 | | Hg(II) + HL ⇆ Hg(II)HL 13.1 3.0<br>H + L ⇆ HL 13.18569 3.0<br>Hg(II) + H + L ⇆ Hg(II)HL 26.28569 3.0<br>I=0: 24.39409 |
| 3 Hg(II) + 2 HL ⇆ 2 H + $Hg(II)_3L_2$ | 24.6 | 3.0 | | 3 Hg(II) + 2 HL ⇆ 2 H + $Hg(II)_3L_2$ 24.6 3.0<br>2 H + 2 L ⇆ 2 HL (2*13.18569) 26.37138 3.0<br>3 Hg(II) + 2 L ⇆ $Hg(II)_3L_2$ 50.97138 3.0<br>I=0: 46.91795 |
| 3 Hg(II) + HL ⇆ 4 H + $Hg(II)_3(OH)_3L$ | 9.4 | 3.0 | | 3 Hg(II) + HL ⇆ 4 H + $Hg(II)_3(OH)_3L$ 9.4 3.0<br>H + L ⇆ HL 13.18569 3.0<br>3 H + 3 OH ⇆ 3 $H_2O$ (3*14.26723) 42.80169 3.0<br>3 Hg(II) + L + 3 OH ⇆ $Hg(II)_3(OH)_3L$ 65.38738 3.0<br>I=0: 62.14464 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pb(II) + HL ⇆ Pb(II)HL | 11.43 | | | Pb(II) + HL ⇆ Pb(II)HL 11.43<br>H + L ⇆ HL 12.375<br>Pb(II) + H + L ⇆ Pb(II)HL 23.805 |
| 3 Pb(II) + 2 L ⇆ $Pb(II)_3L_2$ | 43.53 | | 37 | |
| Al + L ⇆ AlL | 18.34 | 0.15 | 37 | I=0: 20.48087 |
| Ga + L ⇆ GaL | 21.0 | 1.0 | | I=0: 22.82844 |
| In + L ⇆ InL | 21.63 | 1.0 | | I=0: 23.45844 |

## Sulfide ($S^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| HL + H ⇆ $H_2L$ | 7.02 | | | From Morel (see page 96):<br>H + L ⇆ HL 13.9<br>HL + H ⇆ $H_2L$ 7.02<br>2 H + L ⇆ $H_2L$ 20.92 |
| Na + HL ⇆ NaHL | -0.8 | | | Na + HL ⇆ NaHL -0.8<br>H + L ⇆ HL 13.9<br>Na + H + L ⇆ NaHL 13.1 |
| Ag + HL ⇆ AgHL | 13.6 | 0.1 | 20 | Ag + HL ⇆ AgHL 13.6 0.1<br>H + L ⇆ HL 13.47285 0.1<br>Ag + H + L ⇆ AgHL 27.07285 0.1<br>I=0: 27.71358 |
| Ag + 2 HL ⇆ $AgH_2L_2$ | 17.7 | 0.1 | 20 | Ag + 2 HL ⇆ $AgH_2L_2$ 17.7 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.47285) 26.94570 0.1<br>Ag + 2 H + 2 L ⇆ $AgH_2L_2$ 44.64570 0.1<br>I=0: 45.71358 |
| AgHL ⇆ AgL + H | -8.3 | 0.1 | 20 | AgHL ⇆ AgL + H -8.3 0.1<br>Ag + H + L ⇆ AgHL 27.07285 0.1<br>Ag + L ⇆ AgL 18.77285 0.1<br>I=0: 19.2 |
| $AgHL_2$ + H ⇆ $AgH_2L_2$ | 9.5 | 0.1 | 20 | $AgHL_2$ + H ⇆ $AgH_2L_2$ 9.5 0.1<br>$AgH_2L_2$ ⇆ Ag + 2 H + 2 L<br>-44.64570 0.1<br>$AgHL_2$ ⇆ Ag + H + 2 L -35.14570 0.1<br>invert:<br>Ag + H + 2 L ⇆ $AgHL_2$ 35.14570 0.1<br>I=0: 35.78643 |
| $Ag_2H_2L_3$ + $H_2L$ ⇆ $Ag_2H_4L_4$ | -3.2 | 1.0 | 20 | (can not be related to components; not entered) |
| Zn + HL ⇆ ZnL + H | 5.0 | 1.0 | | Zn + HL ⇆ ZnL + H 5.0 1.0<br>H + L ⇆ HL 13.49368 1.0<br>Zn + L ⇆ ZnL 18.49368 1.0<br>I=0: 19.30632 |
| Cd + HL ⇆ CdHL | 7.6 | 1.0 | | Cd + HL ⇆ CdHL 7.6 1.0<br>H + L ⇆ HL 13.49368 1.0<br>Cd + H + L ⇆ CdHL 21.09368 1.0<br>I=0: 21.90632 |
| Cd + 2 HL ⇆ $CdH_2L_2$ | 14.6 | 1.0 | | analogous: 14.6 + (2*13.49368) = 41.58736 (1.0)<br>I=0: 43.00948 |
| Cd + 3 HL ⇆ $CdH_3L_3$ | 16.5 | 1.0 | | analogous: 16.5 + (3*13.49368) = 56.98104 (1.0)<br>I=0: 58.80948 |
| Cd + 4 HL ⇆ $CdH_4L_4$ | 18.9 | 1.0 | | analogous: 18.9 + (4*13.49368) = 72.87472 (1.0)<br>I=0: 74.90632 |
| Hg(II) + 2 HL ⇆ Hg(II)$H_2L_2$ | 37.71 | 1.0 | 20 | analogous: 37.71 + (2*13.49368) = 64.69736 (1.0)<br>I=0: 66.11948 |
| Hg(II)$H_2L_2$ ⇆ Hg(II)$HL_2$ + H | -6.19 | 1.0 | 20 | Hg(II)$H_2L_2$ ⇆ Hg(II)$HL_2$ + H<br>-6.19 1.0<br>Hg(II) + 2 H + 2 L ⇆ Hg(II)$H_2L_2$<br>64.69736 1.0<br>Hg(II) + H + 2 L ⇆ Hg(II)$HL_2$<br>58.50736 1.0<br>I=0: 59.72632 |
| Hg(II)$HL_2$ ⇆ Hg(II)$L_2$ + H | -8.30 | 1.0 | 20 | Hg(II)$HL_2$ ⇆ Hg(II)$L_2$ + H<br>-8.30 1.0<br>Hg(II) + H + 2 L ⇆ Hg(II)$HL_2$<br>58.50736 1.0<br>Hg(II) + 2 L ⇆ Hg(II)$L_2$ 50.20736 1.0<br>I=0: 51.02 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| In + HL $\leftrightarrows$ InHL | 11 | 1.0 | 20 | In + HL $\leftrightarrows$ InHL 11 1.0<br>H + L $\leftrightarrows$ HL 13.49368 1.0<br>In + H + L $\leftrightarrows$ InHL 24.49368 1.0<br>I=0: 25.50948 |
| In + 2 HL $\leftrightarrows$ InH$_2$L$_2$ | 17 | 1.0 | 20 | analogous: 17 + (2*13.49368) = 43.98736 (1.0)<br>I=0: 45.81580 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Be + H$_2$L $\leftrightarrows$ 2 H + BeL | -26.4 | | | Be + H$_2$L $\leftrightarrows$ 2 H + BeL -26.4<br>2 H + L $\leftrightarrows$ H$_2$L 20.92<br>Be + L $\leftrightarrows$ BeL -5.48 |
| Mg + H$_2$L $\leftrightarrows$ 2 H + MgL | -24.7 | | | Analogous: -24.7 + 20.92 = -3.78 |
| Ca + H$_2$L $\leftrightarrows$ 2 H + CaL | -18.2 | | | Analogous: -18.2 + 20.92 = 2.72 |
| Sr + H$_2$L $\leftrightarrows$ 2 H + SrL | -20.9 | | | Analogous: -20.9 + 20.92 = 0.02 |
| Ba + H$_2$L $\leftrightarrows$ 2 H + BaL | -23.2 | | | Analogous: -23.2 + 20.92 = -2.28 |
| Mn(II) + H$_2$L $\leftrightarrows$ 2 H + Mn(II)L | -7.0 | | | Analogous: -7 + 20.92 = 13.92 |
| Fe(II) + H$_2$L $\leftrightarrows$ 2 H + Fe(II)L | -3.0 | | | Analogous: -3.0 + 20.92 = 17.92 |
| Co(II) + H$_2$L $\leftrightarrows$ 2 H + Co(II)L | 4.7 | | | Analogous: 4.7 + 20.92 = 25.62 |
| Ni + H$_2$L $\leftrightarrows$ 2 H + NiL | 5.7 | | | Analogous: 5.7 + 20.92 = 26.62 |
| Cu(II) + H$_2$L $\leftrightarrows$ 2 H + Cu(II)L | 15.2 | | | Analogous: 15.2 + 20.92 = 36.12 |
| 2 Cu(I) + H$_2$L $\leftrightarrows$ 2 H + Cu(I)$_2$L | 27.9 | | | Analogous: 27.9 + 20.92 = 48.82 |
| 2 Ag + H$_2$L $\leftrightarrows$ 2 H + Ag$_2$L | 29.2 | | | Analogous: 29.2 + 20.92 = 50.12 |
| Zn + H$_2$L $\leftrightarrows$ 2 H + ZnL | 3.8 | | | Analogous: 3.8 + 20.92 = 24.72 |
| Cd + H$_2$L $\leftrightarrows$ 2 H + CdL | 7.0 | | | Analogous: 7.0 + 20.92 = 27.92 |
| Hg(II) + H$_2$L $\leftrightarrows$ 2 H + Hg(II)L | 32.1 | | | Analogous: 32.1 + 20.92 = 53.02 |
| Sn(II) + H$_2$L $\leftrightarrows$ 2 H + Sn(II)L | 5.0 | | | Analogous: 5.0 + 20.92 = 25.92 |
| Pb(II) + H$_2$L $\leftrightarrows$ 2 H + Pb(II)L | 7.9 | | | Analogous: 7.9 + 20.92 = 28.82 |
| 2 In + 3 H$_2$L $\leftrightarrows$ In$_2$L$_3$ + 6 H | 15 | 1.0 | 20 | 2 In + 3 H$_2$L $\leftrightarrows$ 6 H + In$_2$L$_3$ 15 1.0<br>6 H + 3 L $\leftrightarrows$ 3 H$_2$L 1.0<br>(3*20.31052) 60.93156<br>2 In + 3 L $\leftrightarrows$ In$_2$L$_3$ 75.93156 1.0<br>I=0: 78.97896 |
| 2 As(III)$_3$L$_6$ + 6 H $\leftrightarrows$ 3 H$_2$L + As(III)$_6$L$_9$ | 35 | 1.0 | 22 | (can not be related to components; not entered) |
| 2 Bi + 3 H$_2$L $\leftrightarrows$ Bi$_2$L$_3$ + 6 H | 20 | | | 2 Bi + 3 H$_2$L $\leftrightarrows$ 6 H + Bi$_2$L$_3$ 20<br>6 H + 3 L $\leftrightarrows$ 3 H$_2$L<br>(3*20.92) 62.76<br>2 Bi + 3 L $\leftrightarrows$ Bi$_2$L$_3$ 82.76 |

Gases:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H$_2$L (aq) $\leftrightarrows$ H$_2$L (g) | 0.99 | | | H$_2$L (aq) $\leftrightarrows$ H$_2$L (g) 0.99<br>2 H + L $\leftrightarrows$ H$_2$L (aq) 20.92<br>2 H + L $\leftrightarrows$ H$_2$L (g) 21.91 |

# Sulfite ($SO_3^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 7.19 | | | |
| HL + H ⇆ $H_2L$ | 1.85 | | | HL + H ⇆ $H_2L$ 1.85<br>H + L ⇆ HL 7.19<br>2 H + L ⇆ $H_2L$ 9.04 |
| 2 HL ⇆ $S_2O_5$ | 1.49 | | | 2 HL ⇆ $S_2O_5$ 1.49<br>2 H + 2 L ⇆ 2 HL<br>(2*7.19) 14.38<br>2 H + 2 L ⇆ $S_2O_5$ 15.87 |
| Na + L ⇆ NaL | 0.42 | 1.0 | | I=0: 0.82632 |
| K + L ⇆ KL | 0.22 | 1.0 | | I=0: 0.62632 |
| Mg + L ⇆ MgL | 2.36 | | | |
| Ca + L ⇆ CaL | 2.62 | | | |
| Ce + L ⇆ CeL | 8.04 | | | |
| (U(VI)$O_2$) + L ⇆ (U(VI)$O_2$)L | 6.7 | | | |
| Mn(II) + L ⇆ Mn(II)L | 3.00 | | | |
| Co(II) + L ⇆ Co(II)L | 3.08 | | | |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | 4.34 | 2.0 | | I=0: 4.28225 |
| Co(II) + 3 L ⇆ Co(II)$L_3$ | 6.48 | 2.0 | | I=0: 6.48000 |
| Ni + L ⇆ NiL | 2.88 | | | |
| Cu(II) + L ⇆ Cu(II)L | 4.26 | 0.5 | 20 | I=0: 5.33355 |
| Fe(III) + L ⇆ Fe(III)L | 6.6 | 0.5 | 20 | I=0: 8.21033 |
| Fe(III)(OH) + L ⇆ Fe(III)(OH)L | 7.3 | 0.5 | 20 | Fe(III)(OH) + L ⇆ Fe(III)(OH)L 7.3 0.5<br>Fe(III) + (OH) ⇆ Fe(III)(OH) 11.00484 0.5<br>Fe(III) + (OH) + L ⇆ Fe(III)(OH)L 18.30484 0.5<br>I=0: 20.18356 |
| Cu(I) + L ⇆ Cu(I)L | 7.85 | 1.0 | | I=0: 8.25632 |
| Cu(I) + 2 L ⇆ Cu(I)$L_2$ | 8.7 | 1.0 | | I=0: 8.7 |
| Cu(I) + 3 L ⇆ Cu(I)$L_3$ | 9.4 | 1.0 | | I=0: 8.18104 |
| Ag + L ⇆ AgL | 5.60 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 8.68 | | | |
| Ag + 3 L ⇆ $AgL_3$ | 9.00 | | | |
| Pd + 4 L ⇆ $PdL_4$ | 29.1 | 0.7 | | I=0: 27.10470 |
| Cd + L ⇆ CdL | 3.29 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 4.2 | 1.0 | | I=0: 5.01264 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 22.33 | 0.5 | | I=0: 23.40355 |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 24.1 | 0.5 | | I=0: 24.1 |

## Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ca + L ⇆ CaL$(H_2O)_{0.5}$ | 6.64 | | | |
| 2 Ag + L ⇆ $Ag_2L$ | 13.82 | | | |

## Gases:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_2L$ ⇆ $SO_2$ (g) | -0.09 | | | $H_2L$ (aq) ⇆ $SO_2$ (g) -0.09<br>2 H + L ⇆ $H_2L$ (aq) 9.05<br>2 H + L ⇆ $SO_2$ (g) 8.96 |

## Sulfate ($SO_4^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H + L \leftrightarrows HL$ | 1.99 | | | |
| $NH_4 + L \leftrightarrows NH_4L$ | 1.03 | | | $NH_4 + L \leftrightarrows NH_4L$ 1.03<br>$NH_3 + H \leftrightarrows NH_4$ 9.244<br>$H + NH_3 + L \leftrightarrows NH_4L$ 10.274 |
| $Li + L \leftrightarrows LiL$ | 0.64 | | | |
| $Na + L \leftrightarrows NaL$ | 0.74 | | | |
| $K + L \leftrightarrows KL$ | 0.85 | | | |
| $Rb + L \leftrightarrows RbL$ | 0.94 | | 37 | |
| $Cs + L \leftrightarrows CsL$ | 1.04 | | 37 | |
| $Be + L \leftrightarrows BeL$ | 2.19 | | | |
| $Be + 2 L \leftrightarrows BeL_2$ | 1.78 | 1.0 | | I=0: 2.59264 |
| $Be + 3 L \leftrightarrows BeL_3$ | 2.08 | 1.0 | | I=0: 2.08 |
| $Mg + L \leftrightarrows MgL$ | 2.26 | | | |
| $Ca + L \leftrightarrows CaL$ | 2.36 | | | |
| $Sr + L \leftrightarrows SrL$ | 2.30 | | | |
| $Ba + L \leftrightarrows BaL$ | 2.13 | | | |
| $Sc + L \leftrightarrows ScL$ | 4.18 | | | |
| $Sc + 2 L \leftrightarrows ScL_2$ | 5.6 | | | |
| $Y + L \leftrightarrows YL$ | 3.48 | | | |
| $Y + 2 L \leftrightarrows YL_2$ | 5.2 | | | |
| $La + L \leftrightarrows LaL$ | 3.64 | | | |
| $La + 2 L \leftrightarrows LaL_2$ | 5.3 | | | |
| $Ce + L \leftrightarrows CeL$ | 3.64 | | | |
| $Ce + 2 L \leftrightarrows CeL_2$ | 5.1 | | | |
| $Pr + L \leftrightarrows PrL$ | 3.64 | | | |
| $Pr + 2 L \leftrightarrows PrL_2$ | 4.9 | | | |
| $Nd + L \leftrightarrows NdL$ | 3.66 | | | |
| $Nd + 2 L \leftrightarrows NdL_2$ | 5.1 | | | |
| $Pm + L \leftrightarrows PmL$ | 1.34 | 2.0 | | I=0: 1.25337 |
| $Pm + 2 L \leftrightarrows PmL_2$ | 1.9 | 2.0 | | I=0: 1.78449 |
| $Sm + L \leftrightarrows SmL$ | 3.67 | | | |
| $Sm + 2 L \leftrightarrows SmL_2$ | 5.1 | | | |
| $Eu + L \leftrightarrows EuL$ | 3.67 | | | |
| $Eu + 2 L \leftrightarrows EuL_2$ | 5.4 | | | |
| $Gd + L \leftrightarrows GdL$ | 3.66 | | | |
| $Gd + 2 L \leftrightarrows GdL_2$ | 5.2 | | | |
| $Tb + L \leftrightarrows TbL$ | 3.64 | | | |
| $Tb + 2 L \leftrightarrows TbL_2$ | 5.1 | | | |
| $Dy + L \leftrightarrows DyL$ | 3.61 | | | |
| $Dy + 2 L \leftrightarrows DyL_2$ | 4.8 | | | |
| $Ho + L \leftrightarrows HoL$ | 3.59 | | | |
| $Ho + 2 L \leftrightarrows HoL_2$ | 4.9 | | | |
| $Er + L \leftrightarrows ErL$ | 3.59 | | | |
| $Er + 2 L \leftrightarrows ErL_2$ | 5.1 | | | |
| $Tm + L \leftrightarrows TmL$ | 3.59 | | | |
| $Tm + 2 L \leftrightarrows TmL_2$ | 5.1 | | | |
| $Yb + L \leftrightarrows YbL$ | 3.55 | | | |
| $Yb + 2 L \leftrightarrows YbL_2$ | 5.2 | | | |
| $Lu + L \leftrightarrows LuL$ | 3.52 | | | |
| $Lu + 2 L \leftrightarrows LuL_2$ | 5.2 | | | |
| $(U(VI)O_2) + L \leftrightarrows (U(VI)O_2)L$ | 3.18 | | | |
| $(U(VI)O_2) + 2 L \leftrightarrows (U(VI)O_2)L_2$ | 4.3 | | | |
| $2 (U(VI)O_2) + 2 L \leftrightarrows (U(VI)O_2)_2(OH)_2L_2 + 2 H$ | -2.73 | 3.5 | | $2 (U(VI)O_2) + 2 L \leftrightarrows (U(VI)O_2)_2(OH)_2L_2 + 2 H$ -2.73 3.5<br>$H + OH \leftrightarrows H_2O$<br>(2*14.40163) 28.80326 3.5<br>$2 (U(VI)O_2) + 2 L + 2 OH \leftrightarrows (U(VI)O_2)_2(OH)_2L_2$ 26.07326 3.5<br>I=0: 23.24088 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 3 $(U(VI)O_2)$ + 3 L ⇆ $(U(VI)O_2)_3(OH)_4L_3$ + 4 H | -8.2 | 3.5 | | 3 $(U(VI)O_2)$ + 3 L ⇆ $(U(VI)O_2)_3(OH)_4L_3$ + 4 H -8.2 3.5<br>H + OH ⇆ $H_2O$<br>(4*14.40163) 57.60652 3.5<br>3 $(U(VI)O_2)$ + 3 L + 4 OH ⇆ $(U(VI)O_2)_3(OH)_4L_3$ 49.40652 3.5<br>I=0: 46.97877 |
| 3 $(U(VI)O_2)$ + 4 L ⇆ $(U(VI)O_2)_3(OH)_4L_4$ + 4 H | -7.8 | 3.5 | | 3 $(U(VI)O_2)$ + 4 L ⇆ $(U(VI)O_2)_3(OH)_4L_4$ + 4 H -7.8 3.5<br>H + OH ⇆ $H_2O$<br>(4*14.40163) 57.60652 3.5<br>3 $(U(VI)O_2)$ + 4 L + 4 OH ⇆ $(U(VI)O_2)_3(OH)_4L_4$ 49.80652 3.5<br>I=0: 50.61577 |
| 5 $(U(VI)O_2)$ + 6 L ⇆ $(U(VI)O_2)_5(OH)_8L_6$ + 8 H | -18.5 | 3.5 | | 5 $(U(VI)O_2)$ + 6 L ⇆ $(U(VI)O_2)_5(OH)_8L_6$ + 8 H -18.5 3.5<br>H + OH ⇆ $H_2O$<br>(8*14.40163) 115.21304 3.5<br>5 $(U(VI)O_2)$ + 6 L + 8 OH ⇆ $(U(VI)O_2)_5(OH)_8L_6$ 96.71304 3.5<br>I=0: 106.42404 |
| Mn(II) + L ⇆ Mn(II)L | 2.25 | | | |
| Fe(II) + L ⇆ Fe(II)L | 2.39 | | | |
| Co(II) + L ⇆ Co(II)L | 2.30 | | | |
| Ni + L ⇆ NiL | 2.30 | | | |
| Cu(II) + L ⇆ Cu(II)L | 2.36 | | | |
| Cr(III) + L ⇆ Cr(III)L | 2.60 | 1.0 | 50 | I=0: 3.81896 |
| Cr(III)L ⇆ Cr(III)L(OH) + H | -4.65 | 0.1 | | Cr(III)L ⇆ Cr(III)L(OH) + H -4.65 0.1<br>Cr(III) + L ⇆ Cr(III)L 2.53751 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Cr(III) + OH + L ⇆ Cr(III)OHL 11.67093 0.1<br>I=0: 13.16596 |
| Fe(III) + L ⇆ Fe(III)L | 4.05 | | | |
| Zr + L ⇆ ZrL | 3.67 | 2.0 | | I=0: 3.55449 |
| Zr + 2 L ⇆ $ZrL_2$ | 6.40 | 2.0 | | I=0: 6.22674 |
| Zr + 3 L ⇆ $ZrL_3$ | 7.4 | 2.0 | | I=0: 7.22674 |
| Hf + L ⇆ HfL | 3.04 | 2.0 | | I=0: 2.92449 |
| Hf + 2 L ⇆ $HfL_2$ | 5.44 | 2.0 | | I=0: 5.26674 |
| Ag + L ⇆ AgL | 1.3 | | | |
| Pd + L ⇆ PdL | 1.28 | 1.0 | | I=0: 2.09264 |
| Zn + L ⇆ ZnL | 2.34 | | | |
| Cd + L ⇆ CdL | 2.37 | | | |
| Hg(II) + L ⇆ Hg(II)L | 1.34 | 0.5 | | I=0: 2.41355 |
| Hg(II) + 2 L ⇆ $Hg(II)L_2$ | 2.4 | 0.5 | | I=0: 3.47355 |
| Pb(II) + L ⇆ Pb(II)L | 2.69 | | | |
| Al + L ⇆ AlL | 3.89 | | | |
| In + L ⇆ InL | 1.80 | 1.0 | 20 | I=0: 3.01896 |
| In + 2 L ⇆ $InL_2$ | 2.55 | 1.0 | 20 | I=0: 4.17528 |
| In + 3 L ⇆ $InL_3$ | 3.0 | 1.0 | 20 | I=0: 4.21896 |
| Si | | | | Complex with $Si(IV)(OH)_4$ not included |
| Bi + L ⇆ BiL | 1.98 | 3.0 | | I=0: 0.35863 |
| Bi + 2 L ⇆ $BiL_2$ | 3.41 | 3.0 | | I=0: 1.24817 |
| Bi + 3 L ⇆ $BiL_3$ | 4.08 | 3.0 | | I=0: 2.45863 |
| Bi + 4 L ⇆ $BiL_4$ | 4.34 | 3.0 | | I=0: 4.34 |
| Bi + 5 L ⇆ $BiL_5$ | 4.60 | 3.0 | | I=0: 7.30229 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ca + L ⇆ $CaL(H_2O)_2$ | 4.61 | | | |
| Sr + L ⇆ SrL | 6.62 | | | |
| Ba + L ⇆ BaL | 9.98 | | | |
| Cu(II) + 1.5 (OH) + 0.25 L ⇆ | 17.19 | | | Cu(II) + 1.5 (OH) + 0.25 L ⇆ Cu(II) |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
| --- | --- | --- | --- | --- |
| Cu(II)$(OH)_{1.5}L_{0.25}$ | | | | $(OH)_{1.5}L_{0.25}$<br>Multiply by 4:<br>4 Cu(II) + 6 (OH) + L ⇆ Cu(II)$_4$(OH)$_6$L<br>log K=4*17.19=68.76 |
| 2 Ag + L ⇆ $Ag_2L$ | 4.82 | | | |
| Pb(II) + L ⇆ Pb(II)L | 7.79 | | | |

## Chloride ($Cl^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Li + L ⇆ LiL | -0.16 | | | |
| Na + L ⇆ NaL | -0.3 | | | |
| K + L ⇆ KL | -0.3 | | | |
| Rb + L ⇆ RbL | -0.3 | | | |
| Cs + L ⇆ CsL | -0.1 | | | |
| Be + L ⇆ BeL | -0.85 | 4.0 | | I=0: -1.93352 |
| Mg + L ⇆ MgL | 0.6 | | | |
| Ca + L ⇆ CaL | 0.4 | | | |
| Sr + L ⇆ SrL | -0.22 | 1.0 | | I=0: 0.18632 |
| Ba + L ⇆ BaL | -0.44 | 1.0 | | I=0: -0.03368 |
| Sc + L ⇆ ScL | -0.12 | 4.0 | | I=0: -1.74528 |
| Y + L ⇆ YL | -0.03 | 1.0 | | I=0: 0.57948 |
| La + L ⇆ LaL | -0.04<br>-0.12 | 1.0 | | -0.04 is for $HClO_4$ as background electrolyte; -0.12 for $NaClO_4$. Used: average of -0.08.<br>I=0: 0.52948 |
| Ce + L ⇆ CeL | -0.04 | 1.0 | | I=0: 0.56948 |
| Pr + L ⇆ PrL | -0.04 | 1.0 | | I=0: 0.56948 |
| Sm + L ⇆ SmL | -0.39 | 3.0 | 20 | I=0: -1.20069 |
| Eu + L ⇆ EuL | -0.04 | 1.0 | | I=0: 0.56948 |
| Gd + L ⇆ GdL | -0.25 | 3.0 | 20 | I=0: -1.06069 |
| Tb + L ⇆ TbL | -0.35 | 3.0 | 20 | I=0: -1.16069 |
| Tm + L ⇆ TmL | -0.1 | 1.0 | 20 | I=0: 0.50948 |
| Yb + L ⇆ YbL | -0.2 | 1.0 | 20 | I=0: 0.40948 |
| Lu + L ⇆ LuL | -0.35 | 4.0 | | I=0: -1.97528 |
| $U(VI)O_2$ + L ⇆ $U(VI)O_2L$ | 0.30 | | | |
| Mn(II) + L ⇆ Mn(II)L | 0.0 | | | |
| Fe(II) + L ⇆ Fe(II)L | -0.3 | | | |
| Co(II) + L ⇆ Co(II)L | -0.35 | | | |
| Ni + L ⇆ NiL | -0.43 | | | |
| Cu(II) + L ⇆ Cu(II)L | 0.3 | | | |
| Cr(III) + L ⇆ Cr(III)L | -1.0 | 1.0 | | I=0: -0.39052 |
| Fe(III) + L ⇆ Fe(III)L | 1.4 | | | |
| Co(III) + L ⇆ Co(III)L | 1.5 | 0.5 | | I=0: 2.30516 |
| Zr + L ⇆ ZrL | 0.2 | 2.0 | | I=0: 0.14225 |
| Zr + 2 L ⇆ $ZrL_2$ | 1.32 | 6.0 | 20 | These data are valid for such high ionic strengths and charges that extrapolation becomes too tricky; NOT entered; instead data taken from Turner, Whitfield & Dickson; see page 98. |
| Zr + 3 L ⇆ $ZrL_3$ | 1.51 | 6.0 | 20 | |
| Hf + L ⇆ HfL | 0.34 | 3.0 | 20 | |
| Cu(I) + L ⇆ Cu(I)L | 3.1 | | | |
| Cu(I) + 2 L ⇆ $Cu(I)L_2$ | 5.42 | | | |
| $Cu(I)L_2$ + L ⇆ $Cu(I)L_3$ | -0.67 | | | $Cu(I)L_2$ + L ⇆ $Cu(I)L_3$ -0.67<br>Cu(I) + 2 L ⇆ $Cu(I)L_2$ 5.42<br>Cu(I) + 3 L ⇆ $Cu(I)L_3$ 4.75 |
| 2 Cu(I) + 4 L ⇆ $Cu(I)_2L_4$ | 13.0 | 5.0 | | I=0: 12.17820 |
| Ag + L ⇆ AgL | 3.31 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 5.25 | | | |
| Ag + 3 L ⇆ $AgL_3$ | 5.2 | | | |
| Ag + 4 L ⇆ $AgL_4$ | 5.32 | 5.0 | | I=0: 6.96360 |
| Pd + L ⇆ PdL | 6.1 | | | |
| Pd + 2 L ⇆ $PdL_2$ | 10.7 | | | |
| Pd + 3 L ⇆ $PdL_3$ | 13.1 | | | |
| Pd + 4 L ⇆ $PdL_4$ | 15.4 | | | |
| $PdL_2$ (cis) ⇆ $PdL_2$ (trans) | -0.32 | 1.0 | | not clear how this one relates to the other one three lines up; NOT entered |
| Zn + L ⇆ ZnL | 0.46 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cd + L ⇆ CdL | 1.98 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 2.60 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 1.96 | 2.0 | | 1.96 using $NaClO_4$ as background electrolyte; 2.13 using $LiClO_4$; used: average of 2.045<br>I=0: 2.00169 |
| Hg(II) + L ⇆ Hg(II)L | 7.30 | | | |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 14.00 | | | |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 15.0 | | | |
| Hg(II) + 4 L ⇆ Hg(II)$L_4$ | 15.6 | | | |
| Hg(II)L ⇆ Hg(II)OHL+ H | -3.05 | 1 | | Hg(II)L ⇆ Hg(II)OHL+ H -3.05 1<br>OH + H ⇆ $H_2O$ 13.79384 1<br>Hg(II) + L ⇆ Hg(II)L 6.89368 1<br>Hg(II) + L + OH ⇆ Hg(II)OHL 17.63752 1<br>I=0: 18.247 |
| Sn(II) + L ⇆ Sn(II)L | 1.64 | | | |
| Sn(II) + 2 L ⇆ Sn(II)$L_2$ | 2.40 | | | |
| Sn(II) + 3 L ⇆ Sn(II)$L_3$ | 1.3 | 2.0 | | I=0: 1.25669 |
| Pb(II) + L ⇆ Pb(II)L | 1.56 | | | |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 1.9 | | | |
| Pb(II) + 3 L ⇆ Pb(II)$L_3$ | 1.8 | | | |
| Al + L ⇆ AlL | -1.0 | 1.0 | | I=0: -0.39052 |
| Ga + L ⇆ GaL | 0.00 | 1.0 | | I=0: 0.60948 |
| In + L ⇆ InL | 2.33 | 1.0 | | I=0: 2.93948 |
| In + 2 L ⇆ $InL_2$ | 3.4 | 1.0 | | I=0: 4.41580 |
| In + 3 L ⇆ $InL_3$ | 3.8 | 1.0 | | I=0: 5.01896 |
| InL ⇆ InOHL + H | -3.9 | 3.0 | | InL ⇆ InOHL + H -3.9 3.0<br>In + L ⇆ InL 3.75017 3.0<br>H + OH ⇆ $H_2O$ 14.26723 3.0<br>In + OH + L ⇆ InOHL 14.11740 3.0<br>I=0: 12.76626 |
| InOHL + In ⇆ $In_2OHL$ | 1.6 | 3.0 | | InOHL + In ⇆ $In_2OHL$ 1.6 3.0<br>In + OH + L ⇆ InOHL 14.11740 3.0<br>2 In + OH + L ⇆ $In_2OHL$ 15.71740 3.0<br>I=0: 15.17694 |
| Bi + L ⇆ BiL | 3.6 | | | |
| Bi + 2 L ⇆ $BiL_2$ | 5.5 | | | |
| Bi + 3 L ⇆ $BiL_3$ | 7.1 | | | |
| Bi + 4 L ⇆ $BiL_4$ | 8.1 | | | |
| Bi + 5 L ⇆ $BiL_5$ | 6.7 | 2.0 | | I=0: 6.62781 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Li + L ⇆ LiL | 6.89 | | | |
| Na + L ⇆ NaL | -1.55 | | | |
| K + L ⇆ KL | -0.90 | | | |
| Cu(II)$(OH)_{1.5}L_{0.5}$ ⇆ Cu(II)$(OH)_{1.5}L_{0.5}$ (s) | 17.3 | | | (can not be related to components; not entered) |
| Cu(I) + L ⇆ Cu(I)L | 6.73 | | | |
| Ag + L ⇆ AgL | 9.750 | | | |
| $Zn(OH)_{1.5}L_{0.5}$ ⇆ $Zn(OH)_{1.5}L_{0.5}$ (s) | 13.4 | | | (can not be related to components; not entered) |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 4.78 | | | |
| Bi + L ⇆ BiOL + 2 H | 7.80 | | | Bi + L ⇆ BiOL + 2 H 7.80<br>H + OH ⇆ $H_2O$<br>(2*13.997) 27.996<br>Bi + 2 OH + L ⇆ BiOL (+$H_2O$) 35.796 |

# Vanadate ($VO_4^{3-}$)

Note: many polynuclear complexes have NOT been entered because they are not likely to occur in significant concentrations at ambient V-levels.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L $\leftrightarrows$ HL | 14.3 | | | |
| HL + H $\leftrightarrows$ $H_2L$ | 8.55 | | | HL + H $\leftrightarrows$ $H_2L$ 8.55<br>H + L $\leftrightarrows$ HL 14.3<br>2 H + L $\leftrightarrows$ $H_2L$ 22.85 |
| $H_2L$ + 2 H $\leftrightarrows$ $VO_2$ | 7.3 | | | $H_2L$ + 2 H $\leftrightarrows$ $VO_2$ 7.3<br>2 H + L $\leftrightarrows$ $H_2L$ 22.85<br>4 H + L $\leftrightarrows$ $VO_2$ 30.15 |
| (many polynuclear complexes for H Li Na K Rb Cs)<br>special case:<br>4 $H_2L$ $\leftrightarrows$ $V_4O_{12}$<br>calculated for solids below but not entered as such | 8.64 | | | 4 H + 4 HL $\leftrightarrows$ $V_4O_{12}$ 42.8<br>4 H + 4 L $\leftrightarrows$ 4 HL<br>(4*14.3) 57.2<br>8 H + 4 L $\leftrightarrows$ $V_4O_{12}$ 100.0 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $VO_2$ $\leftrightarrows$ $(V_2O_5)_{0.5}$ + H | 0.68 | | | $VO_2$ $\leftrightarrows$ $(V_2O_5)_{0.5}$ + H 0.68<br>4 H + L $\leftrightarrows$ $VO_2$ 30.15<br>3 H + L $\leftrightarrows$ $(V_2O_5)_{0.5}$ 30.83<br>multiply by 2:<br>6 H + 2 L $\leftrightarrows$ $(V_2O_5)$ 61.66 |
| $NH_4$ + $H_2L$ $\leftrightarrows$ $(NH_4)VO_3$ | 3.5 | | | $NH_4$ + $H_2L$ $\leftrightarrows$ $(NH_4)VO_3$ 3.5<br>$NH_3$ + H $\leftrightarrows$ $NH_4$ 9.244<br>2 H + L $\leftrightarrows$ $H_2L$ 22.85<br>NH3 + 3 H + L $\leftrightarrows$ $(NH_4)VO_3$ 35.594 |
| Ca + 0.5 $V_4O_{12}$ $\leftrightarrows$ $Ca(VO_3)_2(H_2O)_4$ | 4.10 | 1.0 | 20 | Ca + 0.5 $V_4O_{12}$ $\leftrightarrows$ $Ca(VO_3)_2(H_2O)_4$<br>4.10 1.0<br>multiply by 2:<br>2 Ca + $V_4O_{12}$ $\leftrightarrows$ 2 $Ca(VO_3)_2(H_2O)_4$<br>8.20 1.0<br>8 H + 4 L $\leftrightarrows$ $V_4O_{12}$ 97.15576 1.0<br>2 Ca + 8 H + 4 L $\leftrightarrows$ 2 $Ca(VO_3)_2(H_2O)_4$<br>105.35576 1.0<br>divide by 2:<br>Ca + 4 H + 2 L $\leftrightarrows$ $Ca(VO_3)_2(H_2O)_4$<br>52.67788 1.0<br>I=0: 55.31896 |
| 3 Ca + 2 $VO_4$ $\leftrightarrows$ $Ca_3(VO_4)_2(H_2O)_4$ | 17.48 | 1.0 | 20 | I=0: 20.52740 |
| Sr + 0.5 $V_4O_{12}$ $\leftrightarrows$ $Sr(VO_3)_2(H_2O)_4$ | 9.00 | 1.0 | 20 | like Ca:<br>2 Sr + $V_4O_{12}$ $\leftrightarrows$ 2 $Sr(VO_3)_2(H_2O)_4$<br>18.00 1.0<br>8 H + 4 L $\leftrightarrows$ $V_4O_{12}$ 97.15576 1.0<br>2 Sr + 8 H + 4 L $\leftrightarrows$ 2 $Sr(VO_3)_2(H_2O)_4$<br>115.15576 1.0<br>divide by 2:<br>Sr + 4 H + 2 L $\leftrightarrows$ $Sr(VO_3)_2(H_2O)_4$<br>57.57788 1.0<br>I=0: 60.21896 |
| 3 Sr + 2 $VO_4$ $\leftrightarrows$ $Sr_3(VO_4)_2(H_2O)_4$ | 20.60 | 1.0 | 20 | I=0: 23.64740 |
| Ba + 0.5 $V_4O_{12}$ $\leftrightarrows$ $Ba(VO_3)_2(H_2O)_4$ | 11.92 | 1.0 | 20 | like Ca:<br>2 Ba + $V_4O_{12}$ $\leftrightarrows$ 2 $Ba(VO_3)_2(H_2O)_4$<br>23.84 1.0<br>8 H + 4 L $\leftrightarrows$ $V_4O_{12}$ 97.19576 1.0<br>2 Ba + 8 H + 4 L $\leftrightarrows$ 2 $Ba(VO_3)_2(H_2O)_4$<br>120.99576 1.0<br>divide by 2:<br>Ba + 4 H + 2 L $\leftrightarrows$ $Ba(VO_3)_2(H_2O)_4$<br>60.49788 1.0<br>I=0: 63.13896 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
| --- | --- | --- | --- | --- |
| 3 Ba + 2 $VO_4$ ⇆ $Ba_3(VO_4)_2(H_2O)_4$ | 24.40 | 1.0 | 20 | I=0: 27.44740 |
| (several polynuclear solids for Ca Sr Ba) | | | | |

## Chromate ($CrO_4^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 6.51 | | | |
| HL + H ⇆ $H_2L$ | -0.7 | 1.0 | | HL + H ⇆ $H_2L$ -0.7 1.0<br>H + L ⇆ HL 6.10368 1.0<br>2 H + L ⇆ $H_2L$ 5.40368 1.0<br>I=0: 6.01316 |
| 2 HL ⇆ $Cr_2O_7$ | 1.52 | | | 2 HL ⇆ $Cr_2O_7$ 1.52<br>2 H + 2 L ⇆ 2 HL<br>(2*6.51) 13.02<br>2 H + 2 L ⇆ $Cr_2O_7$ 14.54 |
| K + L ⇆ KL | 0.57 | | 18 | |
| K + $Cr_2O_7$ ⇆ $KCr_2O_7$ | 0.76 | | | K + $Cr_2O_7$ ⇆ $KCr_2O_7$ 0.76<br>2 H + 2 L ⇆ $Cr_2O_7$ 14.56<br>K + 2 H + 2 L ⇆ $KCr_2O_7$ 15.32 |
| $NH_4$ + $Cr_2O_7$ ⇆ $NH_4Cr_2O_7$ | 0.88 | | | $NH_4$ + $Cr_2O_7$ ⇆ $NH_4Cr_2O_7$ 0.88<br>$NH_3$ + H ⇆ $NH_4$ 9.244<br>2 H + 2 L ⇆ $Cr_2O_7$ 14.56<br>$NH_3$ + 3 H + 2 L ⇆ $NH_4Cr_2O_7$<br>24.684 |
| Ni + L ⇆ NiL | 2.40 | | | |
| Cu(II) + L ⇆ Cu(II)L | 3.3 | | | |
| Fe(III) + L ⇆ Fe(III)L | 7.8 | | | |

## Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Na + $Cr_2O_7$ ⇆ $Na_2Cr_2O_7(H_2O)_2$ | -2.42 | | | 2 Na + $Cr_2O_7$ ⇆ $Na_2Cr_2O_7(H_2O)_2$<br>-2.42<br>2 H + 2 L ⇆ $Cr_2O_7$ 14.54<br>2 Na + 2 H + 2 L ⇆ $Na_2Cr_2O_7(H_2O)_2$<br>12.12 |
| Ba + L ⇆ BaL | 9.67 | | | |
| Cu(II) + L ⇆ Cu(II)L | 5.44 | | | |
| 3 Fe(III) + L ⇆ 6 H + $Fe(III)_3(OH)_6L$ | 18.4 | | | Charge of solid is not zero... Not entered... |
| 2 Ag + L ⇆ $Ag_2L$ | 11.59 | | | |
| Pb(II) + L ⇆ Pb(II)L | 12.60 | | | |

## Permanganate ($MnO_4^-$)

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ag + L ⇆ AgL | 9.88 | | | |

## Arsenite ($H_2AsO_3^-$)

Note: the deprotonated ligand is in fact $AsO_3^{3-}$, but this ion can not be entered as component because not all protonation constants are given in NIST. Therefore $H_2AsO_3^-$ was chosen as component.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.32 | | | |
| 2 HL ⇆ $H_2L_2$ | -0.92 | | | 2 HL ⇆ $H_2L_2$ -0.92<br>2 H + 2 L ⇆ 2 HL<br>(2*9.32) 18.64<br>2 H + 2 L ⇆ $H_2L_2$ 17.72 |
| $H_2L_2$ ⇆ $HL_2$ + H | -8.31 | 0.5 | | $H_2L_2$ ⇆ $HL_2$ + H -8.31 0.5<br>2 H + 2 L ⇆ 2 $H_2L_2$ 17.18322 0.5<br>H + 2 L ⇆ $HL_2$ 8.87322 0.5<br>I=0: 9.14161 |
| Ca + L ⇆ CaL | 1.36 | | | |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_3L$ ⇆ $(As_4O_6)_{0.25}$ | 0.69 | | | charges are not OK; personal communication with Dr. Smith: should read:<br>HL ⇆ $(As_4O_6)_{0.25}$ 0.69<br>Multiply by 4:<br>4 HL ⇆ $As_4O_6$ 2.76<br>H + L ⇆ HL<br>(4*9.32) 37.28<br>4 H + 4 L ⇆ $As_4O_6$ 40.04 |
| 3 Ag + $AsO_3^{3-}$ ⇆ $Ag_3AsO_3$ | 31.3 | 0.1 | 20 | charges are not OK; personal communication with Dr. Smith: should read:<br>3 Ag + L ⇆ $Ag_3AsO_3$ + 2 H 31.3 0.1<br>H + OH ⇆ $H_2O$<br>(2*13.99668) 27.99336 0.1<br>3 Ag + L + 2 OH ⇆ $Ag_2AsO_3$<br>59.29336 0.1<br>I=0: 59.93409 |

## Arsenate ($AsO_4^{3-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 11.54 | | | |
| H + HL ⇆ $H_2L$ | 7.00 | | | H + HL ⇆ $H_2L$ 7.00<br>H + L ⇆ HL 11.54<br>2 H + L ⇆ $H_2L$ 18.54 |
| H + $H_2L$ ⇆ $H_3L$ | 2.22 | | | H + $H_2L$ ⇆ $H_3L$ 2.22<br>2 H + L ⇆ $H_2L$ 18.54<br>3 H + L ⇆ $H_3L$ 20.76 |
| Ca + L ⇆ CaL | 4.3 | | 40 | |
| Ca + HL ⇆ CaHL | 2.75 | | 40 | Ca + HL ⇆ CaHL 2.75<br>H + L = HL 11.54<br>Ca + H + L ⇆ CaHL 14.29 |
| Ca + $H_2L$ ⇆ $CaH_2L$ | 1.39 | | 40 | Ca + $H_2L$ ⇆ $CaH_2L$ 1.39<br>2 H + L ⇆ $H_2L$ 18.54<br>Ca + 2 H + L ⇆ $CaH_2L$ 19.93 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Sc + L ⇆ ScL | 26.7 | | | |
| Y + L ⇆ YL | 22.6 | | | |
| La + L ⇆ LaL | 21.4 | | | |
| Pr + L ⇆ PrL | 22.0 | | | |
| Nd + L ⇆ NdL | 21.9 | | | |
| Sm + L ⇆ SmL | 22.7 | | | |
| Eu + L ⇆ EuL | 22.5 | | | |
| Gd + L ⇆ GdL | 21.7 | | | |
| Tb + L ⇆ TbL | 23.1 | | | |
| Dy + L ⇆ DyL | 23.8 | | | |
| Ho + L ⇆ HoL | 22.9 | | | |
| Er + L ⇆ ErL | 22.5 | | | |
| Tm + L ⇆ TmL | 23.1 | | | |
| Yb + L ⇆ YbL | 22.7 | | | |
| Lu + L ⇆ LuL | 22.7 | | | |
| 3 Ag + L ⇆ AgL | 22.2 | 0.1 | 20 | I=0: 23.48145 |

## Selenite ($SeO_3^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 8.40 | | | |
| HL + H ⇆ $H_2L$ | 2.63 | | | HL + H ⇆ $H_2L$ 2.63<br>H + L ⇆ HL 8.40<br>2 H + L ⇆ $H_2L$ 11.03 |
| Fe(III) + HL ⇆ Fe(III)HL | 2.81 | 1.0 | | Fe(III) + HL ⇆ Fe(III)HL<br>2.81 1.0<br>H + L ⇆ HL 7.99368 1.0<br>Fe(III) + H + L ⇆ Fe(III)HL<br>10.80368 1.0<br>I=0: 11.81948 |
| Ag + L ⇆ AgL | 2.4 | 1.0 | | I=0: 2.80632 |
| Ag + 2 L ⇆ $AgL_2$ | 3.76 | 1.0 | | I=0: 3.76 |
| Cd + 2 L ⇆ $CdL_2$ | 5.1 | 1.0 | | I=0: 5.91264 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 12.5 | 1.0 | | I=0: 13.31264 |

### Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Na + L ⇆ $Na_2L(H_2O)_5$ | -1.90 | | | |
| Mg + L ⇆ $MgL(H_2O)_6$ | 5.36 | | 20 | |
| Sr + L ⇆ SrL | 6.10 | | 20 | |
| Ba + L ⇆ BaL | 6.57 | | | |
| Mn(II) + L ⇆ Mn(II)L | 7.27 | | 20 | |
| Co(II) + L ⇆ Co(II)L | 7.08 | | 20 | |
| Cu(II) + L ⇆ Cu(II)L$(H_2O)_2$ | 7.78 | | 20 | |
| 2 Ag + L ⇆ $Ag_2L$ | 15.55 | | | |
| Hg(II) + L ⇆ Hg(II)L | 13.82 | 1.0 | | I=0: 14.63264 |

## Selenate ($SeO_4^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 1.70 | | | |
| Ca + L ⇆ CaL | 2.0 | | | |
| Sc + L ⇆ ScL | 1.78 | 0.5 | | I=0: 3.39033 |
| Sc + 2 L ⇆ $ScL_2$ | 2.64 | 0.5 | | I=0: 4.78711 |
| Mn(II) + L ⇆ Mn(II)L | 2.43 | | | |
| Co(II) + L ⇆ Co(II)L | 2.70 | | | |
| Ni + L ⇆ NiL | 2.67 | | | |
| Zn + L ⇆ ZnL | 2.19 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | 1.38 | 1.0 | | I=0: 2.19264 |
| Cd + L ⇆ CdL | 2.27 | | | |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Li + L ⇆ $Li_2L(H_2O)$ | -2.05 | | | |
| 2 Na + L ⇆ $Na_2L$ | -1.28 | | | |
| 2 K + L ⇆ $K_2L$ | 0.73 | | | |
| 2 Rb + L ⇆ $Rb_2L$ | 0.97 | | | |
| 2 $(NH_4)$ + L ⇆ $(NH_4)_2L$ | -0.45 | | | 2 $(NH_4)$ + L ⇆ $(NH_4)_2L$ -0.45<br>H + $NH_3$ ⇆ $NH_4$<br>(2*9.244) 18.488<br>2 H + 2 $NH_3$ +L ⇆ $(NH_4)_2L$ 18.038 |
| Be + L ⇆ $BeL(H_2O)_4$ | 2.94 | | | |
| Mg + L ⇆ $MgL(H_2O)_6$ | 1.20 | | | |
| Ca + L ⇆ $CaL(H_2O)_2$ | 3.02 | | | |
| Sr + L ⇆ SrL | 4.40 | | | |
| Ba + L ⇆ BaL | 7.46 | | | |
| $(UO_2)$ + L ⇆ $(UO_2)L(H_2O)_4$ | 2.25 | | | |
| Mn(II) + L ⇆ $Mn(II)L(H_2O)_5$ | 2.05 | | | |
| Co(II) + L ⇆ $Co(II)L(H_2O)_6$ | 1.53 | | | |
| Ni + L ⇆ $NiL(H_2O)_6$ | 1.52 | | | |
| Cu(II) + L ⇆ $Cu(II)L(H_2O)_5$ | 2.44 | | | |
| 2 Ag + L ⇆ $Ag_2L$ | 8.91 | | | |
| Zn + L ⇆ $ZnL(H_2O)_6$ | 1.52 | | | |
| Cd + L ⇆ $CdL(H_2O)_2$ | 1.85 | | | |
| Pb(II) + L ⇆ Pb(II)L | 6.84 | | | |

## Bromide ($Br^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cs + L ⇆ CsL | 0.03 | | | |
| Be + L ⇆ BeL | -0.7 | 4.0 | | I=0: -1.78352 |
| Be + 2 L ⇆ $BeL_2$ | -0.8 | 4.0 | | I=0: -2.42528 |
| Mg + L ⇆ MgL | -1.4 | 3.0 | | I=0: -1.94046 |
| Sc + L ⇆ ScL | -0.07 | 0.7 | 20 | I=0: 0.67824 |
| Sc + 2 L ⇆ $ScL_2$ | -0.3 | 0.7 | 20 | I=0: 0.94706 |
| Y + L ⇆ YL | -0.15 | 1.0 | | I=0: 0.45948 |
| Ce + L ⇆ CeL | -0.2 | 1.0 | | I=0: 0.40948 |
| Pr + L ⇆ PrL | -0.2 | 3.0 | | I=0: -1.01069 |
| Sm + L ⇆ SmL | -0.2 | 3.0 | | I=0: -1.01069 |
| Eu + L ⇆ EuL | -0.2 | 1.0 | | I=0: 0.40948 |
| Eu + 2 L ⇆ $EuL_2$ | -0.4 | 1.0 | | I=0: 0.61580 |
| Gd + L ⇆ GdL | -0.4 | 3.0 | 20 | I=0: -1.21069 |
| Tb + L ⇆ TbL | -0.4 | 3.0 | 20 | I=0: -1.21069 |
| Ho + L ⇆ HoL | -0.6 | 3.0 | | I=0: -1.41069 |
| Er + L ⇆ ErL | -0.5 | 3.0 | | I=0: -1.31069 |
| ($UO_2$) + L ⇆ ($UO_2$)L | 0.2 | | | |
| Mn(II) + L ⇆ Mn(II)L | -0.4 | 0.5 | | I=0: 0.13678 |
| Co(II) + L ⇆ Co(II)L | -0.7 | 3.0 | | I=0: -1.24046 |
| Ni + L ⇆ NiL | -0.8 | 3.0 | | I=0: -1.34046 |
| Cu(II) + L ⇆ Cu(II)L | -0.04 | | | |
| Cr(III) + L ⇆ Cr(III)L | 2.52 | | | |
| Cr(III) + 2 L ⇆ Cr(III)$L_2$ | 3.46 | | | |
| Cr(III) + 3 L ⇆ Cr(III)$L_3$ | 4.4 | | | |
| Fe(III) + L ⇆ Fe(III)L | 0.6 | | | |
| Cu(I) + L ⇆ Cu(I)L | 3.53 | | | |
| Cu(I) + 2 L ⇆ Cu(I)$L_2$ | 5.86 | | | |
| Cu(I) + 3 L ⇆ Cu(I)$L_3$ | 6.43 | | | |
| Ag + L ⇆ AgL | 4.6 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 7.5 | | | |
| Ag + 3 L ⇆ $AgL_3$ | 8.1 | | | |
| Ag + 4 L ⇆ $AgL_4$ | 8.7 | | | |
| Pd + L ⇆ PdL | 5.17 | 1.0 | | I=0: 5.57632 |
| Pd + 2 L ⇆ $PdL_2$ | 9.42 | 1.0 | | I=0: 10.02948 |
| Pd + 3 L ⇆ $PdL_3$ | 12.7 | 1.0 | | I=0: 13.30948 |
| Pd + 4 L ⇆ $PdL_4$ | 14.7 | 0.1 | | I=0: 15.12715 |
| $PdL_2$ (cis) ⇆ $PdL_2$ (trans) | -0.78 | 1.0 | | not clear how this one relates to the other one three lines up; NOT entered |
| Zn + L ⇆ ZnL | -0.07 | | | |
| Cd + L ⇆ CdL | 2.15 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 3.0 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 3.0 | | | |
| Cd + 4 L ⇆ $CdL_4$ | 2.9 | | | |
| Hg(II) + L ⇆ Hg(II)L | 9.07 | 0.5 | | I=0: 9.60678 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 17.27 | 0.5 | | I=0: 18.07516 |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 19.7 | 0.5 | | I=0: 20.50516 |
| Hg(II) + 4 L ⇆ Hg(II)$L_4$ | 21.2 | 0.5 | | I=0: 21.73678 |
| Hg(II)L ⇆ Hg(II)(OH)L + H | -3.37 | 0.5 | | Hg(II)L ⇆ Hg(II)(OH)L + H -3.37 0.5<br>Hg(II) + L ⇆ Hg(II)L 9.07 0.5<br>H + OH ⇆ $H_2O$ 13.72861 0.5<br>Hg(II) + L + OH ⇆ Hg(II)(OH)L 19.42861 0.5<br>I=0: 20.23377 |
| Sn(II) + L ⇆ Sn(II)L | 1.16 | | | |
| Sn(II) + 2 L ⇆ Sn(II)$L_2$ | 1.7 | | | |
| Sn(II) + 3 L ⇆ Sn(II)$L_3$ | 1.2 | 3.0 | | I=0: 0.38931 |
| Pb(II) + L ⇆ Pb(II)L | 1.7 | | | |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 2.6 | | | |
| Pb(II) + 3 L ⇆ Pb(II)$L_3$ | 2.2 | 0.5 | | I=0: 3.00516 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Pb(II) + 4\ L \leftrightarrows Pb(II)L_4$ | 2.4 | 2.0 | | I=0: 2.37112 |
| $Ga + L \leftrightarrows GaL$ | -0.10 | 0.7 | 20 | I=0: 0.64824 |
| $In + L \leftrightarrows InL$ | 1.99 | 2.0 | | I=0: 1.94669 |
| $In + 2\ L \leftrightarrows InL_2$ | 2.6 | 2.0 | | I=0: 2.52781 |
| $Bi + L \leftrightarrows BiL$ | 3.24 | | | |
| $Bi + 2\ L \leftrightarrows BiL_2$ | 5.5 | | | |
| $Bi + 3\ L \leftrightarrows BiL_3$ | 7.7 | | | |
| $Bi + 4\ L \leftrightarrows BiL_4$ | 9.0 | | | |
| $Bi + 5\ L \leftrightarrows BiL_5$ | 9.9 | | | |
| $Bi + 6\ L \leftrightarrows BiL_6$ | 8.7 | | | |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Cu(II)(OH)_{1.5}L_{0.5} \leftrightarrows Cu(II)(OH)_{1.5}L_{0.5}$ | 16.70 | 1.0 | | (can not be related to components; not entered) |
| $Cu(I) + L \leftrightarrows Cu(I)L$ | 8.3 | | | |
| $Ag + L \leftrightarrows AgL$ | 12.30 | | | |
| $Pb(II) + 2\ L \leftrightarrows Pb(II)L_2$ | 5.3 | | | |
| $Bi + L \leftrightarrows BiOL + 2\ H$ | 7.45 | | | $Bi + L \leftrightarrows BiOL + 2\ H$ 7.45<br>$H + OH \leftrightarrows H_2O$<br>(2*13.997) 27.996<br>$Bi + 2\ OH + L \leftrightarrows BiOL\ (+H_2O)$ 35.446 |

## Molybdate ($MoO_4^{2-}$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H + L \leftrightarrows HL$ | 3.78 | 0.1 | | I=0: 4.20715 |
| $HL + H \leftrightarrows H_2L$ | 3.77 | 0.1 | | $HL + H \leftrightarrows H_2L$ 3.77 0.1<br>$H + L \leftrightarrows HL$ 3.78 0.1<br>$2H + L \leftrightarrows H_2L$ 7.55 0.1<br>I=0: 8.19073 |
| $8H + 7L \leftrightarrows Mo_7O_{24}$ | 52.99 | 0.1 | | $8H + 7L \leftrightarrows Mo_7O_{24} + 4H_2O$<br>Note 4 $H_2O$ as product.<br>I=0: 52.99 |
| $Mo_7O_{24} + H \leftrightarrows HMo_7O_{24}$ | 5.10 | 0.1 | | $Mo_7O_{24} + H \leftrightarrows HMo_7O_{24}$ 5.10 0.1<br>$8H + 7L \leftrightarrows Mo_7O_{24}$ 52.99 0.1<br>$9H + 7L \leftrightarrows HMo_7O_{24}$ 58.09 0.1<br>I=0: 59.37145 |
| $HMo_7O_{24} + H \leftrightarrows H_2Mo_7O_{24}$ | 3.71 | 0.1 | | $HMo_7O_{24} + H \leftrightarrows H_2Mo_7O_{24}$ 3.71 0.1<br>$9H + 7L \leftrightarrows HMo_7O_{24}$ 58.09 0.1<br>$10H + 7L \leftrightarrows H_2Mo_7O_{24}$ 61.80 0.1<br>I=0: 64.14933 |
| $H_2Mo_7O_{24} + H \leftrightarrows H_3Mo_7O_{24}$ | 2.43 | 1.0 | | $H_2Mo_7O_{24} + H \leftrightarrows H_3Mo_7O_{24}$ 2.43 1.0<br>$10H + 7L \leftrightarrows H_2Mo_7O_{24}$ 61.91457 1.0<br>$11H + 7L \leftrightarrows H_3Mo_7O_{24}$ 64.34457 1.0<br>I=0: 67.39197 |
| $34H + 19L \leftrightarrows Mo_{19}O_{59}$ | 196.3 | 3.0 | | $34H + 19L \leftrightarrows Mo_{19}O_{59} + 17H_2O$<br>I=0: 183.59926 |
| $Al + 6H + 6L \leftrightarrows AlMo_6O_{21}$ | 50.95 | 0.5 | | $Al + 6H + 6L \leftrightarrows AlMo_6O_{21} + 3H_2O$<br>I=0: 54.97582 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $2H + L \leftrightarrows MoO_3$ | 8.0 | | | |
| $Mg + L \leftrightarrows MgL$ | 1.85 | | | |
| $Ca + L \leftrightarrows CaL$ | 7.95 | | | |
| $2Ag + L \leftrightarrows Ag_2L$ | 11.55 | | | |
| $Pb(II) + L \leftrightarrows Pb(II)L$ | 15.62 | | | |

## Iodide ($I^-$)

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| K + L ⇆ KL | -0.4 | | | |
| Rb + L ⇆ RbL | 0.04 | | | |
| Cs + L ⇆ CsL | -0.03 | | | |
| Eu + L ⇆ EuL | -0.4 | 1.0 | | I=0: 0.20948 |
| Hf + L ⇆ HfL | -0.5 | 3.0 | 20 | I=0: -1.58091 |
| Cu(I) + L ⇆ Cu(I)L | 5.7 | 1.0 | | I=0: 5.90316 |
| Cu(I) + 2 L ⇆ Cu(I)$L_2$ | 8.9 | | | |
| Cu(I) + 3 L ⇆ Cu(I)$L_3$ | 10.43 | 5.0 | | I=0: 10.43 |
| Cu(I) + 4 L ⇆ Cu(I)$L_4$ | 9.4 | 5.0 | | I=0: 11.04360 |
| 2 Cu(I) + 6 L ⇆ $Cu(I)_2L_6$ | 22.0 | 5.0 | | I=0: 25.28720 |
| Ag + L ⇆ AgL | 8.1 | 4.0 | | I=0: 7.55824 |
| Ag + 2 L ⇆ $AgL_2$ | 11.0 | 4.0 | | I=0: 10.45824 |
| Ag + 3 L ⇆ $AgL_3$ | 12.6 | | | |
| Ag + 4 L ⇆ $AgL_4$ | 14.2 | 2.0 | | I=0: 14.22888 |
| 2 Ag + 6 L ⇆ $Ag_2L_6$ | 29.7 | 4.0 | | I=0: 31.86704 |
| 3 Ag + 8 L ⇆ $Ag_3L_8$ | 46.4 | 4.0 | | I=0: 50.19232 |
| Pd + L ⇆ PdL | 6.08 | 1.0 | | I=0: 6.48632 |
| Pd + 2 L ⇆ $PdL_2$ | 22 | 1.0 | | I=0: 22.60948 |
| Pd + 3 L ⇆ $PdL_3$ | 25.8 | 1.0 | | I=0: 26.40948 |
| Pd + 4 L ⇆ $PdL_4$ | 28.3 | 1.0 | | I=0: 28.70632 |
| $PdL_3$ + L ⇆ $PdL_4$ | 2.56 | 1.0 | | not entered; already covered by two equilibria above this one |
| 2 $PdL_4$ ⇆ $Pd_2L_6$ + 2 L | 1.32 | 1.0 | | 2 $PdL_4$ ⇆ $Pd_2L_6$ + 2 L 1.32 1.0<br>Pd + 4 L ⇆ $PdL_4$<br>(2*28.3) 56.6 1.0<br>2 Pd + 6 L ⇆ $Pd_2L_6$ 57.92 1.0<br>I=0: 58.93580 |
| Zn + L ⇆ ZnL | -1.5 | 3.0 | | I=0: -2.04046 |
| Cd + L ⇆ CdL | 2.28 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 3.92 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 5.0 | | | |
| Cd + 4 L ⇆ $CdL_4$ | 6.0 | | | |
| Hg(II) + L ⇆ Hg(II)L | 12.87 | 0.5 | | I=0: 13.40678 |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 23.82 | 0.5 | | I=0: 24.62516 |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 27.6 | 0.5 | | I=0: 28.40516 |
| Hg(II) + 4 L ⇆ Hg(II)$L_4$ | 29.8 | 0.5 | | I=0: 30.33678 |
| Hg(II)L ⇆ Hg(II)OHL + H | -4.0 | 0.5 | | Hg(II)L ⇆ Hg(II)OHL + H<br>-4.0 0.5<br>Hg(II) + L ⇆ Hg(II)L 12.87 0.5<br>OH + H ⇆ $H_2O$ 13.72861 0.5<br>Hg(II) + OH + L ⇆ Hg(II)OHL<br>22.59861 0.5<br>I=0: 23.40377 |
| Sn(II) + L ⇆ Sn(II)L | 0.70 | 4.0 | | I=0: -0.38352 |
| Sn(II) + 2 L ⇆ Sn(II)$L_2$ | 1.13 | 4.0 | | I=0: -0.49528 |
| Sn(II) + 3 L ⇆ Sn(II)$L_3$ | 2.1 | 4.0 | | I=0: 0.47472 |
| Sn(II) + 4 L ⇆ Sn(II)$L_4$ | 2.3 | 4.0 | | I=0: 1.21648 |
| Sn(II) + 6 L ⇆ Sn(II)$L_6$ | 2.6 | 4.0 | | I=0: 4.22528 |
| Sn(II) + 8 L ⇆ Sn(II)$L_8$ | 2.1 | 4.0 | | I=0: 8.60112 |
| Pb(II) + L ⇆ Pb(II)L | 2.0 | | | |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 3.2 | | | |
| Pb(II) + 3 L ⇆ Pb(II)$L_3$ | 3.9 | | | |
| Pb(II) + 4 L ⇆ Pb(II)$L_4$ | 4.5 | | | |
| Ga + L ⇆ GaL | -0.2 | 0.7 | 20 | I=0: 0.54824 |
| In + L ⇆ InL | 0.99 | 2.0 | | I=0: 0.94669 |
| In + 2 L ⇆ $InL_2$ | 2.26 | 2.0 | | I=0: 2.18781 |
| Bi + L ⇆ BiL | 3.63 | 0.5 | | I=0: 4.43516 |
| Bi + 4 L ⇆ $BiL_4$ | 15.0 | 2.0 | 20 | I=0: 14.91337 |
| Bi + 5 L ⇆ $BiL_5$ | 16.8 | 2.0 | | I=0: 16.72781 |
| Bi + 6 L ⇆ $BiL_6$ | 18.8 | 2.0 | | I=0: 18.75669 |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cu(I) + L ⇆ Cu(I)L | 12.0 | | | |
| Ag + L ⇆ AgL | 16.08 | | | |
| Pd + 2 L ⇆ $PdL_2$ | 31.15 | 1.0 | | I=0: 31.75948 |
| Hg(II) + 2 L ⇆ $Hg(II)L_2$ | 27.95 | 0.5 | | I=0: 28.75516 |
| Sn(II) + 2 L ⇆ $Sn(II)L_2$ | 5.08 | 4.0 | | I=0: 3.45472 |
| Pb(II) + 2 L ⇆ $Pb(II)L_2$ | 8.10 | | | |
| Bi + 3 L ⇆ $BiL_3$ | 18.09 | 2.0 | 20 | I=0: 18.00337 |

## Tungstate ($WO_4^{2-}$)

NOTE: polynuclear complexes have NOT been entered because they are not likely to occur in significant concentrations at ambient W-levels.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 3.6 | | | |
| 2 H + L ⇆ $H_2L$ | 5.8 | | | |

Solids:

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 H + L ⇆ $WO_3$ | 14.05 | | | |
| 2 Ag + L ⇆ $Ag_2L$ | 12.12 | | | |
| Pb(II) + L ⇆ Pb(II)L | 16.07 | | | |

## Cyanide ($CN^-$)

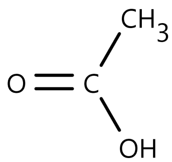
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.21 | | | |
| Mn(II) + L ⇆ Mn(II)L | 1.9 | 1.0 | | I=0: 2.30632 |
| Mn(II) + 2 L ⇆ Mn(II)$L_2$ | 3.36 | 1.0 | | I=0: 3.96948 |
| Fe(II) + 6 L ⇆ Fe(II)$L_6$ | 35.4 | | | |
| Co(II) + 3 L ⇆ Co(II)$L_3$ | 13.7 | 1.0 | | I=0: 14.30948 |
| Co(II) + 5 L ⇆ Co(II)$L_5$ | 23.0 | 1.0 | | I=0: 23.0 |
| Ni + 4 L ⇆ $NiL_4$ | 30.2 | | | |
| $NiL_4$ + H ⇆ $NiHL_4$ | 5.4 | 0.1 | | $NiL_4$ + H ⇆ $NiHL_4$ 5.4 0.1<br>Ni + 4 L ⇆ $NiL_4$ 29.77285 0.1<br>Ni + H + 4 L ⇆ $NiHL_4$ 35.17285 0.1<br>I=0: 36.02715 |
| $NiHL_4$ + H ⇆ $NiH_2L_4$ | 4.5 | 0.1 | | $NiHL_4$ + H ⇆ $NiH_2L_4$ 4.5 0.1<br>Ni + H + 4 L ⇆ $NiHL_4$ 35.17285 0.1<br>Ni + 2 H + 4 L ⇆ $NiH_2L_4$ 39.67285 0.1<br>I=0: 40.74073 |
| $NiH_2L_4$ + H ⇆ $NiH_3L_4$ | 2.6 | 0.1 | | $NiH_2L_4$ + H ⇆ $NiH_3L_4$ 2.6 0.1<br>Ni + 2 H + 4 L ⇆ $NiH_2L_4$ 39.67285 0.1<br>Ni + 3 H + 4 L ⇆ $NiH_3L_4$ 42.27285 0.1<br>I=0: 43.34073 |
| Fe(III) + 6 L ⇆ Fe(III)$L_6$ | 43.6 | | | |
| Cu(I) + 2 L ⇆ Cu(I)$L_2$ | 23.9 | | | |
| Cu(I)$L_2$ + L ⇆ Cu(I)$L_3$ | 5.30 | | | Cu(I)$L_2$ + L ⇆ Cu(I)$L_3$ 5.30<br>Cu(I) + 2 L ⇆ Cu(I)$L_2$ 23.9<br>Cu(I) + 3 L ⇆ Cu(I)$L_3$ 29.2 |
| Cu(I)$L_3$ + L ⇆ Cu(I)$L_4$ | 1.6 | | | Cu(I)$L_3$ + L ⇆ Cu(I)$L_4$ 1.6<br>Cu(I) + 3 L ⇆ Cu(I)$L_3$ 29.2<br>Cu(I) + 4 L ⇆ Cu(I)$L_4$ 30.8 |
| Ag + 2 L ⇆ $AgL_2$ | 20.48 | | | |
| Ag + 3 L ⇆ $AgL_3$ | 21.7 | | | |
| Ag + OH + L ⇆ AgOHL | 13.22 | | | |
| Pd + 4 L ⇆ $PdL_4$ | 42.4 | | | |
| Pd + 5 L ⇆ $PdL_5$ | 45.3 | | | |
| Zn + L ⇆ ZnL | 4.98<br>5.26 | 3.0 | | 4.98 with NaCl-background electrolyte; 5.26 with $NaClO_4$-background electrolyte; used: average (5.12)<br>I=0: 4.57954 |
| Zn + 2 L ⇆ $ZnL_2$ | 11.07 | | | |
| Zn + 3 L ⇆ $ZnL_3$ | 16.05 | | | |
| Zn + 4 L ⇆ $ZnL_4$ | 19.62 | | | |
| Cd + L ⇆ CdL | 6.01 | | | |
| Cd + 2 L ⇆ $CdL_2$ | 11.12 | | | |
| Cd + 3 L ⇆ $CdL_3$ | 15.65 | | | |
| Cd + 4 L ⇆ $CdL_4$ | 17.92 | | | |
| Hg(II) + L ⇆ Hg(II)L | 17.00 | | | |
| Hg(II) + 2 L ⇆ Hg(II)$L_2$ | 32.75 | | | |
| Hg(II) + 3 L ⇆ Hg(II)$L_3$ | 36.31 | | | |
| Hg(II) + 4 L ⇆ Hg(II)$L_4$ | 38.97 | | | |
| Hg(II) + OH + L ⇆ Hg(II)OHL | 28.9 | 2.0 | 30 | I=0: 28.85669 |

### Solids:

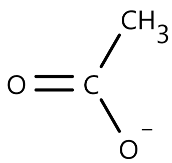
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cu(I) + L ⇆ Cu(I)L | 19.5 | | | |
| Ag + L ⇆ AgL | 15.74 | | | |
| 2 Ag + 2 L ⇆ $Ag_2L_2$ | 10.9 | 0.1 | 20 | This solid is better soluble than the one above and therefore not entered. |
| Zn + 2 L ⇆ $ZnL_2$ | 15.5 | 3.0 | | I=0: 14.68931 |

## Acetate

The ligand in its neutral form is acetic acid (ethanoic acid), $C_2H_4O_2$.



The ligand as it is present in the database is acetate, $C_2H_3O_2^-$.



| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 4.757 | | | |
| Li + L ⇆ LiL | 0.28 | | | |
| Na + L ⇆ NaL | -0.12 | | | |
| K + L ⇆ KL | -0.27 | | | |
| Rb + L ⇆ RbL | -0.37 | 0.1 | | I=0: -0.15642 |
| Cs + L ⇆ CsL | -0.33 | 0.1 | | I=0: -0.11642 |
| Be + L ⇆ BeL | 1.62 | 0.1 | | I=0: 2.04715 |
| Be + 2 L ⇆ $BeL_2$ | 2.36 | 0.1 | | I=0: 3.00073 |
| Mg + L ⇆ MgL | 1.26 | | | |
| Ca + L ⇆ CaL | 1.18 | | | |
| Sr + L ⇆ SrL | 1.12 | | | |
| Ba + L ⇆ BaL | 1.07 | | | |
| Sc + L ⇆ ScL | 3.48 | 0.1 | | I=0: 4.12073 |
| Y + L ⇆ YL | 1.68 | 0.1 | | I=0: 2.32073 |
| Y + 2 L ⇆ $YL_2$ | 3.17 | 0.1 | | I=0: 4.23788 |
| Y + 3 L ⇆ $YL_3$ | 3.5 | 2.0 | | I=0: 3.41337 |
| La + L ⇆ LaL | 2.55 | | | |
| La + 2 L ⇆ $LaL_2$ | 4.12 | | | |
| La + 3 L ⇆ $LaL_3$ | 3.53 | 0.1 | | I=0: 4.81145 |
| Ce + L ⇆ CeL | 1.91 | 0.1 | | I=0: 2.55073 |
| Ce + 2 L ⇆ $CeL_2$ | 3.09 | 0.1 | | I=0: 4.15788 |
| Ce + 3 L ⇆ $CeL_3$ | 3.68 | 0.1 | | I=0: 4.96145 |
| Pr + L ⇆ PrL | 2.01 | 0.1 | | I=0: 2.65073 |
| Pr + 2 L ⇆ $PrL_2$ | 3.41 | 0.1 | | I=0: 4.47788 |
| Pr + 3 L ⇆ $PrL_3$ | 3.33 | 2.0 | | I=0: 3.24337 |
| Nd + L ⇆ NdL | 2.67 | | | |
| Nd + 2 L ⇆ $NdL_2$ | 4.54 | | | |
| Nd + 3 L ⇆ $NdL_3$ | 3.60 | 2.0 | | I=0: 3.51337 |
| Sm + L ⇆ SmL | 2.84 | | | |
| Sm + 2 L ⇆ $SmL_2$ | 4.80 | | | |
| Sm + 3 L ⇆ $SmL_3$ | 3.90 | 2.0 | | I=0: 3.81337 |
| Eu + L ⇆ EuL | 2.13 | 0.1 | | I=0: 2.77073 |
| Eu + 2 L ⇆ $EuL_2$ | 3.64 | 0.1 | | I=0: 4.70788 |
| Eu + 3 L ⇆ $EuL_3$ | 4.24 | 0.1 | | I=0: 5.52145 |
| Gd + L ⇆ GdL | 2.02 | 0.1 | | I=0: 2.66073 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Gd + 2 L ⇆ $GdL_2$ | 3.47 | 0.1 | | I=0: 4.53788 |
| Gd + 3 L ⇆ $GdL_3$ | 4.26 | 0.1 | | I=0: 5.54145 |
| Tb + L ⇆ TbL | 1.91 | 0.1 | | I=0: 2.55073 |
| Tb + 2 L ⇆ $TbL_2$ | 3.23 | 0.1 | | I=0: 4.29788 |
| Tb + 3 L ⇆ $TbL_3$ | 4.39 | 0.1 | | I=0: 5.67145 |
| Dy + L ⇆ DyL | 1.85 | 0.1 | | I=0: 2.49073 |
| Dy + 2 L ⇆ $DyL_2$ | 3.16 | 0.1 | | I=0: 4.22788 |
| Dy + 3 L ⇆ $DyL_3$ | 4.30 | 0.1 | | I=0: 5.58145 |
| Dy + 4 L ⇆ $DyL_4$ | 3.9 | 2.0 | 20 | I=0: 3.81337 |
| Ho + L ⇆ HoL | 1.81 | 0.1 | | I=0: 2.45073 |
| Ho + 2 L ⇆ $HoL_2$ | 3.11 | 0.1 | | I=0: 4.17788 |
| Ho + 3 L ⇆ $HoL_3$ | 4.27 | 0.1 | | I=0: 5.55145 |
| Er + L ⇆ ErL | 1.79 | 0.1 | | I=0: 2.43073 |
| Er + 2 L ⇆ $ErL_2$ | 3.06 | 0.1 | | I=0: 4.12788 |
| Er + 3 L ⇆ $ErL_3$ | 4.20 | 0.1 | | I=0: 5.48145 |
| Er + 4 L ⇆ $ErL_4$ | 3.7 | 2.0 | 20 | I=0: 3.61337 |
| Tm + L ⇆ TmL | 1.83 | 0.1 | | I=0: 2.47073 |
| Tm + 2 L ⇆ $TmL_2$ | 3.02 | 0.1 | | I=0: 4.08788 |
| Tm + 3 L ⇆ $TmL_3$ | 4.17 | 0.1 | | I=0: 5.45145 |
| Yb + L ⇆ YbL | 2.56 | | | |
| Yb + 2 L ⇆ $YbL_2$ | 4.36 | | | |
| Yb + 3 L ⇆ $YbL_3$ | 4.15 | 0.1 | | I=0: 5.43145 |
| Lu + L ⇆ LuL | 1.85 | 0.1 | | I=0: 2.49073 |
| Lu + 2 L ⇆ $LuL_2$ | 3.16 | 0.1 | | I=0: 4.22788 |
| Lu + 3 L ⇆ $LuL_3$ | 4.02 | 0.1 | | I=0: 5.30145 |
| (U(VI)$O_2$) + L ⇆ (U(VI)$O_2$)L | 2.68 | 0.1 | | I=0: 3.10715 |
| (U(VI)$O_2$) + 2 L ⇆ (U(VI)$O_2$)$L_2$ | 4.43 | 1.0 | | I=0: 5.03948 |
| (U(VI)$O_2$) + 3 L ⇆ (U(VI)$O_2$)$L_3$ | 6.45 | 1.0 | | I=0: 7.05948 |
| Mn(II) + L ⇆ Mn(II)L | 1.40 | | | |
| Fe(II) + L ⇆ Fe(II)L | 0.54 | 3.0 | | I=0: -0.00046 |
| Co(II) + L ⇆ Co(II)L | 1.38 | | | |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | 0.8 | 2.0 | | I=0: 0.75669 |
| Ni + L ⇆ NiL | 1.44 | | | |
| Ni + 2 L ⇆ $NiL_2$ | 2.40 | | | |
| Cu(II) + L ⇆ Cu(II)L | 2.21 | | | |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | 3.4 | | | |
| Cu(II) + 3 L ⇆ Cu(II)$L_3$ | 3.3 | 0.1 | | I=0: 3.94073 |
| Cr(III) + L ⇆ Cr(III)L | 4.63 | 0.5 | | I=0: 5.43516 |
| Cr(III) + 2 L ⇆ Cr(III)$L_2$ | 7.08 | 0.5 | | I=0: 8.42194 |
| Cr(III) + 3 L ⇆ Cr(III)$L_3$ | 9.6 | 0.5 | | I=0: 11.21033 |
| Fe(III) + L ⇆ Fe(III)L | 3.6 | 0.1 | | I=0: 4.24073 |
| Fe(III) + 2 L ⇆ Fe(III)$L_2$ | 6.5 | 0.1 | | I=0: 7.56788 |
| 3 Fe(III) + 6 L ⇆<br>Fe(III)$_3$(OH)$_2$$L_6$ + 2 H | 20.0 | 1.0 | | 3 Fe(III) + 6 L ⇆ Fe(III)$_3$(OH)$_2$$L_6$ + 2 H<br>20.0 1<br>OH + H ⇆ $H_2O$<br>(2*13.79384) 27.58768 1<br>3 Fe(III) + 2 OH + 6 L ⇆<br>Fe(III)$_3$(OH)$_2$$L_6$ 47.58768 1<br>I=0: 51.04140 |
| 3 Fe(III) + 2 L ⇆<br>Fe(III)$_3$(OH)$_3$$L_2$ + 3 H | 5.87 | 3.0 | | 3 Fe(III) + 2 L ⇆ Fe(III)$_3$(OH)$_3$$L_2$ + 3 H<br>5.87 3<br>OH + H ⇆ $H_2O$<br>(3*14.26723) 42.80169 3<br>3 Fe(III) + 3 OH + 2 L ⇆<br>Fe(III)$_3$(OH)$_3$$L_2$ 48.67169 3<br>I=0: 46.50986 |
| 7 Fe(III) + 6 L ⇆<br>Fe(III)$_7$(OH)$_9$$L_6$ + 9 H | 17.26 | 3.0 | | 7 Fe(III) + 6 L ⇆ Fe(III)$_7$(OH)$_9$$L_6$ + 9 H<br>17.26 3<br>OH + H ⇆ $H_2O$<br>(9*14.26723) 128.40507 3<br>7 Fe(III) + 9 OH + 6 L ⇆<br>Fe(III)$_7$(OH)$_9$$L_6$ 145.66507 3<br>I=0: 139.99027 |
| Ag + L ⇆ AgL | 0.73 | | | |
| Ag + 2 L ⇆ $AgL_2$ | 0.64 | | | |

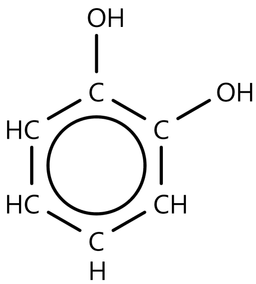
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pd + L $\leftrightarrows$ PdL | 4.34 | 1.0 | | I=0: 4.74632 |
| Zn + L $\leftrightarrows$ ZnL | 1.57 | | | |
| Zn + 2 L $\leftrightarrows$ $ZnL_2$ | 1.1 | 0.5 | | I=0: 1.90516 |
| Zn + 3 L $\leftrightarrows$ $ZnL_3$ | 1.57 | 3.0 | | I=0: 0.75931 |
| Cd + L $\leftrightarrows$ CdL | 1.92 | | | |
| Cd + 2 L $\leftrightarrows$ $CdL_2$ | 1.91 | 0.5 | | I=0: 2.71516 |
| Cd + 3 L $\leftrightarrows$ $CdL_3$ | 2.18 | 0.5 | | I=0: 2.98516 |
| Hg(II) + L $\leftrightarrows$ Hg(II)L | 4.3 | | | |
| Hg(II) + 2 L $\leftrightarrows$ Hg(II)$L_2$ | 8.45 | 3.0 | | I=0: 7.63931 |
| Sn(II) + L $\leftrightarrows$ Sn(II)L | 3.47 | 3.0 | | I=0: 2.92954 |
| Sn(II) + 2 L $\leftrightarrows$ Sn(II)$L_2$ | 6.04 | 3.0 | | I=0: 5.22931 |
| Sn(II) + 3 L $\leftrightarrows$ Sn(II)$L_3$ | 7.27 | 3.0 | | I=0: 6.45931 |
| Pb(II) + L $\leftrightarrows$ Pb(II)L | 2.58 | | | |
| Pb(II) + 2 L $\leftrightarrows$ Pb(II)$L_2$ | 4.02 | | | |
| Pb(II) + 3 L $\leftrightarrows$ Pb(II)$L_3$ | 3.42 | 2.0 | | I=0: 3.37669 |
| $B(OH)_3$ + L $\leftrightarrows$ $B(OH)_3L$ | -0.43 | | | $B(OH)_3$ + L $\leftrightarrows$ $B(OH)_3L$<br>$B(OH)_3$ does not occur as a component in the database, but $H_2BO_3^-$ does.<br>H + $H_2BO_3$ $\leftrightarrows$ $H_3BO_3$ (=$B(OH)_3$) 9.236<br>$B(OH)_3$ + L $\leftrightarrows$ $B(OH)_3L$ -0.43<br>H + $H_2BO_3$ + L $\leftrightarrows$ $B(OH)_3L$ 8.806 |
| Al + L $\leftrightarrows$ AlL | 2.75 | | | |
| Al + 2 L $\leftrightarrows$ $AlL_2$ | 4.6 | | | |
| AlL $\leftrightarrows$ AlOHL + H | -3.1 | 1.0 | | AlL $\leftrightarrows$ AlOHL + H -3.1 1.0<br>Al + L $\leftrightarrows$ AlL 2.14052 1.0<br>OH + H $\leftrightarrows$ $H_2O$ 13.79384 1.0<br>Al + L + OH $\leftrightarrows$ AlOHL 12.83436 1.0<br>I=0: 13.85016 |
| 2 Al + L $\leftrightarrows$ $Al_2(OH)_2L$ + 2 H | -3.49 | 0.5 | | 2 Al + L $\leftrightarrows$ $Al_2(OH)_2L$ + 2 H -3.49 0.5<br>2 OH + 2 H $\leftrightarrows$ 2 $H_2O$ (2*13.72861) 27.45722 0.5<br>2 Al + L + 2 OH $\leftrightarrows$ $Al_2(OH)_2L$ 23.96722 0.5<br>I=0: 25.57755 |
| In + L $\leftrightarrows$ InL | 3.50 | 2.0 | 20 | I=0: 3.45669 |
| In + 2 L $\leftrightarrows$ $InL_2$ | 5.95 | 2.0 | 20 | I=0: 5.87781 |
| In + 3 L $\leftrightarrows$ $InL_3$ | 7.90 | 2.0 | 20 | I=0: 7.81337 |
| In + 4 L $\leftrightarrows$ $InL_4$ | 9.08 | 2.0 | 20 | I=0: 8.99337 |

Solids:

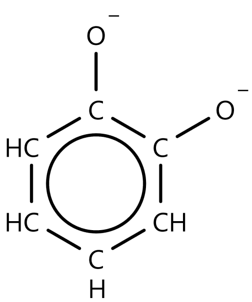
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Ag + L $\leftrightarrows$ AgL | 2.71 | | | |

Catechol

The ligand in its neutral form is 1,2-dihydroxybenzene or catechol, $C_6H_6O_2$.




The ligand as it is present in the database is $C_2H_4O_2^{2-}$.




| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H + L \leftrightarrows HL$ | 13.3 | 0.1 | | I=0: 13.72715 |
| $HL + H \leftrightarrows H_2L$ | 9.45 | | | $HL + H \leftrightarrows H_2L$ 9.45<br>$H + L \leftrightarrows HL$ 13.72715<br>$2H + L \leftrightarrows H_2L$ 23.17715 |
| $Be + H_2L \leftrightarrows BeL + 2H$ | -9.55 | 0.1 | 20 | $Be + H_2L \leftrightarrows BeL + 2H$ -9.55 0.1<br>$2H + L \leftrightarrows H_2L$ 22.53642 0.1<br>$Be + L \leftrightarrows BeL$ 12.98642 0.1<br>I=0: 13.84072 |
| $BeL + H_2L \leftrightarrows BeL_2 + 2H$ | -13.06 | 0.1 | 20 | $BeL + H_2L \leftrightarrows BeL_2 + 2H$ -13.06 0.1<br>$Be + L \leftrightarrows BeL$ 12.98642 0.1<br>$2H + L \leftrightarrows H_2L$ 22.53642 0.1<br>$Be + 2L \leftrightarrows BeL_2$ 22.46284 0.1<br>I=0: 23.31714 |
| $BeL + H \leftrightarrows BeHL$ | 5.16 | 0.1 | 20 | $BeL + H \leftrightarrows BeHL$ 5.16 0.1<br>$Be + L \leftrightarrows BeL$ 12.98642 0.1<br>$Be + H + L \leftrightarrows BeHL$ 18.14642 0.1<br>I=0: 19.00072 |
| $BeL_2 + H \leftrightarrows BeHL_2$ | 6.69 | 0.1 | 20 | $BeL_2 + H \leftrightarrows BeHL_2$ 6.69 0.1<br>$Be + 2L \leftrightarrows BeL_2$ 22.46284 0.1<br>$Be + H + 2L \leftrightarrows BeHL_2$ 29.15284 0.1<br>I=0: 30.43429 |
| $Sc + H_2L \leftrightarrows ScL + 2H$ | -4.90 | 0.1 | | $Sc + H_2L \leftrightarrows ScL + 2H$ -4.90 0.1<br>$2H + L \leftrightarrows H_2L$ 22.53642 0.1<br>$Sc + L \leftrightarrows ScL$ 17.63642 0.1<br>I=0: 18.91787 |
| $La + H_2L \leftrightarrows LaL + 2H$ | -12.48 | 0.1 | | $La + H_2L \leftrightarrows LaL + 2H$ -12.48 0.1<br>$2H + L \leftrightarrows H_2L$ 22.53642 0.1<br>$La + L \leftrightarrows LaL$ 10.05642 0.1<br>I=0: 11.33787 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pr + $H_2L$ ⇆ PrL + 2 H | -11.63 | 0.1 | | Pr + $H_2L$ ⇆ PrL + 2 H -11.63 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Pr + L ⇆ PrL 10.90642 0.1<br>I=0: 12.18787 |
| Nd + $H_2L$ ⇆ NdL + 2 H | -11.44 | 0.1 | | Nd + $H_2L$ ⇆ NdL + 2 H -11.44 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Nd + L ⇆ NdL 11.09642 0.1<br>I=0: 12.37787 |
| Sm + $H_2L$ ⇆ SmL + 2 H | -10.44 | 0.1 | | Sm + $H_2L$ ⇆ SmL + 2 H -10.44 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Sm + L ⇆ SmL 12.09642 0.1<br>I=0: 13.37787 |
| Eu + $H_2L$ ⇆ EuL + 2 H | -10.88 | 0.1 | | Eu + $H_2L$ ⇆ EuL + 2 H -10.88 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Eu + L ⇆ EuL 11.65642 0.1<br>I=0: 12.93787 |
| Gd + $H_2L$ ⇆ GdL + 2 H | -10.74 | 0.1 | | Gd + $H_2L$ ⇆ GdL + 2 H -10.74 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Gd + L ⇆ GdL 11.79642 0.1<br>I=0: 13.07787 |
| Dy + $H_2L$ ⇆ DyL + 2 H | -10.60 | 0.1 | | Dy + $H_2L$ ⇆ DyL + 2 H -10.60 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Dy + L ⇆ DyL 11.93642 0.1<br>I=0: 13.21787 |
| Ho + $H_2L$ ⇆ HoL + 2 H | -10.52 | 0.1 | | Ho + $H_2L$ ⇆ HoL + 2 H -10.52 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Ho + L ⇆ HoL 12.01642 0.1<br>I=0: 13.29787 |
| Er + $H_2L$ ⇆ ErL + 2 H | -10.51 | 0.1 | | Er + $H_2L$ ⇆ ErL + 2 H -10.51 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Er + L ⇆ ErL 12.02642 0.1<br>I=0: 13.30787 |
| Tm + $H_2L$ ⇆ TmL + 2 H | -10.38 | 0.1 | | Tm + $H_2L$ ⇆ TmL + 2 H -10.38 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Tm + L ⇆ TmL 12.15642 0.1<br>I=0: 13.43787 |
| Yb + $H_2L$ ⇆ YbL + 2 H | -10.27 | 0.1 | | Yb + $H_2L$ ⇆ YbL + 2 H -10.27 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Yb + L ⇆ YbL 12.26642 0.1<br>I=0: 13.54787 |
| Lu + $H_2L$ ⇆ LuL + 2 H | -10.63 | 0.1 | | Lu + $H_2L$ ⇆ LuL + 2 H -10.63 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Lu + L ⇆ LuL 11.90642 0.1<br>I=0: 13.18787 |
| $(UO_2)$ + $H_2L$ ⇆ $(UO_2)L$ + 2 H | -7.14 | 0.1 | 20 | $(UO_2)$ + $H_2L$ ⇆ $(UO_2)L$ + 2 H<br>-7.14 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>$(UO_2)$ + L ⇆ $(UO_2)L$ 15.39642 0.1<br>I=0: 16.25072 |
| $(UO_2)L$ + H ⇆ $(UO_2)HL$ | 3.93 | 0.1 | 20 | $(UO_2)L$ + H ⇆ $(UO_2)HL$ 3.93 0.1<br>$(UO_2)$ + L ⇆ $(UO_2)L$ 15.39642 0.1<br>$(UO_2)$ + H + L ⇆ $(UO_2)HL$ 19.32642 0.1<br>I=0: 20.18072 |
| $(UO_2)L$ + $H_2L$ ⇆ $(UO_2)HL_2$ + H | -4.38 | 0.1 | 20 | $(UO_2)L$ + $H_2L$ ⇆ $(UO_2)HL_2$ + H<br>-4.38 0.1<br>$(UO_2)$ + L ⇆ $(UO_2)L$ 15.39642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>$(UO_2)$ + 2 L + H ⇆ $(UO_2)HL_2$<br>33.55284 0.1<br>I=0: 34.83429 |
| $(UO_2)HL_2$ + $H_2L$ ⇆ $(UO_2)H_2L_3$ + H | -5.60 | 0.1 | 20 | $(UO_2)HL_2$ + $H_2L$ ⇆ $(UO_2)H_2L_3$ + H<br>-5.60 0.1<br>$(UO_2)$ + 2 L + H ⇆ $(UO_2)HL_2$<br>33.55284 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>$(UO_2)$ + 3 L + 2 H ⇆ $(UO_2)H_2L_3$<br>50.48926 0.1<br>I=0: 51.98429 |

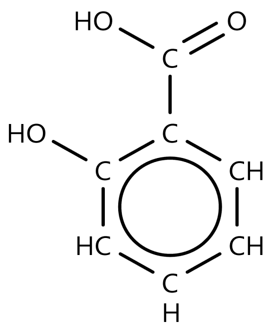
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Mn(II) + $H_2L$ ⇆ Mn(II)L + 2 H | -14.70 | 0.1 | | Mn(II) + $H_2L$ ⇆ Mn(II)L + 2 H<br>-14.70 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Mn(II) + L ⇆ Mn(II)L 7.83642 0.1<br>I=0: 8.69072 |
| Mn(II)L + $H_2L$ ⇆ Mn(II)$L_2$ + 2 H | -17.1 | 0.1 | | Mn(II)L + $H_2L$ ⇆ Mn(II)$L_2$ + 2 H<br>-17.1 0.1<br>Mn(II) + L ⇆ Mn(II)L 7.83642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Mn(II) + 2 L ⇆ Mn(II)$L_2$<br>13.27284 0.1<br>I=0: 14.12714 |
| Fe(II) + $H_2L$ ⇆ Fe(II)L + 2 H | -14.3 | 0.1 | | Fe(II) + $H_2L$ ⇆ Fe(II)L + 2 H<br>-14.3 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Fe(II) + L ⇆ Fe(II)L 8.23642 0.1<br>I=0: 9.09072 |
| Fe(II)L + $H_2L$ ⇆ Fe(II)$L_2$ + 2 H | -16.7 | 1.0 | | Fe(II)L + $H_2L$ ⇆ Fe(II)$L_2$ + 2 H<br>-16.7 1.0<br>Fe(II) + L ⇆ Fe(II)L 8.27808 1.0<br>2 H + L ⇆ $H_2L$ 22.56767 1.0<br>Fe(II) + 2 L ⇆ Fe(II)$L_2$<br>14.14575 1.0<br>I=0: 14.95839 |
| 2 Fe(II) + 2 HL ⇆ Fe(II)$_2$H$L_2$ + H | 10.9 | 0.1 | | 2 Fe(II) + 2 HL ⇆ Fe(II)$_2$H$L_2$ + H<br>10.9 0.1<br>2 H + 2 L ⇆ 2HL<br>(2*13.3) 26.6 0.1<br>2 Fe(II) + 2 H + 2 L ⇆ Fe(II)$_2$H$L_2$<br>37.5 0.1<br>I=0: 39.20860 |
| Co(II) + $H_2L$ ⇆ Co(II)L + 2 H | -13.72 | 0.1 | | Co(II) + $H_2L$ ⇆ Co(II)L + 2 H<br>-13.72 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Co(II) + L ⇆ Co(II)L 8.81642 0.1<br>I=0: 9.67072 |
| Co(II)L + $H_2L$ ⇆ Co(II)$L_2$ + 2 H | -16.1 | 0.1 | | Co(II)L + $H_2L$ ⇆ Co(II)$L_2$ + 2 H<br>-16.1 0.1<br>Co(II) + L ⇆ Co(II)L 8.81642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Co(II) + 2 L ⇆ Co(II)$L_2$ 15.25284 0.1<br>I=0: 16.10714 |
| Ni + $H_2L$ ⇆ NiL + 2 H | -13.33 | 0.1 | | Ni + $H_2L$ ⇆ NiL + 2 H -13.33 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Ni + L ⇆ NiL 9.20642 0.1<br>I=0: 10.06072 |
| NiL + $H_2L$ ⇆ Ni$L_2$ + 2 H | -16.4 | 0.1 | | NiL + $H_2L$ ⇆ Ni$L_2$ + 2 H -16.4 0.1<br>Ni + L ⇆ NiL 9.20642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Ni + 2 L ⇆ Ni$L_2$ 15.34284 0.1<br>I=0: 16.19714 |
| Cu(II) + $H_2L$ ⇆ Cu(II)L + 2 H | -8.10 | | | Cu(II) + $H_2L$ ⇆ Cu(II)L + 2 H<br>-8.10<br>2 H + L ⇆ $H_2L$ 23.17715<br>Cu(II) + L ⇆ Cu(II)L 15.07715 |
| Cu(II)L + $H_2L$ ⇆ Cu(II)$L_2$ + 2 H | -11.75 | | | Cu(II)L + $H_2L$ ⇆ Cu(II)$L_2$ + 2 H<br>-11.75<br>Cu(II) + L ⇆ Cu(II)L 15.07715<br>2 H + L ⇆ $H_2L$ 23.17715<br>Cu(II) + 2 L ⇆ Cu(II)$L_2$ 26.50430 |
| Cu(II)L + H ⇆ Cu(II)HL | 0.85 | 0.1 | | Cu(II)L + H ⇆ Cu(II)HL 0.85 0.1<br>Cu(II) + L ⇆ Cu(II)L 14.22285 0.1<br>Cu(II) + L + H ⇆ Cu(II)HL<br>15.07285 0.1<br>I=0: 15.92715 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Fe(III) + $H_2L$ ⇆ Fe(III)L + 2 H | -2.2 | 0.1 | | Fe(III) + $H_2L$ ⇆ Fe(III)L + 2 H<br>-2.2 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Fe(III) + L ⇆ Fe(III)L 20.33642 0.1<br>I=0: 21.61787 |
| Fe(III)L + $H_2L$ ⇆ Fe(III)$L_2$ + 2 H | -7.53 | 0.1 | | Fe(III)L + $H_2L$ ⇆ Fe(III)$L_2$ + 2 H<br>-7.53 0.1<br>Fe(III) + L ⇆ Fe(III)L 20.33642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Fe(III) + 2 L ⇆ Fe(III)$L_2$<br>35.34284 0.1<br>I=0: 37.05144 |
| Fe(III)$L_2$ + $H_2L$ ⇆ Fe(III)$L_3$ + 2 H | -13.16 | 0.1 | | Fe(III)$L_2$ + $H_2L$ ⇆ Fe(III)$L_3$ + 2 H<br>-13.16 0.1<br>Fe(III) + 2 L ⇆ Fe(III)$L_2$<br>35.34284 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Fe(III) + 3 L ⇆ Fe(III)$L_3$<br>44.71926 0.1<br>I=0: 46.00071 |
| Pd + $H_2L$ ⇆ PdL + 2 H | -2.22 | 0.1 | | Pd + $H_2L$ ⇆ PdL + 2 H -2.22 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Pd + L ⇆ PdL 20.31642 0.1<br>I=0: 21.17072 |
| Zn + $H_2L$ ⇆ ZnL + 2 H | -12.5 | 0.1 | | Zn + $H_2L$ ⇆ ZnL + 2 H -12.5 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Zn + L ⇆ ZnL 10.03642 0.1<br>I=0: 10.89072 |
| ZnL + $H_2L$ ⇆ $ZnL_2$ + 2 H | -14.5 | 0.1 | | ZnL + $H_2L$ ⇆ $ZnL_2$ + 2 H -14.5 0.1<br>Zn + L ⇆ ZnL 10.03642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Zn + 2 L ⇆ $ZnL_2$ 18.07284 0.1<br>I=0: 18.92714 |
| Cd + $H_2L$ ⇆ CdL + 2 H | -13.7 | 0.1 | 30 | Cd + $H_2L$ ⇆ CdL + 2 H -13.7 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Cd + L ⇆ CdL 8.83642 0.1<br>I=0: 9.69072 |
| two complexes with B(III) | | | | (not entered) |
| Al + $H_2L$ ⇆ AlL + 2 H | -6.08 | 0.1 | | Al + $H_2L$ ⇆ AlL + 2 H -6.08 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Al + L ⇆ AlL 16.45642 0.1<br>I=0: 17.73787 |
| AlL + $H_2L$ ⇆ $AlL_2$ + 2 H | -9.20 | 0.1 | | AlL + $H_2L$ ⇆ $AlL_2$ + 2 H -9.20 0.1<br>Al + L ⇆ AlL 16.45642 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Al + 2 L ⇆ $AlL_2$ 29.79284 0.1<br>I=0: 31.50144 |
| $AlL_2$ + $H_2L$ ⇆ $AlL_3$ + 2 H | -13.56 | 0.1 | | $AlL_2$ + $H_2L$ ⇆ $AlL_3$ + 2 H -13.56 0.1<br>Al + 2 L ⇆ $AlL_2$ 29.79284 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Al + 3 L ⇆ $AlL_3$ 38.76926 0.1<br>I=0: 40.05071 |
| $AlL_2$ + H ⇆ $AlHL_2$ | 6.05 | 0.1 | | $AlL_2$ + H ⇆ $AlHL_2$ 6.05 0.1<br>Al + 2 L ⇆ $AlL_2$ 29.79284 0.1<br>Al + H + 2 L ⇆ $AlHL_2$ 35.84284 0.1<br>I=0: 37.76502 |
| $AlL_3$ + H ⇆ $AlHL_3$ | 8.05 | 0.1 | | $AlL_3$ + H ⇆ $AlHL_3$ 8.05 0.1<br>Al + 3 L ⇆ $AlL_3$ 38.76926 0.1<br>Al + 3 L + H ⇆ $AlHL_3$ 46.81926 0.1<br>I=0: 48.74144 |
| 2 Al + 2 L ⇆ $Al_2(OH)_2L_2$ + 2 H | 24.05 | 0.1 | | 2 Al + 2 L ⇆ $Al_2(OH)_2L_2$ + 2 H<br>24.05 0.1<br>2 OH + 2 H ⇆ 2 $H_2O$<br>(2*13.78342) 27.56684 0.1<br>2 Al + 2 L + 2 OH ⇆ $Al_2(OH)_2L_2$<br>51.61684 0.1<br>I=0: 54.60689. |

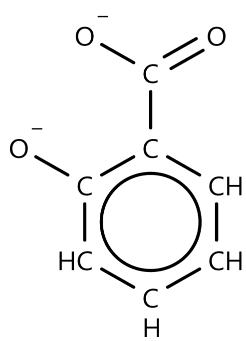
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 3 Al + 3 $H_2L$ ⇆ $Al_3(OH)_3L_3$ + 9 H | -29.91 | 0.5 | | 3 Al + 3 $H_2L$ ⇆ $Al_3(OH)_3L_3$ + 9 H -29.91 0.5<br>6 H + 3 L ⇆ 3 $H_2L$<br>(3*22.37199) 67.11597 0.5<br>3 OH + 3 H ⇆ 3 $H_2O$<br>(3*13.72861) 41.18583 0.5<br>3 Al + 3 OH + 3 L ⇆ $Al_3(OH)_3L_3$ 78.39180 0.5<br>I=0: 84.02795 |
| Ga + $H_2L$ ⇆ GaL + 2 H | -3.0 | 0.1 | 20 | Ga + $H_2L$ ⇆ GaL + 2 H -3.0 0.1<br>2 H + L ⇆ $H_2L$ 22.53642 0.1<br>Ga + L ⇆ GaL 19.53642 0.1<br>I=0: 20.81787 |
| two complexes with As(III), one with Si(IV) and two with As(V) | | | | (not entered) |

Salicylate

The ligand in its neutral form is salicylic acid (2-hydroxybenzoic acid), $C_7H_6O_3$.



The ligand as it is present in the database is salicylate, $C_7H_4O_3^{2-}$.



| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 13.7 | | | |
| HL + H ⇆ $H_2L$ | 2.972 | | | HL + H ⇆ $H_2L$ 2.972<br>H + L ⇆ HL 13.7<br>2 H + L ⇆ $H_2L$ 16.672 |
| Na + HL ⇆ NaHL | -0.5 | 0.1 | | Na + HL ⇆ NaHL -0.5 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Na + H + L ⇆ NaHL 12.77285 0.1<br>I=0: 13.41358 |
| K + HL ⇆ KHL | -0.5 | 0.1 | | K + HL ⇆ KHL -0.5 0.1<br>H + L ⇆ HL 13.27285 0.1<br>K + H + L ⇆ KHL 12.77285 0.1<br>I=0: 13.41358 |
| Be + HL ⇆ BeL + H | -0.63 | 0.1 | | Be + HL ⇆ BeL + H -0.63 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Be + L ⇆ BeL 12.64285 0.1<br>I=0: 13.49715 |
| BeL + HL ⇆ $BeL_2$ + H | -3.4 | 0.1 | | BeL + HL ⇆ $BeL_2$ + H -3.4 0.1<br>Be + L ⇆ BeL 12.64285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Be + 2 L ⇆ $BeL_2$ 22.51570 0.1<br>I=0: 23.37000 |
| Be + HL ⇆ BeHL | 1.6 | 1.0 | | Be + HL ⇆ BeHL 1.6 1.0<br>H + L ⇆ HL 13.29368 1.0<br>Be + H + L ⇆ BeHL 14.89368 1.0<br>I=0: 15.70632 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Be + 2 HL ⇆ $BeH_2L_2$ | 3.8 | 1.0 | | Be + 2 HL ⇆ $BeH_2L_2$ 3.8 1.0<br>2 H + 2 L ⇆ 2 HL<br>(2*13.29368) 26.58736 1.0<br>Be + 2 H + 2 L ⇆ $BeH_2L_2$ 30.38736 1.0<br>I=0: 31.80948 |
| BeL ⇆ BeOHL + H | -7.1 | 1.0 | | BeL ⇆ BeOHL + H -7.1 1.0<br>Be + L ⇆ BeL 12.68451 1.0<br>OH + H ⇆ $H_2O$ 13.79384 1.0<br>Be + L + OH ⇆ BeOHL 19.37835 1.0<br>I=0: 20.19099 |
| $BeHL_2$ + H ⇆ $BeH_2L_2$ | 2.9 | 1.0 | | $BeHL_2$ + H ⇆ $BeH_2L_2$ 2.9 1.0<br>invert:<br>$BeH_2L_2$ ⇆ $BeHL_2$ + H -2.9 1.0<br>Be + 2 H + 2 L ⇆ $BeH_2L_2$ 30.38736 1.0<br>Be + H + 2 L ⇆ $BeHL_2$ 27.48736 1.0<br>I=0: 28.70632 |
| 3 Be + 3 HL ⇆ $Be_3L_3(OH)_3$ + 6 H | -16.2 | 1.0 | | 3 Be + 3 HL ⇆ $Be_3L_3(OH)_3$ + 6 H<br>-16.2 1.0<br>3 H + 3 L ⇆ 3 HL<br>(3*13.29368) 39.88104 1.0<br>3 OH + 3 H ⇆ 3 $H_2O$<br>(3*13.79384) 41.38152 1.0<br>3 Be + 3 L + 3 OH ⇆ $Be_3L_3(OH)_3$<br>65.06256 1.0<br>I=0: 66.89100 |
| Mg + HL ⇆ MgL + H | -8.48 | 0.5 | | Mg + HL ⇆ MgL + H -8.48 0.5<br>H + L ⇆ HL 13.16322 0.5<br>Mg + L ⇆ MgL 4.68322 0.5<br>I=0: 5.75677 |
| Mg + HL ⇆ MgHL | 0.4 | | | Mg + HL ⇆ MgHL 0.4<br>H + L ⇆ HL 13.7<br>Mg + H + L ⇆ MgHL 14.1 |
| Ca + HL ⇆ CaL + H | -10.19 | 0.5 | | Ca + HL ⇆ CaL + H -10.19 0.5<br>H + L ⇆ HL 13.16322 0.5<br>Ca + L ⇆ CaL 2.97322 0.5<br>I=0: 4.04677 |
| Ca + HL ⇆ CaHL | 0.5 | | | Ca + HL ⇆ CaHL 0.5<br>H + L ⇆ HL 13.7<br>Ca + H + L ⇆ CaHL 14.2 |
| Ba + HL ⇆ BaHL | 0.3 | | | Ba + HL ⇆ BaHL 0.3<br>H + L ⇆ HL 13.7<br>Ba + H + L ⇆ BaHL 14.0 |
| La + HL ⇆ LaHL | 2.08 | | | La + HL ⇆ LaHL 2.08<br>H + L ⇆ HL 13.7<br>La + H + L ⇆ LaHL 15.78 |
| La + 2 HL ⇆ $LaH_2L_2$ | 3.6 | 0.1 | | La + 2 HL ⇆ $LaH_2L_2$ 3.6 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>La + 2 H + 2 L ⇆ $LaH_2L_2$ 30.14570 0.1<br>I=0: 32.06788 |
| Pr + HL ⇆ PrHL | 1.9 | 0.1 | | Pr + HL ⇆ PrHL 1.9 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Pr + H + L ⇆ PrHL 15.17285 0.1<br>I=0: 16.24073 |
| Pr + 2 HL ⇆ $PrH_2L_2$ | 3.7 | 0.1 | | Pr + 2 HL ⇆ $PrH_2L_2$ 3.7 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Pr + 2 H + 2 L ⇆ $PrH_2L_2$ 30.24570 0.1<br>I=0: 32.16788 |
| Nd + HL ⇆ NdHL | 1.9 | 0.1 | | Nd + HL ⇆ NdHL 1.9 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Nd + H + L ⇆ NdHL 15.17285 0.1<br>I=0: 16.24073 |
| Nd + 2 HL ⇆ $NdH_2L_2$ | 3.6 | 0.1 | | Nd + 2 HL ⇆ $NdH_2L_2$ 3.6 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Nd + 2 H + 2 L ⇆ $NdH_2L_2$ 30.14570 0.1<br>I=0: 32.06788 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Sm + HL ⇆ SmHL | 2.1 | 0.1 | | Sm + HL ⇆ SmHL 2.1 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Sm + H + L ⇆ SmHL 15.37285 0.1<br>I=0: 16.44073 |
| Sm + 2 HL ⇆ $SmH_2L_2$ | 3.8 | 0.1 | | Sm + 2 HL ⇆ $H_2L_2$ 3.8 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Sm + 2 H + 2 L ⇆ $H_2L_2$ 30.34570 0.1<br>I=0: 32.26788 |
| Eu + HL ⇆ EuHL | 2.0 | 0.1 | | Eu + HL ⇆ EuHL 2.0 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Eu + H + L ⇆ EuHL 15.27285 0.1<br>I=0: 16.34073 |
| Eu + 2 HL ⇆ $EuH_2L_2$ | 3.8 | 0.1 | | Eu + 2 HL ⇆ $EuH_2L_2$ 3.8 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Eu + 2 H + 2 L ⇆ $EuH_2L_2$ 30.34570 0.1<br>I=0: 32.26788 |
| Gd + HL ⇆ GdHL | 1.9 | 0.1 | | Gd + HL ⇆ GdHL 1.9 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Gd + H + L ⇆ Gd HL 15.17285 0.1<br>I=0: 16.24073 |
| Gd + 2 HL ⇆ $GdH_2L_2$ | 3.8 | 0.1 | | Gd + 2 HL ⇆ $GdH_2L_2$ 3.8 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Gd + 2 H + 2 L ⇆ $GdH_2L_2$ 30.34570 0.1<br>I=0: 32.26788 |
| Tb + HL ⇆ TbHL | 1.9 | 0.1 | | Tb + HL ⇆ TbHL 1.9 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Tb + H + L ⇆ TbHL 15.17285 0.1<br>I=0: 16.24073 |
| Tb + 2 HL ⇆ $TbH_2L_2$ | 3.9 | 0.1 | | Tb + 2 HL ⇆ $TbH_2L_2$ 3.9 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Tb + 2 H + 2 L ⇆ $TbH_2L_2$ 30.44570 0.1<br>I=0: 32.36788 |
| Dy + HL ⇆ DyHL | 1.7 | 0.1 | | Dy + HL ⇆ DyHL 1.7 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Dy + H + L ⇆ DyHL 14.97285 0.1<br>I=0: 16.04073 |
| Dy + 2 HL ⇆ $DyH_2L_2$ | 3.8 | 0.1 | | Dy + 2 HL ⇆ $DyH_2L_2$ 3.8 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Dy + 2 H + 2 L ⇆ $DyH_2L_2$ 30.34570 0.1<br>I=0: 32.26788 |
| Ho + HL ⇆ HoHL | 1.8 | 0.1 | | Ho + HL ⇆ HoHL 1.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Ho + H + L ⇆ HoHL 15.07285 0.1<br>I=0: 16.14073 |
| Ho + 2 HL ⇆ $HoH_2L_2$ | 3.8 | 0.1 | | Ho + 2 HL ⇆ $HoH_2L_2$ 3.8 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Ho + 2 H + 2 L ⇆ $HoH_2L_2$ 30.34570 0.1<br>I=0: 32.26788 |
| Er + HL ⇆ ErHL | 1.8 | 0.1 | | Er + HL ⇆ ErHL 1.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Er + H + L ⇆ ErHL 15.07285 0.1<br>I=0: 16.14073 |
| Er + 2 HL ⇆ $ErH_2L_2$ | 3.6 | 0.1 | | Er + 2 HL ⇆ $ErH_2L_2$ 3.6 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Er + 2 H + 2 L ⇆ $HEr_2L_2$ 30.14570 0.1<br>I=0: 32.06788 |
| Tm + HL ⇆ TmHL | 1.8 | 0.1 | | Tm + HL ⇆ TmHL 1.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Tm + H + L ⇆ TmHL 15.07285 0.1<br>I=0: 16.14073 |

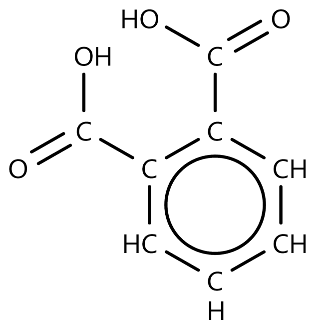
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Tm + 2 HL ⇆ $TmH_2L_2$ | 3.7 | 0.1 | | Tm + 2 HL ⇆ $TmH_2L_2$ 3.7 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Tm + 2 H + 2 L ⇆ $TmH_2L_2$ 30.24570 0.1<br>I=0: 32.16788 |
| Yb + HL ⇆ YbHL | 1.8 | 0.1 | | Yb + HL ⇆ YbHL 1.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Yb + H + L ⇆ YbHL 15.07285 0.1<br>I=0: 16.14073 |
| Yb + 2 HL ⇆ $YbH_2L_2$ | 3.5 | 0.1 | | Yb + 2 HL ⇆ $YbH_2L_2$ 3.5 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Yb + 2 H + 2 L ⇆ $YbH_2L_2$ 30.04570 0.1<br>I=0: 31.96788 |
| Lu + HL ⇆ LuHL | 1.7 | 0.1 | | Lu + HL ⇆ LuHL 1.7 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Lu + H + L ⇆ LuHL 14.97285 0.1<br>I=0: 16.04073 |
| Lu + 2 HL ⇆ Lu $H_2L_2$ | 3.7 | 0.1 | | Lu + 2 HL ⇆ $LuH_2L_2$ 3.7 0.1<br>2 H + 2 L ⇆ 2 HL<br>(2*13.27285) 26.54570 0.1<br>Lu + 2 H + 2 L ⇆ $LuH_2L_2$ 30.24570 0.1<br>I=0: 32.16788 |
| $(UO_2)$ + HL ⇆ $(UO_2)L$ + H | -0.57 | | | $(UO_2)$ + HL ⇆ $(UO_2)L$ + H -0.57<br>H + L ⇆ HL 13.7<br>$(UO_2)$ + L ⇆ $(UO_2)L$ 13.13 |
| $(UO_2)L$ + HL ⇆ $(UO_2)L_2$ + H | -3.0 | 0.1 | | $(UO_2)L$ + HL ⇆ $(UO_2)L_2$ + H<br>-3.0 0.1<br>$(UO_2)$ + L ⇆ $(UO_2)L$ 12.27570 0.1<br>H + L ⇆ HL 13.27285 0.1<br>$(UO_2)$ + 2 L ⇆ $(UO_2)L_2$ 22.54855 0.1<br>I=0: 23.40285 |
| $(UO_2)$ + HL ⇆ $(UO_2)HL$ | 1.61 | 0.1 | | $(UO_2)$ + HL ⇆ $(UO_2)HL$ 1.61 0.1<br>H + L ⇆ HL 13.27285 0.1<br>$(UO_2)$ + H + L ⇆ $(UO_2)HL$ 14.88285 0.1<br>I=0: 15.73715 |
| Mn(II) + HL ⇆ Mn(II)L + H | -7.5 | 0.1 | 20 | Mn(II) + HL ⇆ Mn(II)L + H<br>-7.5 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Mn(II) + L ⇆ Mn(II)L 5.77285 0.1<br>I=0: 6.62715 |
| Mn(II)L + HL ⇆ Mn(II)$L_2$ + H | -9.7 | 0.1 | 20 | Mn(II)L + HL ⇆ Mn(II)$L_2$ + H<br>-9.7 0.1<br>Mn(II) + L ⇆ Mn(II)L 5.77285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Mn(II) + 2 L ⇆ Mn(II)$L_2$ 9.34570 0.1<br>I=0: 10.20000 |
| Fe(II) + HL ⇆ Fe(II)L + H | -6.8 | 0.1 | 20 | Fe(II) + HL ⇆ Fe(II)L + H<br>-6.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Fe(II) + L ⇆ Fe(II)L 6.47285 0.1<br>I=0: 7.32715 |
| Fe(II)L + HL ⇆ Fe(II)$L_2$ + H | -8.9 | 0.1 | 20 | Fe(II)L + HL ⇆ Fe(II)$L_2$ + H<br>-8.9 0.1<br>Fe(II) + L ⇆ Fe(II)L 6.47285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Fe(II) + 2 L ⇆ Fe(II)$L_2$ 10.84570 0.1<br>I=0: 11.70000 |
| Co(II) + HL ⇆ Co(II)L + H | -6.2 | 0.1 | | Co(II) + HL ⇆ Co(II)L + H<br>-6.2 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Co(II) + L ⇆ Co(II)L 7.07285 0.1<br>I=0: 7.92715 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Co(II)L + HL ⇆ Co(II)L$_2$ + H | -8.9 | 0.1 | 20 | Co(II)L + HL ⇆ Co(II)L$_2$ + H<br>-8.9 0.1<br>Co(II) + L ⇆ Co(II)L 7.07285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Co(II) + 2 L ⇆ Co(II)L$_2$ 11.44570 0.1<br>I=0: 12.30000 |
| Ni + HL ⇆ NiL + H | -6.0 | 0.1 | | Ni + HL ⇆ NiL + H -6.0 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Ni + L ⇆ NiL 7.27285 0.1<br>I=0: 8.12715 |
| NiL + HL ⇆ NiL$_2$ + H | -8.8 | 0.1 | 20 | NiL + HL ⇆ NiL$_2$ + H -8.8 0.1<br>Ni + L ⇆ NiL 7.27285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Ni + 2 L ⇆ NiL$_2$ 11.74570 0.1<br>I=0: 12.60000 |
| Cu(II) + HL ⇆ Cu(II)L + H | -2.78 | 0.1 | | Cu(II) + HL ⇆ Cu(II)L + H<br>-2.78 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Cu(II) + L ⇆ Cu(II)L 10.49285 0.1<br>I=0: 11.34715 |
| Cu(II)L + HL ⇆ Cu(II)L$_2$ + H | -5.0 | 0.1 | | Cu(II)L + HL ⇆ Cu(II)L$_2$ + H<br>-5.0 0.1<br>Cu(II) + L ⇆ Cu(II)L 10.49285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Cu(II) + 2 L ⇆ Cu(II)L$_2$ 18.76570 0.1<br>I=0: 19.62000 |
| Fe(III) + HL ⇆ Fe(III)L + H | 3.85 | | | Fe(III) + HL ⇆ Fe(III)L + H<br>3.85<br>H + L ⇆ HL 13.7<br>Fe(III) + L ⇆ Fe(III)L 17.55 |
| Fe(III)L + HL ⇆ Fe(III)L$_2$ + H | -1.7 | 0.1 | | Fe(III)L + HL ⇆ Fe(III)L$_2$ + H<br>-1.7 0.1<br>Fe(III) + L ⇆ Fe(III)L 16.26855 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Fe(III) + 2 L ⇆ Fe(III)L$_2$<br>27.84140 0.1<br>I=0: 29.55000 |
| Fe(III) + HL ⇆ Fe(III)HL | 4.4 | 0.1 | | Fe(III) + HL ⇆ Fe(III)HL 4.4 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Fe(III) + H + L ⇆ Fe(III)HL<br>17.67285 0.1<br>I=0: 18.74073 |
| Zn + HL ⇆ ZnL + H | -6.5 | 0.1 | 20 | Zn + HL ⇆ ZnL + H -6.5 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Zn + L ⇆ ZnL 6.77285 0.1<br>I=0: 7.62715 |
| Cd + HL ⇆ CdL + H | -7.8 | 0.1 | 20 | Cd + HL ⇆ CdL + H -7.8 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Cd + L ⇆ CdL 5.47285 0.1<br>I=0: 6.32715 |
| one complex with B(III) | | | | (not entered) |
| Al + HL ⇆ AlL + H | -0.18 | 0.1 | | Al + HL ⇆ AlL + H -0.18 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Al + L ⇆ AlL 13.09285 0.1<br>I=0: 14.37430 |
| AlL + HL ⇆ AlL$_2$ + H | -2.89 | 0.1 | | AlL + HL ⇆ AlL$_2$ + H -2.89 0.1<br>Al + L ⇆ AlL 13.09285 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Al + 2 L ⇆ AlL$_2$ 23.47570 0.1<br>I=0: 25.18430 |
| AlL$_2$ ⇆ Al(OH)L$_2$ + H | -7.13 | 0.1 | | AlL$_2$ ⇆ Al(OH)L$_2$ + H -7.13 0.1<br>Al + 2 L ⇆ AlL$_2$ 23.47570 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + 2 L + OH ⇆ Al(OH)L$_2$<br>30.12912 0.1<br>I=0: 31.62415 |

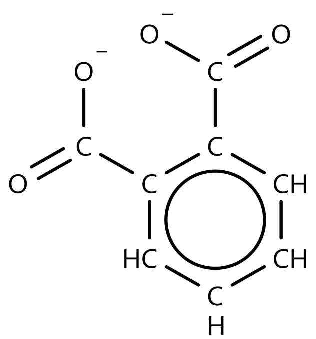
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Al(OH)L_2$ ⇆ $Al(OH)_2L_2$ + H | -9.3 | 0.5 | | $Al(OH)L_2$ ⇆ $Al(OH)_2L_2$ + H -9.3 0.5<br>Al + 2 L + OH ⇆ $Al(OH)L_2$<br>29.74543 0.5<br>OH + H ⇆ $H_2O$ 13.72861 0.5<br>Al + 2 L + 2 OH ⇆ $Al(OH)_2L_2$<br>34.17404 0.5<br>I=0: 35.51598 |
| 2 Al + 2 L ⇆ $Al_2(OH)_2L_2$ + 2 H | 17.9 | 0.1 | | 2 Al + 2 L ⇆ $Al_2(OH)_2L_2$ + 2 H<br>17.9 0.1<br>2 OH + 2 H ⇆ 2 $H_2O$<br>(2*13.78342) 27.56684 0.1<br>2 Al + 2 L + 2 OH ⇆ $Al_2(OH)_2L_2$<br>45.46684 0.1<br>I=0: 48.45689 |
| Ga + HL ⇆ GaL + H | 0.73 | 0.1 | | Ga + HL ⇆ GaL + H 0.73 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Ga + L ⇆ GaL 14.00285 0.1<br>I=0: 15.28430 |
| Ga + HL ⇆ GaHL | 1.9 | 0.1 | | Ga + HL ⇆ GaHL 1.9 0.1<br>H + L ⇆ HL 13.27285 0.1<br>Ga + H + L ⇆ GaHL 15.17285 0.1<br>I=0: 16.24073 |

## Phthalate

The ligand in its neutral form is phthalic acid (benzene-1,2-dicarboxylic acid), $C_8H_6O_4$.




The ligand as it is present in the database is phthalate, $C_8H_4O_4^{2-}$.



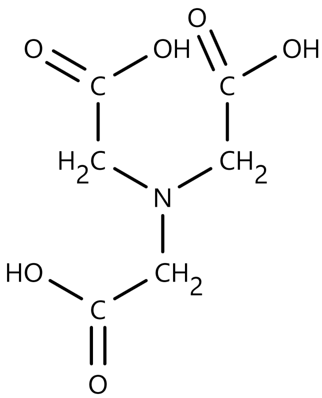

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 5.411 | | | |
| HL + H ⇆ $H_2L$ | 2.950 | | | HL + H ⇆ $H_2L$ 2.950<br>H + L ⇆ HL 5.411<br>2 H + L ⇆ $H_2L$ 8.361 |
| Li + L ⇆ LiL | 0.9 | | | |
| Na + L ⇆ NaL | 0.8 | | | |
| K + L ⇆ KL | 0.7 | | | |
| $NH_4$ + L ⇆ $NH_4L$ | 1.3 | | | $NH_4$ + L ⇆ $NH_4L$ 1.3<br>$NH_3$ + H ⇆ $NH_4$ 9.244<br>H + $NH_3$ + L ⇆ $NH_4L$ 10.544 |
| Be + L ⇆ BeL | 3.17 | 0.5 | | I=0: 4.24355 |
| Be + 2 L ⇆ $BeL_2$ | 5.32 | 0.5 | | I=0: 6.39355 |
| $Be_3(OH)_3$ + L ⇆ $Be_3(OH)_3L$ | 2.44 | 0.5 | | $Be_3(OH)_3$ + L ⇆ $Be_3(OH)_3L$ 2.44 0.5<br>3 Be + 3 OH ⇆ $Be_3OH_3$ 32.29484 0.5<br>3 Be + 3 OH + L ⇆ $Be_3(OH)_3L$<br>34.73484 0.5<br>I=0: 37.15033 |
| Mg + L ⇆ MgL | 2.52 | | | |
| Ca + L ⇆ CaL | 2.45 | | | |
| Ca + HL ⇆ CaHL | 1.02 | | | Ca + HL ⇆ CaHL 1.02<br>H + L ⇆ HL 5.411<br>Ca + H + L ⇆ CaHL 6.431 |
| Sr + L ⇆ SrL | 2.38 | | | |
| Ba + L ⇆ BaL | 2.30 | | | |
| Y + L ⇆ YL | 3.46 | 0.1 | | I=0: 4.74145 |
| La + L ⇆ LaL | 4.74 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pr + L ⇆ PrL | 3.56 | 0.1 | | I=0: 4.84145 |
| Nd + L ⇆ NdL | 3.88 | 0.1 | | I=0: 5.16145 |
| Sm + L ⇆ SmL | 3.70 | 0.1 | | I=0: 4.98145 |
| Eu + L ⇆ EuL | 3.70 | 0.1 | | I=0: 4.98145 |
| Gd + L ⇆ GdL | 3.63 | 0.1 | | I=0: 4.91145 |
| Tb + L ⇆ TbL | 3.46 | 0.1 | | I=0: 4.74145 |
| Dy + L ⇆ DyL | 3.48 | 0.1 | | I=0: 4.76145 |
| Ho + L ⇆ HoL | 3.55 | 0.1 | | I=0: 4.83145 |
| Er + L ⇆ ErL | 3.76 | 0.1 | | I=0: 5.04145 |
| Tm + L ⇆ TmL | 3.53 | 0.1 | | I=0: 4.81145 |
| Yb + L ⇆ YbL | 3.48 | 0.1 | | I=0: 4.76145 |
| Lu + L ⇆ LuL | 3.65 | 0.1 | | I=0: 4.93145 |
| $(U(VI)O_2)$+ L ⇆ $(U(VI)O_2)L$ | 4.81 | 0.1 | | I=0: 5.66430 |
| $(U(VI)O_2)$ + 2 L ⇆ $(U(VI)O_2)L_2$ | 7.73 | 0.1 | | I=0: 8.58430 |
| 2 $(U(VI)O_2)$ + 2 L ⇆ $(U(VI)O_2)_2(OH)_2L_2$ + 2 H | 2.37 | 0.1 | | 2 $(U(VI)O_2)$ + 2 L ⇆ $(U(VI)O_2)_2(OH)_2L_2$ + 2 H 2.37 0.1<br>2 H + 2 OH ⇆ 2 $H_2O$ (2*13.78342) 27.56684 0.1<br>2 $(U(VI)O_2)$ + 2 L + 2 OH ⇆ $(U(VI)O_2)_2L_2(OH)_2$ 29.93684 0.1<br>I=0: 31.43187 |
| Mn(II) + L ⇆ Mn(II)L | 2.74 | | | |
| Co(II) + L ⇆ Co(II)L | 2.83 | | | |
| Co(II) + HL ⇆ Co(II)HL | 1.28 | 0.5 | | Co(II) + HL ⇆ Co(II)HL 1.28 0.5<br>H + L ⇆ HL 4.87422 0.5<br>Co(II) + H + L ⇆ Co(II)HL 6.15422 0.5<br>I=0: 7.22777 |
| Ni + L ⇆ NiL | 2.95 | | | |
| Ni + HL ⇆ NiHL | 0.7 | 0.5 | | Ni + HL ⇆ NiHL 0.7 0.5<br>H + L ⇆ HL 4.87422 0.5<br>Ni + H + L ⇆ NiHL 5.57422 0.5<br>I=0: 6.64777 |
| Cu(II) + L ⇆ Cu(II)L | 4.02 | | | |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | 5.3 | | | |
| Cu(II) + HL ⇆ Cu(II)HL | 1.3 | 0.1 | | Cu(II) + HL ⇆ Cu(II)HL 1.3 0.1<br>H + L ⇆ HL 4.98385 0.1<br>Cu(II) + H + L ⇆ Cu(II)HL 6.28385 0.1<br>I=0: 7.13815 |
| Fe(III) + L ⇆ Fe(III)L | 6.07 | 0.1 | 30 | I=0: 7.35145 |
| Fe(III) + 2 L ⇆ Fe(III)$L_2$ | 10.56 | 0.1 | 30 | I=0: 12.26860 |
| Fe(III) + 3 L ⇆ Fe(III)$L_3$ | 13.26 | 0.1 | 30 | I=0: 14.54145 |
| Zn + L ⇆ ZnL | 2.91 | | | |
| Zn + 2 L ⇆ $ZnL_2$ | 4.2 | | | |
| Cd + L ⇆ CdL | 2.5 | 0.1 | | I=0: 3.35430 |
| Cd + 2 L ⇆ $CdL_2$ | 2.88 | 1.0 | | I=0: 3.69264 |
| Cd + HL ⇆ CdHL | 0.48 | 1.0 | | Cd + HL ⇆ CdHL 0.48 1.0<br>H + L ⇆ HL 5.00468 1.0<br>Cd + H + L ⇆ CdHL 5.48468 1.0<br>I=0: 6.29732 |
| $CdL_2$ + H ⇆ $CdHL_2$ | 3.60 | 1.0 | | $CdL_2$ + H ⇆ $CdHL_2$ 3.60 1.0<br>Cd + 2 L ⇆ $CdL_2$ 2.88 1.0<br>Cd + 2 L + H ⇆ $CdHL_2$ 6.48 1.0<br>I=0: 7.76145 |
| Pb(II) + L ⇆ Pb(II)L | 2.78 | 1.0 | | I=0: 3.59264 |
| Pb(II) + 2 L ⇆ Pb(II)$L_2$ | 4.01 | 1.0 | | I=0: 4.82264 |
| Pb(II) + HL ⇆ Pb(II)HL | 1.16 | 1.0 | | Pb(II) + HL ⇆ Pb(II)HL 1.16 1.0<br>H + L ⇆ HL 5.00468 1.0<br>Pb(II) + H + L ⇆ Pb(II)HL 6.16468 1.0<br>I=0: 6.97732 |

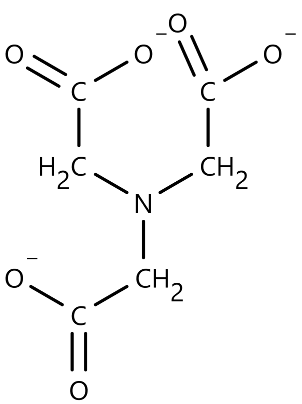
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Pb(II)L_2 + H \leftrightarrows Pb(II)HL_2$ | 3.77 | 1.0 | | $Pb(II)L_2 + H \leftrightarrows Pb(II)HL_2$ 3.77 1.0<br>$Pb(II) + 2 L \leftrightarrows Pb(II)L_2$ 4.01 1.0<br>$Pb(II) + 2 L \leftrightarrows H \leftrightarrows Pb(II)HL_2$<br>7.78 1.0<br>I=0: 8.99896 |
| $B(OH)_3 + L \leftrightarrows B(OH)_3L$ | -0.07 | | | $B(OH)_3 + L \leftrightarrows B(OH)_3L$ -0.07<br>$H + H_2BO_3 \leftrightarrows H_3BO_3$ 9.236<br>$H + H_2BO_3 + L \leftrightarrows B(OH)_3L$ 9.166 |
| $B(OH)_3 + HL \leftrightarrows B(OH)_3HL$ | -1 | | | $B(OH)_3 + HL \leftrightarrows B(OH)_3HL$ -1<br>$H + H_2BO_3 \leftrightarrows H_3BO_3$ 9.236<br>$H + L \leftrightarrows HL$ 5.411<br>$2 H + H_2BO_3 + L \leftrightarrows B(OH)_3HL$<br>13.647 |
| $Al + L \leftrightarrows AlL$ | 2.94 | 0.5 | | I=0: 4.55033 |
| $Al + 2 L \leftrightarrows AlL_2$ | 5.0 | 0.5 | | I=0: 7.14711 |
| $2 Al + L \leftrightarrows Al_2(OH)_2L + 2 H$ | -2.50 | 0.5 | | $2 Al + L \leftrightarrows Al_2(OH)_2L + 2 H$<br>-2.50 0.5<br>$2 OH + 2 H \leftrightarrows 2 H_2O$<br>(2*13.72861) 27.45722 0.5<br>$2 Al + L + 2 OH \leftrightarrows Al_2(OH)_2L$<br>24.95722 0.5<br>I=0: 27.64110 |
| $3 Al + L \leftrightarrows Al_3(OH)_4L + 4 H$ | -8.47 | 0.5 | | $3 Al + L \leftrightarrows Al_3(OH)_4L + 4 H$<br>-8.47 0.5<br>$4 OH + 4 H \leftrightarrows 4 H_2O$<br>(4*13.72861) 54.91444 0.5<br>$3 Al + L + 4 OH \leftrightarrows Al_3(OH)_4L$<br>46.44444 0.5<br>I=0: 49.93349 |
| $2 Al + 2 L \leftrightarrows Al_2(OH)_2L_2 + 2 H$ | -0.07 | 0.5 | | $2 Al + 2 L \leftrightarrows Al_2(OH)_2L_2 + 2 H$<br>-0.07 0.5<br>$2 OH + 2 H \leftrightarrows 2 H_2O$<br>(2*13.72861) 27.45722 0.5<br>$2 Al + 2 L + 2 OH \leftrightarrows Al_2(OH)_2L_2$<br>27.38722 0.5<br>I=0: 31.14465 |
| $Ga + L \leftrightarrows GaL$ | 5.15 | 0.1 | | I=0: 6.43145 |

## NTA

The ligand in its neutral form is NTA (nitrilotriacetic acid), $C_6H_9NO_6$.




The ligand as it is present in the database is the NTA-anion, $C_6H_6NO_6^{3-}$.




| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.46<br>9.66<br>9.84 | 0.1 | | Values are for three background electrolytes (Na/K/N(alkyl)$_4$); the average is used (28.96/3 = 9.65333 at I=0.1)<br>I=0: 10.29406 |
| HL + H ⇆ $H_2L$ | 2.52 | 0.1 | | HL + H ⇆ $H_2L$ 2.52 0.1<br>H + L ⇆ HL 9.65333 0.1<br>2 H + L ⇆ $H_2L$ 12.17333 0.1<br>I=0: 13.24121 |
| $H_2L$ + H ⇆ $H_3L$ | 2.0 | | | $H_2L$ + H ⇆ $H_3L$ 2.0<br>2 H + L ⇆ $H_2L$ 13.24121<br>3 H + L ⇆ $H_3L$ 15.24121 |
| $H_3L$ + H ⇆ $H_4L$ | 1.0 | 0.1 | | $H_3L$ + H ⇆ $H_4L$ 1.0 0.1<br>3 H + L ⇆ $H_3L$ 13.95976 0.1<br>4 H + L ⇆ $H_4L$ 14.95976 0.1<br>I=0: 16.24121 |
| Li + L ⇆ LiL | 2.45 | 0.1 | | I=0: 3.09073 |
| Na + L ⇆ NaL | 1.2 | 0.1 | | I=0: 1.84073 |
| K + L ⇆ KL | 0.6 | 0.1 | | I=0: 1.24073 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Rb + L ⇆ RbL | 0.4 | 0.1 | | I=0: 1.04073 |
| Cs + L ⇆ CsL | 0.2 | 0.1 | | I=0: 0.84073 |
| Be + L ⇆ BeL | 7.79 | 0.1 | | I=0: 9.07145 |
| Mg + L ⇆ MgL | 5.50 | 0.1 | | I=0: 6.78145 |
| Ca + L ⇆ CaL | 6.3<br>6.44<br>6.64 | 0.1 | | as for the first equilibrium: three different background electrolytes; used: average: 6.46<br>I=0: 7.74145 |
| Ca + 2 L ⇆ $CaL_2$ | 8.81<br>9.27 | 0.1 | | similarly: values for K and $N(alkyl)_4$ background; used: 9.04<br>I=0: 9.68073 |
| Sr + L ⇆ SrL | 4.99 | 0.1 | | I=0: 6.27145 |
| Ba + L ⇆ BaL | 4.81 | 0.1 | | I=0: 6.09145 |
| Sc + L ⇆ ScL | 12.7 | 0.1 | | I=0: 14.62218 |
| Sc + 2 L ⇆ $ScL_2$ | 24.1 | 0.1 | 20 | I=0: 26.02218 |
| ScL + OH ⇆ Sc(OH)L | 7.44 | 0.1 | 20 | ScL + OH ⇆ Sc(OH)L 7.44 0.1<br>Sc + L ⇆ ScL 12.7 0.1<br>Sc + L + OH ⇆ Sc(OH)L 20.14 0.1<br>I=0: 22.06218 |
| Y + L ⇆ YL | 11.42 | 0.1 | | I=0: 13.34218 |
| Y + 2 L ⇆ $YL_2$ | 20.41 | 0.1 | | I=0: 22.33218 |
| YL + OH ⇆ Y(OH)L | 6.39 | 0.1 | | YL + OH ⇆ Y(OH)L 6.39 0.1<br>Y + L ⇆ YL 11.42 0.1<br>Y + OH + L ⇆ Y(OH)L 17.81 0.1<br>I=0: 19.73218 |
| La + L ⇆ LaL | 10.47 | 0.1 | | I=0: 12.39218 |
| La + 2 L ⇆ $LaL_2$ | 17.84 | 0.1 | | I=0: 19.76218 |
| LaL + OH ⇆ La(OH)L | 5.9 | 0.1 | | LaL + OH ⇆ La(OH)L 5.9 0.1<br>La + L ⇆ LaL 10.47 0.1<br>La + OH + L ⇆ La(OH)L 16.37 0.1<br>I=0: 18.29218 |
| Ce + L ⇆ CeL | 10.70 | 0.1 | | I=0: 12.62218 |
| Ce + 2 L ⇆ $CeL_2$ | 18.66 | 0.1 | | I=0: 20.58218 |
| CeL + OH ⇆ Ce(OH)L | 5.78 | 0.1 | 20 | CeL + OH ⇆ Ce(OH)L 5.78 0.1<br>Ce + L ⇆ CeL 10.70 0.1<br>Ce + OH + L ⇆ Ce(OH)L 16.48 0.1<br>I=0: 18.40218 |
| Pr + L ⇆ PrL | 10.87 | 0.1 | | I=0: 12.79218 |
| Pr + 2 L ⇆ $PrL_2$ | 19.02 | 0.1 | | I=0: 20.94218 |
| PrL + OH ⇆ Pr(OH)L | 5.72 | 0.1 | | PrL + OH ⇆ Pr(OH)L 5.72 0.1<br>Pr + L ⇆ PrL 10.87 0.1<br>Pr + OH + L ⇆ Pr(OH)L 16.59 0.1<br>I=0: 18.51218 |
| Nd + L ⇆ NdL | 11.10 | 0.1 | | I=0: 13.02218 |
| Nd + 2 L ⇆ $NdL_2$ | 19.51 | 0.1 | | I=0: 21.43218 |
| NdL + OH ⇆ Nd(OH)L | 5.86 | 0.1 | | NdL + OH ⇆ Nd(OH)L 5.86 0.1<br>Nd + L ⇆ NdL 11.10 0.1<br>Nd + OH + L ⇆ Nd(OH)L 16.96 0.1<br>I=0: 18.88218 |
| Pm + 2 L ⇆ $PmL_2$ | 19.7 | 0.1 | 20 | I=0: 21.62218 |
| Sm + L ⇆ SmL | 11.32 | 0.1 | | I=0: 13.24218 |
| Sm + 2 L ⇆ $SmL_2$ | 20.43 | 0.1 | | I=0: 22.35218 |
| SmL + OH ⇆ Sm(OH)L | 6.59 | 0.1 | | SmL + OH ⇆ Sm(OH)L 6.59 0.1<br>Sm + L ⇆ SmL 11.32 0.1<br>Sm + OH + L ⇆ Sm(OH)L 17.91 0.1<br>I=0: 19.83218 |
| Eu + L ⇆ EuL | 11.32 | 0.1 | | I=0: 13.24218 |
| Eu + 2 L ⇆ $EuL_2$ | 20.64 | 0.1 | | I=0: 22.56218 |
| EuL + OH ⇆ Eu(OH)L | 6.84 | 0.1 | | EuL + OH ⇆ Eu(OH)L 6.84 0.1<br>Eu + L ⇆ EuL 11.32 0.1<br>Eu + OH + L ⇆ Eu(OH)L 18.16 0.1<br>I=0: 20.08218 |
| Gd + L ⇆ GdL | 11.35 | 0.1 | | I=0: 13.27218 |
| Gd + 2 L ⇆ $GdL_2$ | 20.66 | 0.1 | | I=0: 22.58218 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| GdL + OH ⇆ Gd(OH)L | 6.54 | 0.1 | | GdL + OH ⇆ Gd(OH)L 6.54 0.1<br>Gd + L ⇆ GdL 11.35 0.1<br>Gd + OH + L ⇆ Gd(OH)L 17.89 0.1<br>I=0: 19.81218 |
| Tb + L ⇆ TbL | 11.50 | 0.1 | | I=0: 13.42218 |
| Tb + 2 L ⇆ $TbL_2$ | 20.95 | 0.1 | | I=0: 22.87218 |
| TbL + OH ⇆ Tb(OH)L | 6.67 | 0.1 | | TbL + OH ⇆ Tb(OH)L 6.67 0.1<br>Tb + L ⇆ TbL 11.50 0.1<br>Tb + OH + L ⇆ Tb(OH)L 18.17 0.1<br>I=0: 20.09218 |
| Dy + L ⇆ DyL | 11.63 | 0.1 | | I=0: 13.55218 |
| Dy + 2 L ⇆ $DyL_2$ | 20.98 | 0.1 | | I=0: 22.90218 |
| DyL + OH ⇆ Dy(OH)L | 6.84 | 0.1 | | DyL + OH ⇆ Dy(OH)L 6.84 0.1<br>Dy + L ⇆ DyL 11.63 0.1<br>Dy + OH + L ⇆ Dy(OH)L 18.47 0.1<br>I=0: 20.39218 |
| Ho + L ⇆ HoL | 11.76 | 0.1 | | I=0: 13.68218 |
| Ho + 2 L ⇆ $HoL_2$ | 21.06 | 0.1 | | I=0: 22.98218 |
| HoL + OH ⇆ Ho(OH)L | 6.66 | 0.1 | | HoL + OH ⇆ Ho(OH)L 6.66 0.1<br>Ho + L ⇆ HoL 11.76 0.1<br>Ho + OH + L ⇆ Ho(OH)L 18.42 0.1<br>I=0: 20.34218 |
| Er + L ⇆ ErL | 11.90 | 0.1 | | I=0: 13.82218 |
| Er + 2 L ⇆ $ErL_2$ | 21.09 | 0.1 | | I=0: 23.01218 |
| ErL + OH ⇆ Er(OH)L | 6.56 | 0.1 | | ErL + OH ⇆ Er(OH)L 6.56 0.1<br>Er + L ⇆ ErL 11.90 0.1<br>Er + OH + L ⇆ Er(OH)L 18.46 0.1<br>I=0: 20.38218 |
| Tm + L ⇆ TmL | 12.07 | 0.1 | | I=0: 13.99218 |
| Tm + 2 L ⇆ $TmL_2$ | 21.22 | 0.1 | | I=0: 23.14218 |
| TmL + OH ⇆ Tm(OH)L | 6.24 | 0.1 | | TmL + OH ⇆ Tm(OH)L 6.24 0.1<br>Tm + L ⇆ TmL 12.07 0.1<br>Tm + OH + L ⇆ Tm(OH)L 18.31 0.1<br>I=0: 20.23218 |
| Yb + L ⇆ YbL | 12.21 | 0.1 | | I=0: 14.13218 |
| Yb + 2 L ⇆ $YbL_2$ | 21.41 | 0.1 | | I=0: 23.33218 |
| YbL + OH ⇆ Yb(OH)L | 6.29 | 0.1 | | YbL + OH ⇆ Yb(OH)L 6.29 0.1<br>Yb + L ⇆ YbL 12.21 0.1<br>Yb + OH + L ⇆ Yb(OH)L 18.50 0.1<br>I=0: 20.42218 |
| Lu + L ⇆ LuL | 12.32 | 0.1 | | I=0: 14.24218 |
| Lu + 2 L ⇆ $LuL_2$ | 21.65 | 0.1 | | I=0: 23.57218 |
| LuL + OH ⇆ Lu(OH)L | 6.30 | 0.1 | | LuL + OH ⇆ Lu(OH)L 6.30 0.1<br>Lu + L ⇆ LuL 12.32 0.1<br>Lu + OH + L ⇆ Lu(OH)L 18.62 0.1<br>I=0: 20.54218 |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 9.50 | 0.1 | | I=0: 10.78145 |
| Mn(II) + L ⇆ Mn(II)L | 7.27<br>7.46 | 0.1 | | 7.46 is for K as background electrolyte; 7.27 for Na as background electrolyte; used: average 7.365<br>I=0: 8.64645 |
| Mn(II) + 2 L ⇆ Mn(II)$L_2$ | 10.44<br>10.94 | 0.1 | | for resp. Na and K as background electrolyte; used: average 10.69<br>I=0: 11.33073 |
| Fe(II) + L ⇆ Fe(II)L | 8.90 | 0.1 | | I=0: 10.18145 |
| Fe(II) + 2 L ⇆ Fe(II)$L_2$ | 11.98 | 0.1 | | I=0: 12.62073 |
| Fe(II)L ⇆ Fe(II)(OH)L + H | -10.82 | 0.1 | | Fe(II)L ⇆ Fe(II)(OH)L + H -10.82 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(II) + L ⇆ Fe(II)L 8.90 0.1<br>Fe(II) + L + OH ⇆ Fe(II)(OH)L 11.86342 0.1<br>I=0: 12.93130 |
| Co(II) + L ⇆ Co(II)L | 10.38 | 0.1 | | I=0: 11.66145 |
| Co(II) + 2 L ⇆ Co(II)$L_2$ | 14.33 | 0.1 | | I=0: 14.97073 |

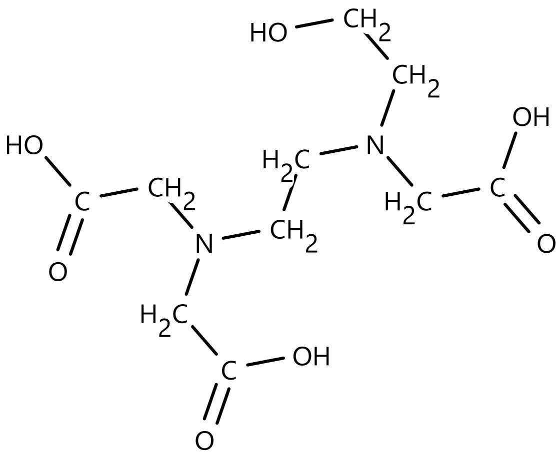
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Co(II)L ⇆ Co(II)(OH)L + H | -10.80 | 0.1 | | Co(II)L ⇆ Co(II)(OH)L + H<br>-10.80 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Co(II) + L ⇆ Co(II)L 10.38 0.1<br>Co(II) + L + OH ⇆ Co(II)(OH)L<br>13.36342 0.1<br>I=0: 14.43130 |
| Ni + L ⇆ NiL | 11.51 | 0.1 | | I=0: 12.79145 |
| Ni + 2 L ⇆ $NiL_2$ | 16.32 | 0.1 | | I=0: 16.96073 |
| NiL ⇆ Ni(OH)L + H | -10.86 | 0.1 | | NiL ⇆ Ni(OH)L + H -10.86 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ni + L ⇆ NiL 11.50 0.1<br>Ni + L + OH ⇆ Ni(OH)L 14.42342 0.1<br>I=0: 15.49130 |
| Cu(II) + L ⇆ Cu(II)L | 12.7<br>13.0<br>13.3 | 0.1 | | three values for resp. Na as background electrolyte; "corrected for background electrolyte" and K as background electrolyte; used: average: 13.0<br>I=0: 14.28145 |
| Cu(II) + 2 L ⇆ Cu(II)$L_2$ | 17.4 | 0.1 | | I=0: 18.04073 |
| Cu(II)L + H ⇆ Cu(II)HL | 1.6 | 0.1 | | Cu(II)L + H ⇆ Cu(II)HL 1.6 0.1<br>Cu(II) + L ⇆ Cu(II)L 13.0 0.1<br>Cu(II) + L + H ⇆ Cu(II)HL<br>14.6 0.1<br>I=0: 16.09503 |
| Cu(II)L ⇆ Cu(II)(OH)L + H | -9.2 | 0.1 | | Cu(II)L ⇆ Cu(II)(OH)L + H<br>-9.2 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Cu(II) + L ⇆ Cu(II)L 13.0 0.1<br>Cu(II) + L + OH ⇆ Cu(II)(OH)L<br>17.58342 0.1<br>I=0: 18.65130 |
| Cr(III)L ⇆ Cr(III)(OH)L + H | -6.23 | 0.1 | 20 | (can not be related to components; not entered) |
| Cr(III)(OH)L ⇆ Cr(III)$(OH)_2$L + H | -8.45 | 0.1 | 20 | (can not be related to components; not entered) |
| Fe(III) + L ⇆ Fe(III)L | 16.00 | 0.1 | | I=0: 17.92218 |
| Fe(III) + 2 L ⇆ Fe(III)$L_2$ | 24.0 | 0.1 | | I=0: 25.92218 |
| Fe(III)L + H ⇆ Fe(III)HL | 1.0 | 0.5 | | Fe(III)L + H ⇆ Fe(III)HL 1.0 0.5<br>Fe(III) + L ⇆ Fe(III)L 15.50669 0.5<br>Fe(III) + L + H ⇆ Fe(III)HL<br>16.50669 0.5<br>I=0: 18.92218 |
| Fe(III)L ⇆ Fe(III)(OH)L + H | -4.36 | 0.1 | | Fe(III)L ⇆ Fe(III)(OH)L + H<br>-4.36 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + L ⇆ Fe(III)L 16.00 0.1<br>Fe(III) + L + OH ⇆ Fe(III)(OH)L<br>25.42342 0.1<br>I=0: 27.34560 |
| Fe(III)(OH)L ⇆ Fe(III)$(OH)_2$L + H | -7.58 | 0.1 | | Fe(III)(OH)L ⇆ Fe(III)$(OH)_2$L + H<br>-7.58 0.1<br>Fe(III) + L + OH ⇆ Fe(III)(OH)L<br>25.42342 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + 2 OH + L ⇆ Fe(III)$(OH)_2$L<br>31.62684 0.1<br>I=0: 33.33544 |
| Fe(III)$(OH)_2$L ⇆ Fe(III)$(OH)_3$L + H | -10.72 | 0.1 | | Fe(III)$(OH)_2$L ⇆ Fe(III)$(OH)_3$L + H<br>-10.72 0.1<br>Fe(III) + 2 OH + L ⇆ Fe(III)$(OH)_2$L<br>31.62684 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + 3 OH + L ⇆ Fe(III)$(OH)_3$L<br>34.69026 0.1<br>I=0: 35.97171 |
| 2 Fe(III) + 2 L ⇆ Fe$(III)_2L_2$ | 30.9 | 0.5 | | I=0: 35.73099 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Fe(III)(OH)L ⇆ $Fe(III)_2(OH)_2L_2$ | 9.14 | 0.5 | | 2 Fe(III)(OH)L ⇆ $Fe(III)_2(OH)_2L_2$ 9.14 0.5<br>2 Fe(III) + 2 L + 2 OH ⇆ 2 Fe(III)(OH)L (2*24.93011) 49.86022 0.5<br>2 Fe(III) + 2 L + 2 OH ⇆ $Fe(III)_2(OH)_2L_2$ 59.00022 0.5<br>I=0: 63.56282 |
| Co(III)L ⇆ Co(III)(OH)L + H | -6.84 | 0.1 | 20 | (can not be related to components; not entered) |
| Co(III)(OH)L ⇆ $Co(III)(OH)_2L$ + H | -9.66 | 0.1 | 20 | (can not be related to components; not entered) |
| Zr + L ⇆ ZrL | 24.1 | | | |
| Hf + L ⇆ HfL | 23.6 | | | |
| Ag + L ⇆ AgL | 4.85<br>5.08 | 0.1 | | for resp. Na and K background; used: average (9.93/2=4.965)<br>I=0: 5.60573 |
| AgL + H ⇆ AgHL | 7.0 | 1.0 | | AgL + H ⇆ AgHL 7.0 1.0<br>Ag + L ⇆ AgL 4.99625 1.0<br>Ag + H + L ⇆ AgHL 11.99625 1.0<br>I=0: 13.01205 |
| Pd + L ⇆ PdL | 17.0 | 1.0 | 20 | I=0: 18.21896 |
| Pd + 2 L ⇆ $PdL_2$ | 23.7 | 1.0 | 20 | I=0: 24.30948 |
| PdL + H ⇆ PdHL | 7.82 | 1.0 | 20 | PdL + H ⇆ PdHL 7.82 1.0<br>Pd + L ⇆ PdL 17.0 1.0<br>Pd + H + L ⇆ PdHL 24.82 1.0<br>I=0: 26.24212 |
| PdHL + H ⇆ $PdH_2L$ | 0.5 | 1.0 | 20 | PdHL + H ⇆ $PdH_2L$ 0.5 1.0<br>Pd + H + L ⇆ PdHL 24.82 1.0<br>Pd + 2 H + L ⇆ $PdH_2L$ 25.32 1.0<br>I=0: 26.74212 |
| 2 PdL ⇆ $Pd_2L_2$ | 2 | 1.0 | 20 | 2 PdL ⇆ $Pd_2L_2$ 2 1.0<br>Pd + L ⇆ PdL (2*17.0) 34.0 1.0<br>2 Pd + 2 L ⇆ $Pd_2L_2$ 36.0 1.0<br>I=0: 38.23476 |
| PdL + PdOHL ⇆ $Pd_2OHL_2$ | 3.1 | 1.0 | 20 | constant for PdOHL is not given; therefore $Pd_2OHL_2$ can not be calculated |
| Zn + L ⇆ ZnL | 10.45<br>10.66 | 0.1 | | 10.45 for KCl as background electrolyte; 10.66 for $KNO_3$; used: average of 10.555<br>I=0: 11.83645 |
| Zn + 2 L ⇆ $ZnL_2$ | 14.24 | 0.1 | | I=0: 14.88073 |
| ZnL ⇆ Zn(OH)L + H | -10.1<br>-10.06 | 0.1 | | -10.1 for $NaNO_3$ as background electrolyte; -10.06 for $KNO_3$; used: average of -10.08<br>ZnL ⇆ Zn(OH)L + H -10.08 0.1<br>Zn + L ⇆ ZnL 10.66 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Zn + L + OH ⇆ Zn(OH)L 14.36342 0.1<br>I=0: 15.43130 |
| Cd + L ⇆ CdL | 9.76 | 0.1 | | I=0: 11.04145 |
| Cd + 2 L ⇆ $CdL_2$ | 14.47 | 0.1 | | I=0: 15.11073 |
| CdL ⇆ Cd(OH)L + H | -11.25 | 0.1 | | CdL ⇆ Cd(OH)L + H -11.25 0.1<br>Cd + L ⇆ CdL 9.76 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Cd + L + OH ⇆ Cd(OH)L 12.29342 0.1<br>I=0: 13.36130 |
| Hg(II) + L ⇆ Hg(II)L | 14.3 | 0.1 | | I=0: 15.58145 |
| Pb(II) + L ⇆ Pb(II)L | 11.48 | 0.1 | | I=0: 12.76145 |
| Pb(II) + 2 L ⇆ $Pb(II)L_2$ | 12.8 | 0.1 | 20 | I=0: 13.44073 |
| Pb(II)L + H ⇆ Pb(II)HL | 2.3 | 0.5 | | Pb(II)L + H ⇆ Pb(II)HL 2.3 0.5<br>Pb(II) + L ⇆ Pb(II)L 11.15112 0.5<br>Pb(II) + H + L ⇆ Pb(II)HL 13.45112 0.5<br>I=0: 15.32984 |
| Al + L ⇆ AlL | 11.4 | 0.1 | | I=0: 13.32218 |

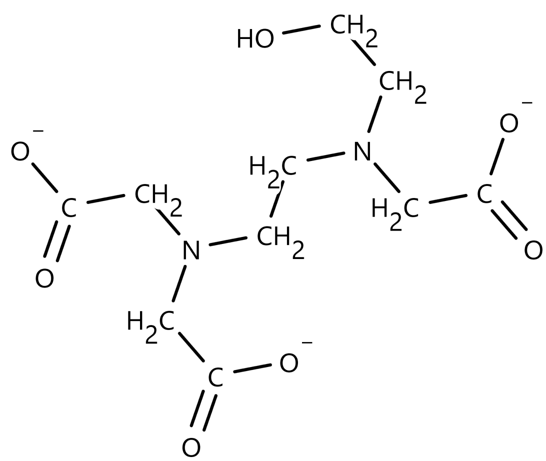
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| AlL + H ⇆ AlHL | 1.90 | 0.1 | | AlL + H ⇆ AlHL 1.90 0.1<br>Al + L ⇆ AlL 11.4 0.1<br>Al + H + L ⇆ AlHL 13.3 0.1<br>I=0: 15.22218 |
| AlL ⇆ Al(OH)L + H | -5.09 | 0.1 | | AlL ⇆ Al(OH)L + H -5.09 0.1<br>Al + L ⇆ AlL 11.4 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + L + OH ⇆ Al(OH)L 20.09342 0.1<br>I=0: 22.01560 |
| Al(OH)L ⇆ $Al(OH)_2L$ + H | -8.28 | 0.1 | | Al(OH)L ⇆ $Al(OH)_2L$ + H -8.28 0.1<br>Al + L + OH ⇆ Al(OH)L 20.09342 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + L + 2 OH ⇆ $Al(OH)_2L$<br>25.59684 0.1<br>I=0: 27.30544 |
| 2 Al(OH)L ⇆ $Al_2(OH)_2L_2$ | 1.82 | 0.5 | | 2 Al(OH)L ⇆ $Al_2(OH)_2L_2$ 1.82 0.5<br>2 Al + 2 OH + 2 L ⇆ 2 Al(OH)L<br>(2*19.60011) 39.20022 0.5<br>2 Al + 2 OH + 2 L ⇆ $Al_2(OH)_2L_2$<br>41.02022 0.5<br>I=0: 45.58282 |
| Ga + L ⇆ GaL | 13.6<br>13.9 | 0.1 | 20 | 13.6 for Na as background electrolyte;<br>13.9 for K<br>used: average (13.75)<br>I=0: 15.67218 |
| GaL ⇆ GaOHL + H | -4.27 | 0.1 | | GaL ⇆ GaOHL + H -4.27 0.1<br>Ga + L ⇆ GaL 13.75 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ga + L + OH ⇆ GaOHL 23.26342 0.1<br>I=0: 25.18560 |
| GaOHL ⇆ $Ga(OH)_2L$ + H | -7.64 | 0.1 | | GaOHL ⇆ $Ga(OH)_2L$ + H -7.64 0.1<br>Ga + L + OH ⇆ GaOHL 23.26342 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ga + 2 OH + L ⇆ $Ga(OH)_2L$ 29.40684 0.1<br>I=0: 31.11544 |
| In + L ⇆ InL | 13.81 | 0.1 | | I=0: 15.73218 |
| In + 2 L ⇆ $InL_2$ | 23.70 | 0.1 | | I=0: 25.62218 |
| $InL_2$ + H ⇆ $InHL_2$ | 2.87 | 0.1 | | $InL_2$ + H ⇆ $InHL_2$ 2.87 0.1<br>In + 2 L ⇆ $InL_2$ 23.70 0.1<br>In + H + 2 L ⇆ InHL2 26.57 0.1<br>I=0: 29.13290 |
| Bi + L ⇆ BiL | 18.2 | 0.1 | | I-0: 20.12218 |
| Bi + 2 L ⇆ $BiL_2$ | 26.6 | 1.0 | 20 | I=0: 28.42844 |
| As(III)$(OH)_2$ + H + L ⇆ As(III)$(OH)_2$HL | 15.3 | 0.1 | | (can not be related to components; not entered) |

## HEDTA

The ligand in its neutral form is HEDTA (N-(2-hydroxyethyl)ethylenedinitrilotriacetic acid), $C_{10}H_{18}N_2O_7$.



The ligand as it is present in the database is the HEDTA-anion, $C_{10}H_{15}N_2O_7^{3-}$.



| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 9.70<br>9.87 | 0.1 | | Values are for two background electrolytes (Na/K); the average is used (19.57/2 = 9.785 at I=0.1)<br>I=0: 10.42573 |
| HL + H ⇆ $H_2L$ | 5.38 | 0.1 | | HL + H ⇆ $H_2L$ 5.38 0.1<br>H + L ⇆ HL 9.785 0.1<br>2 H + L ⇆ $H_2L$ 15.165 0.1<br>I=0: 16.23288 |
| $H_2L$ + H ⇆ $H_3L$ | 2.62 | 0.1 | | $H_2L$ + H ⇆ $H_3L$ 2.62 0.1<br>2 H + L ⇆ $H_2L$ 15.165 0.1<br>3 H + L ⇆ $H_3L$ 17.785 0.1<br>I=0: 19.06645 |

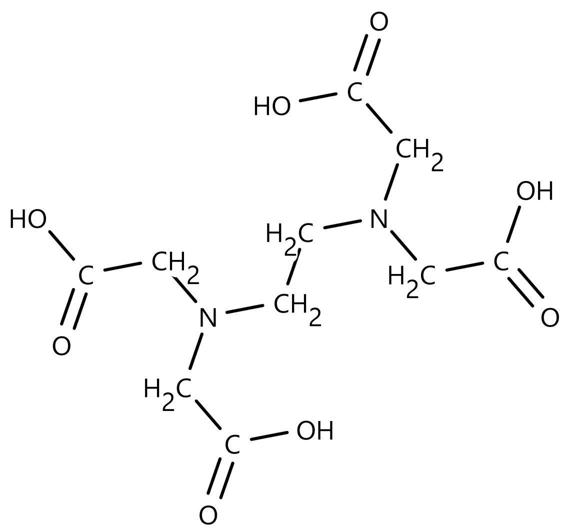
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_3L$ + H ⇆ $H_4L$ | 1.6 | 1.0 | | $H_3L$ + H ⇆ $H_4L$ 1.6 1.0<br>3 H + L ⇆ $H_3L$ 17.84749 1.0<br>4 H + L ⇆ $H_4L$ 19.44749 1.0<br>I=0: 20.66645 |
| Mg + L ⇆ MgL | 7.0 | 0.1 | | I=0: 8.28145 |
| Ca + L ⇆ CaL | 8.1 | 0.1 | | I=0: 9.38145 |
| Sr + L ⇆ SrL | 6.8 | 0.1 | | I=0: 8.08145 |
| Ba + L ⇆ BaL | 6.2 | 0.1 | | I=0: 7.48145 |
| Sc + L ⇆ ScL | 17.3 | 0.1 | | I=0: 19.22218 |
| Y + L ⇆ YL | 14.72 | 0.1 | | I=0: 16.64218 |
| YL + OH ⇆ YOHL | 4.76 | 0.1 | 20 | YL + OH ⇆ YOHL 4.76 0.1<br>Y + L ⇆ YL 14.72 0.1<br>Y + OH + L ⇆ YOHL 19.48 0.1<br>I=0: 21.40218 |
| La + L ⇆ LaL | 13.48 | 0.1 | | I=0: 15.40218 |
| LaL + OH ⇆ LaOHL | 3.46 | 0.1 | 20 | LaL + OH ⇆ LaOHL 3.46 0.1<br>La + L ⇆ LaL 13.48 0.1<br>La + OH + L ⇆ LaOHL 16.94 0.1<br>I=0: 18.86218 |
| Ce + L ⇆ CeL | 14.09 | 0.1 | | I=0: 16.01218 |
| Pr + L ⇆ PrL | 14.61 | 0.1 | | I=0: 16.53218 |
| PrL + OH ⇆ PrOHL | 3.69 | 0.1 | 20 | PrL + OH ⇆ PrOHL 3.69 0.1<br>Pr + L ⇆ PrL 14.61 0.1<br>Pr + OH + L ⇆ PrOHL 18.40 0.1<br>I=0: 20.32218 |
| Nd + L ⇆ NdL | 14.88 | 0.1 | | I=0: 16.80218 |
| NdL + OH ⇆ NdOHL | 3.59 | 0.1 | 20 | NdL + OH ⇆ NdOHL 3.59 0.1<br>Nd + L ⇆ NdL 14.88 0.1<br>Nd + OH + L ⇆ NdOHL 18.47 0.1<br>I=0: 20.39218 |
| Sm + L ⇆ SmL | 15.31 | 0.1 | | I=0: 17.23218 |
| SmL + OH ⇆ SmOHL | 3.70 | 0.1 | 20 | SmL + OH ⇆ SmOHL 3.70 0.1<br>Sm + L ⇆ SmL 15.31 0.1<br>Sm + OH + L ⇆ SmOHL 19.01 0.1<br>I=0: 20.93218 |
| Eu + L ⇆ EuL | 15.34 | 0.1 | | I=0: 17.26218 |
| EuL + OH ⇆ EuOHL | 4.03 | 0.1 | 20 | EuL + OH ⇆ EuOHL 4.03 0.1<br>Eu + L ⇆ EuL 15.34 0.1<br>Eu + OH + L ⇆ EuOHL 19.37 0.1<br>I=0: 21.29218 |
| Gd + L ⇆ GdL | 15.20 | 0.1 | | I=0: 17.12218 |
| GdL + OH ⇆ GdOHL | 3.98 | 0.1 | 20 | GdL + OH ⇆ GdOHL 3.98 0.1<br>Gd + L ⇆ GdL 15.20 0.1<br>Gd + OH + L ⇆ GdOHL 19.18 0.1<br>I=0: 21.10218 |
| Tb + L ⇆ TbL | 15.28 | 0.1 | | I=0: 17.20218 |
| TbL + OH ⇆ TbOHL | 4.52 | 0.1 | 20 | TbL + OH ⇆ TbOHL 4.52 0.1<br>Tb + L ⇆ TbL 15.28 0.1<br>Tb + OH + L ⇆ TbOHL 19.80 0.1<br>I=0: 21.72218 |
| Dy + L ⇆ DyL | 15.26 | 0.1 | | I=0: 17.18218 |
| DyL + OH ⇆ DyOHL | 4.88 | 0.1 | 20 | DyL + OH ⇆ DyOHL 4.88 0.1<br>Dy + L ⇆ DyL 15.26 0.1<br>Dy + OH + L ⇆ DyOHL 20.14 0.1<br>I=0: 22.06218 |
| Ho + L ⇆ HoL | 15.28 | 0.1 | | I=0: 17.20218 |
| HoL + OH ⇆ HoOHL | 5.12 | 0.1 | 20 | HoL + OH ⇆ HoOHL 5.12 0.1<br>Ho + L ⇆ HoL 15.28 0.1<br>Ho + OH + L ⇆ HoOHL 20.40 0.1<br>I=0: 22.32218 |
| Er + L ⇆ ErL | 15.38 | 0.1 | | I=0: 17.30218 |
| ErL + OH ⇆ ErOHL | 5.14 | 0.1 | 20 | ErL + OH ⇆ ErOHL 5.14 0.1<br>Er + L ⇆ ErL 15.38 0.1<br>Er + OH + L ⇆ ErOHL 20.52 0.1<br>I=0: 22.44218 |
| Tm + L ⇆ TmL | 15.56 | 0.1 | | I=0: 17.48218 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| TmL + OH ⇆ TmOHL | 5.11 | 0.1 | 20 | TmL + OH ⇆ TmOHL 5.11 0.1<br>Tm + L ⇆ TmL 15.56 0.1<br>Tm + OH + L ⇆ TmOHL 20.67 0.1<br>I=0: 22.59218 |
| Yb + L ⇆ YbL | 15.83 | 0.1 | | I=0: 17.75218 |
| YbL + OH ⇆ YbOHL | 5.21 | 0.1 | 20 | YbL + OH ⇆ YbOHL 5.21 0.1<br>Yb + L ⇆ YbL 15.83 0.1<br>Yb + OH + L ⇆ YbOHL 21.04 0.1<br>I=0: 22.96218 |
| Lu + L ⇆ LuL | 15.93 | 0.1 | | I=0: 17.85218 |
| LuL + OH ⇆ LuOHL | 5.13 | 0.1 | 20 | LuL + OH ⇆ LuOHL 5.13 0.1<br>Lu + L ⇆ LuL 15.93 0.1<br>Lu + OH + L ⇆ LuOHL 21.06 0.1<br>I=0: 22.98218 |
| Mn(II) + L ⇆ Mn(II)L | 11.1 | 0.1 | | I=0: 12.38145 |
| Fe(II) + L ⇆ Fe(II)L | 12.2 | 0.1 | | I=0: 13.48145 |
| Fe(II) + HL ⇆ Fe(II)HL | 5.12 | 0.1 | | Fe(II) + HL ⇆ Fe(II)HL 5.12 0.1<br>H + L ⇆ HL 9.785 0.1<br>Fe(II) + H + L ⇆ Fe(II)HL<br>14.905 0.1<br>I=0: 16.40003 |
| Co(II) + L ⇆ Co(II)L | 14.5 | 0.1 | | I=0: 15.78145 |
| Co(II)L + H ⇆ Co(II)HL | 2.24 | 0.1 | | Co(II)L + H ⇆ Co(II)HL 2.24 0.1<br>Co(II) + L ⇆ Co(II)L 14.5 0.1<br>Co(II) + H + L ⇆ Co(II)HL<br>16.74 0.1<br>I=0: 18.23503 |
| Ni + L ⇆ NiL | 17.1 | 0.1 | | I-0: 18.38145 |
| NiL + H ⇆ NiHL | 2.54 | 1.0 | | NiL + H ⇆ NiHL 2.54 1.0<br>Ni + L ⇆ NiL 17.16249 1.0<br>Ni + H + L ⇆ NiHL 19.80249 1.0<br>I=0: 21.22461 |
| Cu(II) + L ⇆ Cu(II)L | 17.4 | 0.1 | | I=0: 18.68145 |
| Cu(II)L + H ⇆ Cu(II)HL | 2.45 | 0.1 | | Cu(II)L + H ⇆ Cu(II)HL 2.45 0.1<br>Cu(II) + L ⇆ Cu(II)L 17.4 0.1<br>Cu(II) + H + L ⇆ Cu(II)HL<br>19.85 0.1<br>I=0: 21.34503 |
| Cr(III)OHL + H ⇆ Cr(III)L | 6.08 | 0.1 | | (can not be related to components; not entered) |
| Cr(III)(OH)L ⇆ Cr(III)(OH)$_2$L + H | -9.85 | 0.1 | | (can not be related to components; not entered) |
| Fe(III) + L ⇆ Fe(III)L | 19.7 | 0.1 | | I=0: 21.62218 |
| Fe(III)L ⇆ Fe(III)OHL + H | -3.88 | 0.1 | | Fe(III)L ⇆ Fe(III)OHL + H<br>-3.88 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + L ⇆ Fe(III)L 19.7 0.1<br>Fe(III) + L + OH ⇆ Fe(III)OHL<br>29.60342 0.1<br>I=0: 31.52560 |
| Fe(III)OHL ⇆ Fe(III)(OH)$_2$L + H | -8.83 | 0.1 | | Fe(III)OHL ⇆ Fe(III)(OH)$_2$L + H<br>-8.83 0.1<br>Fe(III) + L + OH ⇆ Fe(III)OHL<br>29.60342 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + L + 2 OH ⇆ Fe(III)(OH)$_2$L<br>34.55684 0.1<br>I=0: 36.26544 |
| Fe(III)(OH)$_2$L ⇆ Fe(III)(OH)$_3$L + H | -10.00 | 0.1 | | Fe(III)(OH)$_2$L ⇆ Fe(III)(OH)$_3$L + H<br>-10.00 0.1<br>Fe(III) + 2 OH + L ⇆ Fe(III)(OH)$_2$L<br>34.55684 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + 3 OH +L ⇆ Fe(III)(OH)$_3$L<br>38.34026 0.1<br>I=0: 39.62171 |

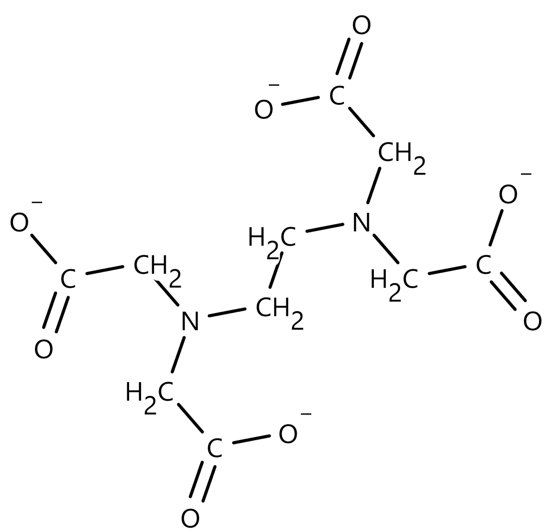
| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Fe(III)OHL ⇆ $Fe(III)_2(OH)_2L_2$ | 2.38 | 1.0 | | 2 Fe(III)OHL ⇆ $Fe(III)_2(OH)_2L_2$ 2.38 1.0<br>2 Fe(III) + 2 OH + 2 L ⇆ 2 Fe(III)OHL (2*29.69716) 59.39432 1.0<br>2 Fe(III) + 2 OH + 2 L ⇆ $Fe(III)_2(OH)_2L_2$ 61.77432 1.0<br>I=0: 65.22804 |
| Co(III) + L ⇆ Co(III)L | 37.2 | 0.1 | | I=0: 39.12218 |
| Ag + L ⇆ AgL | 6.67 | 0.1 | | I=0: 7.31073 |
| Zn + L ⇆ ZnL | 14.6 | 0.1 | | I=0: 15.88145 |
| Cd + L ⇆ CdL | 13.7 | 0.1 | | I=0: 14.98145 |
| CdL + H ⇆ CdHL | 2.30 | 1.0 | | CdL + H ⇆ CdHL 2.30 1.0<br>Cd + L ⇆ CdL 13.76249 1.0<br>Cd + H + L ⇆ CdHL 16.06249 1.0<br>I=0: 17.55752 |
| Hg(II) + L ⇆ Hg(II)L | 20.1 | 0.1 | | I=0: 21.38145 |
| Hg(II)L ⇆ Hg(II)OHL + H | -8.4 | 0.1 | | Hg(II)L ⇆ Hg(II)OHL + H -8.4 0.1<br>Hg(II) + L ⇆ Hg(II)L 20.1 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Hg(II) + OH + L ⇆ Hg(II)OHL 25.48342 0.1<br>I=0: 26.55130 |
| Pb(II) + L ⇆ Pb(II)L | 15.6 | 0.1 | | I=0: 16.88145 |
| Pb(II)L + H ⇆ Pb(II)HL | 2.14 | 1.0 | | Pb(II)L + H ⇆ Pb(II)HL 2.14 1.0<br>Pb(II) + L ⇆ Pb(II)L 15.66249 1.0<br>Pb(II) + L + H ⇆ Pb(II)HL 17.80249 1.0<br>I=0: 19.22461 |
| Al + L ⇆ AlL | 14.4 | 0.1 | | I=0: 16.32218 |
| AlL + H ⇆ AlHL | 2.14 | 0.1 | | AlL + H ⇆ AlHL 2.14 0.1<br>Al + L ⇆ AlL 14.4 0.1<br>Al + L + H ⇆ AlHL 16.54 0.1<br>I=0: 18.46218 |
| AlL ⇆ AlOHL + H | -4.89 | 0.1 | | AlL ⇆ AlOHL + H -4.89 0.1<br>Al + L ⇆ AlL 14.4 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + L + OH ⇆ AlOHL 23.29342 0.1<br>I=0: 26.21560 |
| AlOHL ⇆ $Al(OH)_2L$ + H | -9.19 | 0.1 | | AlOHL ⇆ $Al(OH)_2L$ + H -9.19 0.1<br>Al + L + OH ⇆ AlOHL 23.29342 0.1<br>OH + H ⇆ H2O 13.78342 0.1<br>Al + L + 2 OH ⇆ $Al(OH)_2L$ 27.88684 0.1<br>I=0: 29.59544 |
| Ga + L ⇆ GaL | 18.1 | 0.1 | | I=0: 20.02218 |
| GaL ⇆ GaOHL + H | -4.38 | 0.1 | | GaL ⇆ GaOHL + H -4.38 0.1<br>Ga + L ⇆ GaL 18.1 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ga + L + OH ⇆ GaOHL 27.50342 0.1<br>I=0: 29.42560 |
| In + L ⇆ InL | 20.2 | 0.1 | 20 | I=0: 22.12218 |
| Bi + L ⇆ BiL | 22.3 | 1.0 | | I=0: 24.12844 |
| BiL ⇆ BiOHL + H | -5.45 | 1.0 | | BiL ⇆ BiOHL + H -5.45 1.0<br>Bi + L ⇆ BiL 22.3 1.0<br>OH + H ⇆ $H_2O$ 13.79384 1.0<br>Bi + OH + L ⇆ BiOHL 30.64384 1.0<br>I=0: 32.47228 |

## EDTA

The ligand in its neutral form is EDTA (ethylenedinitrilotetraacetic acid), $C_{10}H_{16}N_2O_8$.



The ligand as it is present in the database is the EDTA-anion, $C_{10}H_{12}N_2O_8^{4-}$.



| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| H + L ⇆ HL | 10.948 | | | |
| HL + H ⇆ $H_2L$ | 6.273 | | | HL + H ⇆ $H_2L$ 6.273<br>H + L ⇆ HL 10.948<br>2 H + L ⇆ $H_2L$ 17.221 |
| $H_2L$ + H ⇆ $H_3L$ | 2.69 | 0.1 | | $H_2L$ + H ⇆ $H_3L$ 2.69 0.1<br>2 H + L ⇆ $H_2L$ 15.72597 0.1<br>3 H + L ⇆ $H_3L$ 18.41597 0.1<br>I=0: 20.33815 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H_3L$ + H ⇆ $H_4L$ | 2.00 | 0.1 | | $H_3L$ + H ⇆ $H_4L$ 2.00 0.1<br>3 H + L ⇆ $H_3L$ 18.41597 0.1<br>4 H + L ⇆ $H_4L$ 20.41597 0.1<br>I=0: 22.55172 |
| $H_4L$ + H ⇆ $H_5L$ | 1.5 | 0.1 | | $H_4L$ + H ⇆ $H_5L$ 1.5 0.1<br>4 H + L ⇆ $H_4L$ 20.41597 0.1<br>5 H + L ⇆ $H_5L$ 21.91597 0.1<br>I=0: 24.05172 |
| $H_5L$ + H ⇆ $H_6L$ | 0.0 | 1.0 | | $H_5L$ + H ⇆ $H_6L$ 0.0 1.0<br>5 H + L ⇆ $H_5L$ 22.02012 1.0<br>6 H + L ⇆ $H_6L$ 22.02012 1.0<br>I=0: 23.94230 |
| Li + L ⇆ LiL | 2.95 | 0.1 | | I=0: 3.80430 |
| Na + L ⇆ NaL | 1.86 | 0.1 | | I=0: 2.71430 |
| K + L ⇆ KL | 0.8 | 0.1 | | I=0: 1.65430 |
| Rb + L ⇆ RbL | 0.6 | 0.1 | | I=0: 1.45430 |
| Cs + L ⇆ CsL | 0.2 | 0.1 | | I=0: 1.05430 |
| Be + L ⇆ BeL | 9.7 | 0.1 | | I=0: 11.40860 |
| Mg + L ⇆ MgL | 8.79<br>8.96 | 0.1 | | for two background electrolytes: K and tetraalkyl ammonium; used: average (8.79+8.96=17.75/2=8.875)<br>I=0: 10.58360 |
| MgL + H ⇆ MgHL | 4.0 | 0.1 | | MgL + H ⇆ MgHL 4.0 0.1<br>Mg + L ⇆ MgL 8.875 0.1<br>Mg + H + L ⇆ MgHL 12.875 0.1<br>I=0: 15.01075 |
| Ca + L ⇆ CaL | 10.65<br>10.81 | | | for two background electrolytes: K and tetraalkyl ammonium; used: average (10.65+10.81=21.46/2=10.73)<br>I=0: 12.43860 |
| CaL + H ⇆ CaHL | 3.1 | 0.1 | | CaL + H ⇆ CaHL 3.1 0.1<br>Ca + L ⇆ CaL 10.73 0.1<br>Ca + H + L ⇆ CaHL 13.83 0.1<br>I=0: 15.96575 |
| Sr + L ⇆ SrL | 8.72 | 0.1 | | I=0: 10.42860 |
| SrL + H ⇆ SrHL | 3.93 | 0.1 | 20 | SrL + H ⇆ SrHL 3.93 0.1<br>Sr + L ⇆ SrL 8.72 0.1<br>Ca + H + L ⇆ CaHL 12.65 0.1<br>I=0: 14.78575 |
| Ba + L ⇆ BaL | 7.88 | 0.1 | | I=0: 9.58860 |
| Sc + L ⇆ ScL | 23.1 | 0.1 | 20 | I=0: 25.66290 |
| ScL + H ⇆ ScHL | 2.0 | 0.1 | 20 | ScL + H ⇆ ScHL 2.0 0.1<br>Sc + L ⇆ ScL 23.1 0.1<br>Sc + H + L ⇆ ScHL 25.1 0.1<br>I=0: 27.87648 |
| ScL ⇆ Sc(OH)L + H | -10.66 | 0.1 | 20 | ScL ⇆ Sc(OH)L + H -10.66 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Sc + L ⇆ ScL 23.1 0.1<br>Sc + L + OH ⇆ Sc(OH)L 26.22342 0.1<br>I=0: 28.57275 |
| Y + L ⇆ YL | 18.08 | 0.1 | | I=0: 20.64290 |
| La + L ⇆ LaL | 15.36 | 0.1 | | I=0: 17.92290 |
| LaL + H ⇆ LaHL | 2.24 | 0.1 | | LaL + H ⇆ LaHL 2.24 0.1<br>La + L ⇆ LaL 15.36 0.1<br>La + H + L ⇆ LaHL 17.60 0.1<br>I=0: 20.37648 |
| Ce + L ⇆ CeL | 15.93 | 0.1 | | I=0: 18.49290 |
| CeL + H ⇆ CeHL | 1.7 | 1.0 | | CeL + H ⇆ CeHL 1.7 1.0<br>Ce + L ⇆ CeL 16.05498 1.0<br>Ce + H + L ⇆ CeHL 17.75498 1.0<br>I=0: 20.39606 |
| Pr + L ⇆ PrL | 16.30 | 0.1 | | I=0: 18.86290 |
| PrL + H ⇆ PrHL | 1.6 | 1.0 | | PrL + H ⇆ PrHL 1.6 1.0<br>Pr + L ⇆ PrL 16.42498 1.0<br>Pr + H + L ⇆ PrHL 18.02498 1.0<br>I=0: 20.66606 |
| Nd + L ⇆ NdL | 16.51 | 0.1 | | I=0: 19.07290 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| NdL + H ⇆ NdHL | 1.5 | 1.0 | | NdL + H ⇆ NdHL 1.5 1.0<br>Nd + L ⇆ NdL 16.63498 1.0<br>Nd + H + L ⇆ NdHL 18.13498 1.0<br>I=0: 20.77606 |
| Pm + L ⇆ PmL | 16.9 | 0.1 | | I=0: 19.46290 |
| Sm + L ⇆ SmL | 17.06 | 0.1 | | I=0: 19.62290 |
| SmL + H ⇆ SmHL | 1.5 | 1.0 | | SmL + H ⇆ SmHL 1.5 1.0<br>Sm + L ⇆ SmL 17.18498 1.0<br>Sm + H + L ⇆ SmHL 18.68498 1.0<br>I=0: 21.32606 |
| Eu + L ⇆ EuL | 17.25 | 0.1 | | I=0: 19.81290 |
| EuL + H ⇆ EuHL | 1.4 | 1.0 | | EuL + H ⇆ EuHL 1.4 1.0<br>Sc + L ⇆ ScL 17.37498 1.0<br>Sc + H + L ⇆ ScHL 18.77498 1.0<br>I=0: 21.41606 |
| Gd + L ⇆ GdL | 17.35 | 0.1 | | I=0: 19.91290 |
| GdL + H ⇆ GdHL | 1.3 | 1.0 | | GdL + H ⇆ GdHL 1.3 1.0<br>Gd + L ⇆ GdL 17.47498 1.0<br>Gd + H + L ⇆ GdHL 18.77498 1.0<br>I=0: 21.41606 |
| Tb + L ⇆ TbL | 17.87 | 0.1 | | I=0: 20.43290 |
| TbL + H ⇆ TbHL | 0.9 | 1.0 | | TbL + H ⇆ TbHL 0.9 1.0<br>Tb + L ⇆ TbL 17.99498 1.0<br>Tb + H + L ⇆ TbHL 18.89498 1.0<br>I=0: 21.53606 |
| Dy + L ⇆ DyL | 18.30 | 0.1 | | I=0: 20.86290 |
| DyL + H ⇆ DyHL | 0.7 | 1.0 | | DyL + H ⇆ DyHL 0.7 1.0<br>Dy + L ⇆ DyL 18.42498 1.0<br>Dy + H + L ⇆ DyHL 19.12498 1.0<br>I=0: 21.76606 |
| Ho + L ⇆ HoL | 18.56 | 0.1 | | I=0: 21.12290 |
| HoL + H ⇆ HoHL | 0.5 | 1.0 | | HoL + H ⇆ HoHL 0.5 1.0<br>Ho + L ⇆ HoL 18.68498 1.0<br>Ho + H + L ⇆ HoHL 19.18498 1.0<br>I=0: 21.82606 |
| Er + L ⇆ ErL | 18.89 | 0.1 | | I=0: 21.45290 |
| Tm + L ⇆ TmL | 19.32 | 0.1 | | I=0: 21.88290 |
| Yb + L ⇆ YbL | 19.49 | 0.1 | | I=0: 22.05290 |
| Lu + L ⇆ LuL | 19.74 | 0.1 | | I=0: 22.30290 |
| $(UO_2)$ + L ⇆ $(UO_2)L$ | 9.28 | 1.0 | | I=0: 10.90528 |
| $(UO_2)$ + HL ⇆ $(UO_2)HL$ | 7.40 | 0.1 | | $(UO_2)$ + HL ⇆ $(UO_2)HL$ 7.40 0.1<br>H + L ⇆ HL 10.09370 0.1<br>$(UO_2)$ + H + L ⇆ $(UO_2)HL$ 17.49370 0.1<br>I=0: 19.62945 |
| 2 $(UO_2)$ + L ⇆ $(UO_2)_2L$ | 17.87 | 0.1 | | I=0: 20.43290 |
| $(UO_2)_2L$ ⇆ $(UO_2)_2(OH)L$ + H | -4.81 | 1.0 | | $(UO_2)_2L$ ⇆ $(UO_2)_2(OH)L$ + H<br>-4.81 1.0<br>2 $(UO_2)$ + L ⇆ $(UO_2)_2L$ 17.99498 1.0<br>OH + H ⇆ $H_2O$ 13.79384 1.0<br>2 $(UO_2)$ + L + OH ⇆ $(UO_2)_2(OH)L$<br>26.97882 1.0<br>I=0: 29.41674 |
| $(UO_2)_2L$ + L ⇆ $(UO_2)_2L_2$ | 8.90 | 1.0 | | $(UO_2)_2L$ + L ⇆ $(UO_2)_2L_2$ 8.90 1.0<br>2 $(UO_2)$ + L ⇆ $(UO_2)_2L$ 17.99498 1.0<br>2 $(UO_2)$ + 2 L ⇆ $(UO_2)_2L_2$ 26.89498 1.0<br>I=0: 29.33290 |
| 4 $(UO_2)$ + 2 L ⇆ $(UO_2)_4(OH)_4L_2$ + 4 H | 15.34 | 1.0 | | 4 $(UO_2)$ + 2 L ⇆ $(UO_2)_4(OH)_4L_2$ + 4 H<br>15.34 1.0<br>4 OH + 4 H ⇆ 4 $H_2O$<br>(4*13.79384) 55.17536 1.0<br>4 $(UO_2)$ + 2 L + 4 (OH) ⇆ $(UO_2)_4(OH)_4L_2$<br>70.51536 1.0<br>I=0: 74.17224 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 6 $(UO_2)$ + 3 L ⇆ $(UO_2)_6(OH)_4L_3$ + 4 H | 34.3 | 1.0 | | 6 $(UO_2)$ + 3 L ⇆ $(UO_2)_6(OH)_4L_3$ + 4 H 34.3 1.0<br>4 OH + 4 H ⇆ 4 $H_2O$ (4*13.79384) 55.17536 1.0<br>6 $(UO_2)$ + 3 L + 4 (OH) ⇆ $(UO_2)_6(OH)_4L_3$ 89.47536 1.0<br>I=0: 95.57016 |
| Mn(II) + L ⇆ Mn(II)L | 13.89 | 0.1 | | I=0: 15.59860 |
| Mn(II)L + H ⇆ Mn(II)HL | 3.1 | 0.1 | | Mn(II)L + H ⇆ Mn(II)HL 3.1 0.1<br>Mn(II) + L ⇆ Mn(II)L 13.89 0.1<br>Mn(II) + H + L ⇆ Mn(II)HL 16.99 0.1<br>I=0: 19.12575 |
| Fe(II) + L ⇆ Fe(II)L | 14.30 | 0.1 | | I=0: 16.00860 |
| Fe(II) + HL ⇆ Fe(II)HL | 6.82 | 0.1 | | Fe(II) + HL ⇆ Fe(II)HL 6.82 0.1<br>H + L ⇆ HL 10.09370 0.1<br>Fe(II) + H + L ⇆ Fe(II)HL 16.91370 0.1<br>I=0: 19.04945 |
| Co(II) + L ⇆ Co(II)L | 16.45 | 0.1 | | I=0: 18.15860 |
| Co(II)L + H ⇆ Co(II)HL | 3.0 | 0.1 | | Co(II)L + H ⇆ Co(II)HL 3.0 0.1<br>Co(II) + L ⇆ Co(II)L 16.45 0.1<br>Co(II) + H + L ⇆ Co(II)HL 19.45 0.1<br>I=0: 21.58575 |
| Co(II)HL + H ⇆ Co(II)$H_2L$ | 1.7 | 1.0 | | Co(II)HL + H ⇆ Co(II)$H_2L$ 1.7 1.0<br>Co(II) + H + L ⇆ Co(II)HL 19.55415 1.0<br>Co(II) + 2 H + L ⇆ Co(II)$H_2L$ 21.25415 1.0<br>I=0: 23.48891 |
| Ni + L ⇆ NiL | 18.4 | 0.1 | | I=0: 20.10860 |
| NiL + H ⇆ NiHL | 3.1 | 0.1 | | NiL + H ⇆ NiHL 3.1 0.1<br>Ni + L ⇆ NiL 18.4 0.1<br>Ni + H + L ⇆ NiHL 21.5 0.1<br>I=0: 23.63575 |
| NiHL + H ⇆ $NiH_2L$ | 0.9 | 1.0 | | NiHL + H ⇆ $NiH_2L$ 0.9 1.0<br>Ni + H + L ⇆ NiHL 21.60415 1.0<br>Ni + 2 H + L ⇆ $NiH_2L$ 22.50415 1.0<br>I=0: 24.73891 |
| NiL ⇆ NiOHL + H | -11.9 | 0.1 | | NiL ⇆ NiOHL + H -11.9 0.1<br>Ni + L ⇆ NiL 18.4 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ni + L + OH ⇆ NiOHL 20.28342 0.1<br>I=0: 21.56487 |
| Cu(II) + L ⇆ Cu(II)L | 18.78 | 0.1 | | I=0: 20.48860 |
| Cu(II)L + H ⇆ Cu(II)HL | 3.1 | 0.1 | | Cu(II)L + H ⇆ Cu(II)HL 3.1 0.1<br>Cu(II) + L ⇆ Cu(II)L 18.78 0.1<br>Cu(II) + H + L ⇆ Cu(II)HL 21.88 0.1<br>I=0: 24.01575 |
| Cu(II)HL + H ⇆ Cu(II)$H_2L$ | 2.0 | 0.1 | | Cu(II)HL + H ⇆ Cu(II)$H_2L$ 2.0 0.1<br>Cu(II) + H + L ⇆ Cu(II)HL 21.88 0.1<br>Cu(II) + 2 H + L ⇆ Cu(II)$H_2L$ 23.88 0.1<br>I=0: 26.22933 |
| Cu(II)L ⇆ Cu(II)OHL + H | -11.4 | 0.1 | | Cu(II)L ⇆ Cu(II)OHL + H -11.4 0.1<br>Cu(II) + L ⇆ Cu(II)L 18.78 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Cu(II) + L + OH ⇆ Cu(II)OHL 21.16342 0.1<br>I=0: 22.44487 |
| Cr(III) + L ⇆ Cr(III)L | 23.4 | 0.1 | 20 | I=0: 25.96290 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Cr(III)L + H ⇆ Cr(III)HL | 1.7 | 0.1 | | Cr(III)L + H ⇆ Cr(III)HL<br>1.7 0.1<br>Cr(III) + L ⇆ Cr(III)L 23.4 0.1<br>Cr(III) + H + L ⇆ Cr(III)HL<br>25.1 0.1<br>I=0: 27.87648 |
| Cr(III)L ⇆ Cr(III)OHL + H | -7.37 | 0.1 | | Cr(III)L ⇆ Cr(III)OHL + H<br>-7.37 0.1<br>Cr(III) + L ⇆ Cr(III)L 23.4 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Cr(III) + L + OH ⇆ Cr(III)OHL<br>29.81342 0.1<br>I=0: 32.16275 |
| Fe(III) + L ⇆ Fe(III)L | 25.1 | 0.1 | | I=0: 27.66290 |
| Fe(III)L + H ⇆ Fe(III)HL | 1.3 | 0.1 | | Fe(III)L + H ⇆ Fe(III)HL<br>1.3 0.1<br>Fe(III) + L ⇆ Fe(III)L 25.1 0.1<br>Fe(III) + L + H ⇆ Fe(III)HL<br>26.4 0.1<br>I=0: 29.17648 |
| Fe(III)L ⇆ Fe(III)OHL + H | -7.39 | 0.1 | | Fe(III)L ⇆ Fe(III)OHL + H<br>-7.39 0.1<br>Fe(III) + L ⇆ Fe(III)L 25.1 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Fe(III) + L + OH ⇆ Fe(III)OHL<br>31.49342 0.1<br>I=0: 33.84275 |
| 2 Fe(III)OHL ⇆ Fe(III)$_2$(OH)$_2$L$_2$ | 2.8 | 1.0 | | 2 Fe(III)OHL ⇆ Fe(III)$_2$(OH)$_2$L$_2$<br>2.8 1.0<br>2 Fe(III) + 2 OH + 2 L ⇆ 2 Fe(III)OHL<br>(2*31.60799) 63.21598 1.0<br>2 Fe(III) + 2 OH + 2 L ⇆<br>Fe(III)$_2$(OH)$_2$L$_2$ 66.01598 1.0<br>I=0: 69.67286 |
| Co(III) + L ⇆ Co(III)L | 41.4 | 0.1 | | I=0: 43.96290 |
| Co(III)L + H ⇆ Co(III)HL | 2.98 | 0.1 | 20 | Co(III)L + H ⇆ Co(III)HL<br>2.98 0.1<br>Co(III) + L ⇆ Co(III)L 41.4 0.1<br>Co(III) + H + L ⇆ Co(III)HL<br>44.38 0.1<br>I=0: 47.15648 |
| Zr + L ⇆ ZrL | 32.8 | | | |
| ZrL ⇆ ZrOHL + H | -6.2 | 0.1 | | ZrL ⇆ ZrOHL + H -6.2 0.1<br>Zr + L ⇆ ZrL 29.38280 0.1<br>H + OH ⇆ $H_2O$ 13.78342 0.1<br>Zr + OH + L ⇆ ZrOHL 36.96622 0.1<br>I=0: 40.38342 |
| 2 ZrOHL ⇆ Zr$_2$(OH)$_2$L$_2$ | 3.5 | 0.1 | | 2 ZrOHL ⇆ Zr$_2$(OH)$_2$L$_2$ 3.5 0.1<br>2 Zr + 2 OH + 2 L ⇆ 2 ZrOHL<br>(2*36.96622) 73.93244 0.1<br>2 Zr + 2 OH + 2 L ⇆ Zr$_2$(OH)$_2$L$_2$<br>77.43244 0.1<br>I=0: 84.05327 |
| Hf + L ⇆ HfL | 33.7 | | | |
| Ag + L ⇆ AgL | 7.20 | 0.1 | | I=0: 8.05430 |
| AgL + H ⇆ AgHL | 6.04 | 0.1 | | AgL + H ⇆ AgHL 6.04 0.1<br>Ag + L ⇆ AgL 7.20 0.1<br>Ag + H + L ⇆ AgHL 13.24 0.1<br>I=0: 14.73503 |
| 2 Ag + L ⇆ Ag$_2$L | 7.6 | 1.0 | | I=0: 9.02212 |
| Pd + L ⇆ PdL | 25.6 | 0.1 | 20 | I=0: 27.30860 |
| PdL + H ⇆ PdHL | 3.01 | 1.0 | 20 | PdL + H ⇆ PdHL 3.01 1.0<br>Pd + L ⇆ PdL 25.68332 1.0<br>Pd + H + L ⇆ PdHL 28.69332 1.0<br>I=0: 30.72492 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| PdHL + H ⇆ PdH$_2$L | 2.31 | 1.0 | 20 | PdHL + H ⇆ PdH$_2$L 2.31 1.0<br>Pd + H + L ⇆ PdHL 28.69332 1.0<br>Pd + 2 H + L ⇆ PdH$_2$L 31.00332 1.0<br>I=0: 33.23808 |
| PdH$_2$L + H ⇆ PdH$_3$L | 0.9 | 1.0 | 20 | PdH$_2$L + H ⇆ PdH$_3$L 0.9 1.0<br>Pd + 2 H + L ⇆ PdH$_2$L 31.00332 1.0<br>Pd + 3 H + L ⇆ PdH$_3$L 31.90332 1.0<br>I=0: 34.13808 |
| Zn + L ⇆ ZnL | 18.0 | | | |
| ZnL + H ⇆ ZnHL | 3.0 | 0.1 | | ZnL + H ⇆ ZnHL 3.0 0.1<br>Zn + L ⇆ ZnL 16.29140 0.1<br>Zn + H + L ⇆ ZnHL 19.29140 0.1<br>I=0: 21.42715 |
| ZnHL + H ⇆ ZnH$_2$L | 1.2 | 1.0 | | ZnHL + H ⇆ ZnH$_2$L 1.2 1.0<br>Zn + H + L ⇆ ZnHL 19.39555 1.0<br>Zn + 2 H + L ⇆ ZnH$_2$L 20.59555 1.0<br>I=0: 22.83031 |
| ZnL ⇆ ZnOHL + H | -11.6 | 0.1 | | ZnL ⇆ ZnOHL + H -11.6 0.1<br>Zn + L ⇆ ZnL 16.29140 0.1<br>OH + H ⇆ H$_2$O 13.78342 0.1<br>Zn + L + OH ⇆ ZnOHL 18.47482 0.1<br>I=0: 19.75627 |
| Cd + L ⇆ CdL | 18.1 | | | |
| CdL + H ⇆ CdHL | 2.9 | 0.1 | | CdL + H ⇆ CdHL 2.9 0.1<br>Cd + L ⇆ CdL 16.39140 0.1<br>Cd + H + L ⇆ CdHL 19.29140 0.1<br>I=0: 21.42715 |
| CdHL + H ⇆ CdH$_2$L | 1.6 | 1.0 | | CdHL + H ⇆ CdH$_2$L 1.6 1.0<br>Cd + H + L ⇆ CdHL 19.39555 1.0<br>Cd + 2 H + L ⇆ CdH$_2$L 20.99555 1.0<br>I=0: 23.23031 |
| CdL ⇆ CdOHL + H | -13.2 | 1.0 | | CdL ⇆ CdOHL + H -13.2 1.0<br>Cd + L ⇆ CdL 16.47472 1.0<br>OH + H ⇆ H$_2$O 13.79384 1.0<br>Cd + OH + L ⇆ CdOHL 17.06856 1.0<br>I=0: 18.28752 |
| Hg(II) + L ⇆ Hg(II)L | 21.5 | 0.1 | | I=0: 23.20860 |
| Hg(II)L + H ⇆ Hg(II)HL | 3.2 | 0.1 | | Hg(II)L + H ⇆ Hg(II)HL 3.2 0.1<br>Hg(II) + L ⇆ Hg(II)L 21.5 0.1<br>Hg(II) + H + L ⇆ Hg(II)HL<br>24.7 0.1<br>I=0: 26.83575 |
| Hg(II)HL + H ⇆ Hg(II)H$_2$L | 2.1 | 1.0 | | Hg(II)HL + H ⇆ Hg(II)H$_2$L 2.1 1.0<br>Hg(II) + H + L ⇆ Hg(II)HL<br>24.80415 1.0<br>Hg(II) + 2 H + L ⇆ Hg(II)H$_2$L<br>26.90415 1.0<br>I=0: 29.13891 |
| Hg(II)L ⇆ Hg(II)OHL + H | -8.9 | 0.1 | | Hg(II)L ⇆ Hg(II)OHL + H<br>-8.9 0.1<br>Hg(II) + L ⇆ Hg(II)L 21.5 0.1<br>OH + H ⇆ H$_2$O 13.78342 0.1<br>Hg(II) + L + OH ⇆ Hg(II)(OH)L<br>26.38342 0.1<br>I=0: 27.66487 |
| Sn(II) + L ⇆ Sn(II)L | 18.3 | 1.0 | 20 | I=0: 19.92528 |
| Sn(II)L + H ⇆ Sn(II)HL | 2.5 | 1.0 | 20 | Sn(II)L + H ⇆ Sn(II)HL 2.5 1.0<br>Sn + L ⇆ SnL 18.3 1.0<br>Sn + H + L ⇆ SnHL 20.8 1.0<br>I=0: 22.83160 |
| Sn(II)HL + H ⇆ Sn(II)H$_2$L | 1.5 | 1.0 | 20 | Sn(II)HL + H ⇆ Sn(II)H$_2$L 1.5 1.0<br>Sn + H + L ⇆ SnHL 20.8 1.0<br>Sn + 2 H + L ⇆ SnH$_2$L 22.3 1.0<br>I=0: 24.53476 |
| Pb(II) + L ⇆ Pb(II)L | 18.0 | 0.1 | | I=0: 19.70860 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Pb(II)L + H ⇆ Pb(II)HL | 2.4 | 1.0 | | Pb(II)L + H ⇆ Pb(II)HL 2.4 0.1<br>Pb + L ⇆ PbL 18.0 0.1<br>Pb + H + L ⇆ PbHL 20.4 0.1<br>I=0: 22.53575 |
| Pb(II)HL + H ⇆ Pb(II)$H_2$L | 1.7 | 1.0 | | Pb(II)HL + H ⇆ Pb(II)$H_2$L 1.7 1.0<br>Pb + H + L ⇆ PbHL 20.50415 1.0<br>Pb + 2 H + L ⇆ Pb$H_2$L 22.20415 1.0<br>I=0: 24.43891 |
| Pb(II)$H_2$L + H ⇆ Pb(II)$H_3$L | 1.2 | 1.0 | | Pb(II)$H_2$L + H ⇆ Pb(II)$H_3$L<br>1.2 1.0<br>Pb + 2 H + L ⇆ Pb$H_2$L 22.20415 1.0<br>Pb + 3 H + L ⇆ Pb$H_3$L 23.40415 1.0<br>I=0: 25.63891 |
| Al + L ⇆ AlL | 16.4 | 0.1 | | I=0: 18.96290 |
| AlL + H ⇆ AlHL | 2.6 | 0.1 | | AlL + H ⇆ AlHL 2.6 0.1<br>Al + L ⇆ AlL 16.4 0.1<br>Al + H + L ⇆ AlHL 19.0 0.1<br>I=0: 21.77648 |
| AlL ⇆ AlOHL + H | -5.9 | 0.1 | | AlL ⇆ AlOHL + H -5.9 0.1<br>Al + L ⇆ AlL 16.4 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + OH + L ⇆ AlOHL 24.28342 0.1<br>I=0: 26.63275 |
| AlOHL ⇆ Al$(OH)_2$L + H | -10.31 | 0.1 | | AlOHL ⇆ Al$(OH)_2$L + H -10.31 0.1<br>Al + OH + L ⇆ AlOHL 24.28342 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Al + 2 OH + L ⇆ Al$(OH)_2$L<br>27.75684 0.1<br>I=0: 29.67902 |
| Ga + L ⇆ GaL | 21.7 | 0.1 | | I=0: 24.26290 |
| GaL + H ⇆ GaHL | 1.7 | 0.1 | | GaL + H ⇆ GaHL 1.7 0.1<br>Ga + L ⇆ GaL 21.7 0.1<br>Ga + H + L ⇆ GaHL 23.4 0.1<br>I=0: 26.17648 |
| GaL ⇆ GaOHL + H | -5.58 | 0.1 | | GaL ⇆ GaOHL + H -5.58 0.1<br>Ga + L ⇆ GaL 21.7 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Ga + L + OH ⇆ GaOHL 29.90342 0.1<br>I=0: 32.25275 |
| In + L ⇆ InL | 25.0 | 0.1 | | I=0: 27.56290 |
| InL + H ⇆ InHL | 0.7 | 0.5 | | InL + H ⇆ InHL 0.7 0.5<br>In + L ⇆ InL 24.34224 0.5<br>In + H + L ⇆ InHL 25.04224 0.5<br>I=0: 28.53129 |
| InL ⇆ InOHL + H | -8.43 | 0.1 | | InL ⇆ InOHL + H -8.43 0.1<br>In + L ⇆ InL 25.0 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>In + L + OH ⇆ InOHL 30.35342 0.1<br>I=0: 32.70275 |
| As(III)$(OH)_2$ + HL ⇆ As(III)$(OH)_2$HL | 9.2 | 0.1 | 20 | (can not be related to components; not entered) |
| Bi + L ⇆ BiL | 26.5 | 1.0 | | I=0: 28.93792 |
| BiL + H ⇆ BiHL | 1.4 | 0.1 | | BiL + H ⇆ BiHL 1.4 0.1<br>Bi + L ⇆ BiL 26.37502 0.1<br>Bi + H + L ⇆ BiHL 27.77502 0.1<br>I=0: 30.55150 |
| BiL ⇆ BiOHL + H | -10.6 | 0.1 | | BiL ⇆ BiOHL + H -10.6 0.1<br>Bi + L ⇆ BiL 26.37502 0.1<br>OH + H ⇆ $H_2O$ 13.78342 0.1<br>Bi + L + OH ⇆ BiOHL 29.55844 0.1<br>I=0: 31.90777 |

## Part II: other references

As already stated in the introduction, the NIST data were extended with data from other sources. In part II, you will find these data, grouped by (1) type of equilibria/species and (2) source. See the appendix for comparison of common data between the NIST and these sources.

### *II.1 Complexes*

#### II.1.1 Turner et al.

Since Turner *et al.* state their values with two decimals, all calculations were done with two decimals.

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Be + 3 $H_2O$ ⇆ $Be(OH)_3$ + 3 H | -23.25 | | | Be + 3 $H_2O$ ⇆ $Be(OH)_3$ + 3 H -23.25<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Be + 3 OH ⇆ $Be(OH)_3$ 18.75 |
| Be + 4 $H_2O$ ⇆ $Be(OH)_4$ + 4 H | -37.41 | | | Be + 4 $H_2O$ ⇆ $Be(OH)_4$ + 4 H -37.41<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Be + 4 OH ⇆ $Be(OH)_4$ 18.59 |
| Be + 2 Cl ⇆ $BeCl_2$ | -0.54 | | | |
| Na + $HVO_4$ ⇆ $NaHVO_4$ | 1.16 | | | Na + $HVO_4$ ⇆ $NaHVO_4$ 1.16<br>H + $VO_4$ ⇆ $HVO_4$ 14.3<br>Na + H + $VO_4$ ⇆ $NaHVO_4$ 15.46 |
| Na + $(CrO_4)$ ⇆ $Na(CrO_4)$ | 0.70 | | | |
| Mg + $(PO_4)$ ⇆ $Mg(PO_4)$ | 4.85 | | | |
| Al + $CO_3$ ⇆ $Al(CO_3)$ | 8.43 | | | |
| Al + 5 F ⇆ $AlF_5$ | 20.73 | | | |
| Al + 6 F ⇆ $AlF_6$ | 20.46 | | | |
| K + $HVO_4$ ⇆ $KHVO_4$ | | | | K + $HVO_4$ ⇆ $KHVO_4$ 0.90<br>H + $VO_4$ ⇆ $HVO_4$ 14.3<br>K + H + $VO_4$ ⇆ $KHVO_4$ 15.20 |
| Ca + $(PO_4)$ ⇆ $Ca(PO_4)$ | 6.46 | | | |
| Sc + $CO_3$ ⇆ $Sc(CO_3)$ | 10.10 | | | |
| Sc + 2 Cl ⇆ $ScCl_2$ | 1.57 | | | |
| Cr(III) + 3 $H_2O$ ⇆ $Cr(III)(OH)_3$ + 3 H | -18.00 | | | Cr(III) + 3 $H_2O$ ⇆ $Cr(III)(OH)_3$ + 3 H -18.00<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Cr(III) + 3 OH ⇆ $Cr(III)(OH)_3$ 24.00 |
| Cr(III) + 4 $H_2O$ ⇆ $Cr(III)(OH)_4$ + 4 H | -27.40 | | | Cr(III) + 4 $H_2O$ ⇆ $Cr(III)(OH)_4$ + 4 H -27.40<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Cr(III) + 4 OH ⇆ $Cr(III)(OH)_4$ 28.60 |
| Mn(II) + 2 $H_2O$ ⇆ $Mn(II)(OH)_2$ + 2 H | -22.20 | | | Mn(II) + 2 $H_2O$ ⇆ $Mn(II)(OH)_2$ + 2 H -22.20<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Mn(II) + 2 OH ⇆ $Mn(II)(OH)_2$ 5.80 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Mn(II) + 3 $H_2O$ ⇆ Mn(II)$(OH)_3$ + 3 H | -34.80 | | | Mn(II) + 3 $H_2O$ ⇆ Mn(II)$(OH)_3$ + 3 H -34.80<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Mn(II) + 3 OH ⇆ Mn(II)$(OH)_3$ 7.20 |
| Fe(II) + 4 $H_2O$ ⇆ Fe(II)$(OH)_4$ + 4 H | -46.00 | | | Fe(II) + 4 $H_2O$ ⇆ Fe(II)$(OH)_4$ + 4 H -46.00<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Fe(II) + 4 OH ⇆ Fe(II)$(OH)_4$ 10.00 |
| Fe(II) + $CO_3$ ⇆ Fe(II)$(CO_3)$ | 4.73 | | | |
| Fe(III) + $CO_3$ ⇆ Fe(III)$(CO_3)$ | 9.72 | | | |
| Fe(III) + 2 $(SO_4)$2 ⇆ Fe(III) $(SO_4)_2$ | 5.38 | | | |
| Fe(III) + 3 Cl ⇆ Fe(III)$Cl_3$ | 0.99 | | | |
| Co(II) + 4 $H_2O$ ⇆ Co(II)$(OH)_4$ + 4 H | -46.30 | | | Co(II) + 4 $H_2O$ ⇆ Co(II)$(OH)_4$ + 4 H -46.30<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Co(II) + 4 OH ⇆ Co(II) $(OH)_4$ 9.70 |
| Ni + 4 $H_2O$ ⇆ Ni$(OH)_4$ + 4 H | -44.00 | | | Ni + 4 $H_2O$ ⇆ Ni$(OH)_4$ + 4 H -44.00<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Ni + 4 OH ⇆ Ni$(OH)_4$ 12.00 |
| Ni + 2 $SO_4$ ⇆ Ni$(SO_4)_2$ | 3.2 | | | |
| Cu(II) + 2 $H_2O$ ⇆ Cu(II) $(OH)_2$ + 2 H | -17.30 | | | Cu(II) + 2 $H_2O$ ⇆ Cu(II) $(OH)_2$ + 2 H -17.30<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Cu(II) + 2 OH ⇆ Cu(II) $(OH)_2$ 10.70 |
| Cu(II) + 3 $H_2O$ ⇆ Cu(II) $(OH)_3$ + 3 H | -27.80 | | | Cu(II) + 3 $H_2O$ ⇆ Cu(II) $(OH)_3$ + 3 H -27.80<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Cu(II) + 3 OH ⇆ Cu(II) $(OH)_3$ 14.20 |
| Cu(II) + 4 $H_2O$ ⇆ Cu(II) $(OH)_4$ + 4 H | -39.60 | | | Cu(II) + 4 $H_2O$ ⇆ Cu(II) $(OH)_4$ + 4 H -39.60<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Cu(II) + 4 OH ⇆ Cu(II) $(OH)_4$ 16.40 |
| Zn + 2 $SO_4$ ⇆ Zn$(SO_4)_2$ | 3.63 | | | |
| Zn + 3 $SO_4$ ⇆ Zn$(SO_4)_3$ | 2.70 | | | |
| Zn + 4 $SO_4$ ⇆ Zn$(SO_4)_4$ | -0.82 | | | |
| Zn + 2 Cl ⇆ $ZnCl_2$ | 0.62 | | | |
| Zn + 3 Cl ⇆ $ZnCl_3$ | 0.51 | | | |
| Zn + 4 Cl ⇆ $ZnCl_4$ | 0.20 | | | |
| Ga + 3 $H_2O$ ⇆ Ga$(OH)_3$ + 3 H | -10.30 | | | Ga + 3 $H_2O$ ⇆ Ga$(OH)_3$ + 3 H -10.30<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Ga + 3 OH ⇆ Ga$(OH)_3$ 31.70 |
| Ga + 4 $H_2O$ ⇆ Ga$(OH)_4$ + 4 H | -16.60 | | | Ga + 4 $H_2O$ ⇆ Ga$(OH)_4$ + 4 H -16.60<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Ga + 4 OH ⇆ Ga$(OH)_4$ 39.40 |
| Ga + $CO_3$ ⇆ Ga$(CO_3)$ | 8.79 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Y + 2 H_2O \leftrightarrows Y(OH)_2 + 2 H$ | -16.40 | | | $Y + 2 H_2O \leftrightarrows Y(OH)_2 + 2 H$ -16.40<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$Y + 2 OH \leftrightarrows Y(OH)_2$ 11.60 |
| $Y + 3 H_2O \leftrightarrows Y(OH)_3 + 3 H$ | -26.00 | | | $Y + 3 H_2O \leftrightarrows Y(OH)_3 + 3 H$ -26.00<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$Y + 3 OH \leftrightarrows Y(OH)_3$ 16.00 |
| $Y + 4 H_2O \leftrightarrows Y(OH)_4 + 4 H$ | -36.50 | | | $Y + 4 H_2O \leftrightarrows Y(OH)_4 + 4 H$ -36.50<br>$4 H + 4 OH \leftrightarrows 4 H_2O$<br>(4*14.00) 56.00<br>$Y + 4 OH \leftrightarrows Y(OH)_4$ 19.50 |
| $Zr + 2 H_2O \leftrightarrows Zr(OH)_2 + 2 H$ | -1.70 | | | $Zr + 2 H_2O \leftrightarrows Zr(OH)_2 + 2 H$ -1.70<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$Zr + 2 OH \leftrightarrows Zr(OH)_2$ 26.30 |
| $Zr + 3 H_2O \leftrightarrows Zr(OH)_3 + 3 H$ | -5.10 | | | $Zr + 3 H_2O \leftrightarrows Zr(OH)_3 + 3 H$ -5.10<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$Zr + 3 OH \leftrightarrows Zr(OH)_3$ 36.90 |
| $Zr + 2 Cl \leftrightarrows ZrCl_2$ | 1.47 | | | Note: data for these equilibria do occur in the NIST database but for ionic strengths of 6.5 M; see page 45. |
| $Zr + 3 Cl \leftrightarrows ZrCl_3$ | 0.80 | | | |
| $Cd + 2 F \leftrightarrows CdF_2$ | 1.41 | | | |
| $Cd + 2 SO_4 \leftrightarrows Cd(SO_4)_2$ | 3.44 | | | |
| $Cd + 3 SO_4 \leftrightarrows Cd(SO_4)_3$ | 3.09 | | | |
| $Cd + 4 SO_4 \leftrightarrows Cd(SO_4)_4$ | -0.72 | | | |
| $Cd + 4 Cl \leftrightarrows CdCl_4$ | 1.47 | | | |
| $In + CO_3 \leftrightarrows InCO_3$ | 7.60 | | | |
| $Sn(IV) + H_2O \leftrightarrows Sn(IV)(OH) + H$ | 1.50 | | | $Sn(IV) + H_2O \leftrightarrows Sn(IV)(OH) + H$ 1.50<br>$H + OH \leftrightarrows H_2O$ 14.00<br>$Sn(IV) + OH \leftrightarrows Sn(IV)(OH)$ 15.50 |
| $Sn(IV) + 2 H_2O \leftrightarrows Sn(IV)(OH)_2 + 2 H$ | 1.31 | | | $Sn(IV) + 2 H_2O \leftrightarrows Sn(IV)(OH)_2 + 2 H$ 1.31<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$Sn(IV) + 2 OH \leftrightarrows Sn(IV)(OH)_2$ 29.31 |
| $Sn(IV) + 3 H_2O \leftrightarrows Sn(IV)(OH)_3 + 3 H$ | 1.70 | | | $Sn(IV) + 3 H_2O \leftrightarrows Sn(IV)(OH)_3 + 3 H$ 1.70<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$Sn(IV) + 3 OH \leftrightarrows Sn(IV)(OH)_3$ 43.70 |
| $Sn(IV) + 4 H_2O \leftrightarrows Sn(IV)(OH)_4 + 4 H$ | 0.51 | | | $Sn(IV) + 4 H_2O \leftrightarrows Sn(IV)(OH)_4 + 4 H$ 0.51<br>$4 H + 4 OH \leftrightarrows 4 H_2O$<br>(4*14.00) 56.00<br>$Sn(IV) + 4 OH \leftrightarrows Sn(IV)(OH)_4$ 56.51 |
| $Ba + 2 SO_4 \leftrightarrows Ba(SO_4)_2$ | 3.20 | | | |
| $La + 2 H_2O \leftrightarrows La(OH)_2 + 2 H$ | -17.40 | | | $La + 2 H_2O \leftrightarrows La(OH)_2 + 2 H$ -17.40<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$La + 2 OH \leftrightarrows La(OH)_2$ 10.60 |
| $La + 3 H_2O \leftrightarrows La(OH)_3 + 3 H$ | -27.50 | | | $La + 3 H_2O \leftrightarrows La(OH)_3 + 3 H$ -27.50<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$La + 3 OH \leftrightarrows La(OH)_3$ 14.50 |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $La + 4\ H_2O \leftrightarrows La(OH)_4 + 4\ H$ | -38.80 | | | $La + 4\ H_2O \leftrightarrows La(OH)_4 + 4\ H$ -38.80<br>$4\ H + 4\ OH \leftrightarrows 4\ H_2O$<br>(4*14.00) 56.00<br>$La + 4\ OH \leftrightarrows La(OH)_4$ 17.20 |
| $La + 2\ Cl \leftrightarrows LaCl_2$ | -0.29 | | | |
| $Ce + 2\ H_2O \leftrightarrows Ce(OH)_2 + 2\ H$ | -17.10 | | | $Ce + 2\ H_2O \leftrightarrows Ce(OH)_2 + 2\ H$ -17.10<br>$2\ H + 2\ OH \leftrightarrows 2\ H_2O$<br>(2*14.00) 28.00<br>$Ce + 2\ OH \leftrightarrows Ce(OH)_2$ 10.90 |
| $Ce + 3\ H_2O \leftrightarrows Ce(OH)_3 + 3\ H$ | -26.80 | | | $Ce + 3\ H_2O \leftrightarrows Ce(OH)_3 + 3\ H$ -26.80<br>$3\ H + 3\ OH \leftrightarrows 3\ H_2O$<br>(3*14.00) 42.00<br>$Ce + 3\ OH \leftrightarrows Ce(OH)_3$ 15.20 |
| $Ce + 4\ H_2O \leftrightarrows Ce(OH)_4 + 4\ H$ | -37.60 | | | $Ce + 4\ H_2O \leftrightarrows Ce(OH)_4 + 4\ H$ -37.60<br>$4\ H + 4\ OH \leftrightarrows 4\ H_2O$<br>(4*14.00) 56.00<br>$Ce + 4\ OH \leftrightarrows Ce(OH)_4$ 18.40 |
| $Ce + 2\ Cl \leftrightarrows CeCl_2$ | 1.19 | | | |
| $Pr + 2\ H_2O \leftrightarrows Pr(OH)_2 + 2\ H$ | -17.00 | | | $Pr + 2\ H_2O \leftrightarrows Pr\ (OH)_2 + 2\ H$ -17.00<br>$2\ H + 2\ OH \leftrightarrows 2\ H_2O$<br>(2*14.00) 28.00<br>$Pr + 2\ OH \leftrightarrows Pr(OH)_2$ 11.00 |
| $Pr + 3\ H_2O \leftrightarrows Pr(OH)_3 + 3\ H$ | -26.60 | | | $Pr + 3\ H_2O \leftrightarrows Pr(OH)_3 + 3\ H$ -26.60<br>$3\ H + 3\ OH \leftrightarrows 3\ H_2O$<br>(3*14.00) 42.00<br>$Pr + 3\ OH \leftrightarrows Pr(OH)_3$ 15.40 |
| $Pr + 4\ H_2O \leftrightarrows Pr(OH)_4 + 4\ H$ | -37.20 | | | $Pr + 4\ H_2O \leftrightarrows Pr(OH)_4 + 4\ H$ -37.20<br>$4\ H + 4\ OH \leftrightarrows 4\ H_2O$<br>(4*14.00) 56.00<br>$Pr + 4\ OH \leftrightarrows Pr(OH)_4$ 18.80 |
| $Pr + 2\ Cl \leftrightarrows PrCl_2$ | -0.29 | | | |
| $Nd + 2\ H_2O \leftrightarrows Nd(OH)_2 + 2\ H$ | -16.90 | | | $Nd + 2\ H_2O \leftrightarrows Nd(OH)_2 + 2\ H$ -16.90<br>$2\ H + 2\ OH \leftrightarrows 2\ H_2O$<br>(2*14.00) 28.00<br>$Nd + 2\ OH \leftrightarrows Nd(OH)_2$ 11.10 |
| $Nd + 3\ H_2O \leftrightarrows Nd(OH)_3 + 3\ H$ | -26.50 | | | $Nd + 3\ H_2O \leftrightarrows Nd(OH)_3 + 3\ H$ -26.50<br>$3\ H + 3\ OH \leftrightarrows 3\ H_2O$<br>(3*14.00) 42.00<br>$Nd + 3\ OH \leftrightarrows Nd(OH)_3$ 15.50 |
| $Nd + Cl \leftrightarrows NdCl$ | 0.80 | | | |
| $Nd + 2\ Cl \leftrightarrows NdCl_2$ | -0.29 | | | |
| $Sm + 2\ H_2O \leftrightarrows Sm(OH)_2 + 2\ H$ | -16.60 | | | $Sm + 2\ H_2O \leftrightarrows Sm(OH)_2 + 2\ H$ -16.60<br>$2\ H + 2\ OH \leftrightarrows 2\ H_2O$<br>(2*14.00) 28.00<br>$Sm + 2\ OH \leftrightarrows Sm(OH)_2$ 11.40 |
| $Sm + 3\ H_2O \leftrightarrows Sm(OH)_3 + 3\ H$ | -25.80 | | | $Sm + 3\ H_2O \leftrightarrows Sm(OH)_3 + 3\ H$ -25.80<br>$3\ H + 3\ OH \leftrightarrows 3\ H_2O$<br>(3*14.00) 42.00<br>$Sm + 3\ OH \leftrightarrows Sm(OH)_3$ 16.20 |
| $Sm + 4\ H_2O \leftrightarrows Sm(OH)_4 + 4\ H$ | -35.70 | | | $Sm + 4\ H_2O \leftrightarrows Sm(OH)_4 + 4\ H$ -35.70<br>$4\ H + 4\ OH \leftrightarrows 4\ H_2O$<br>(4*14.00) 56.00<br>$Sm + 4\ OH \leftrightarrows Sm(OH)_4$ 20.30 |
| $Sm + 2\ Cl \leftrightarrows SmCl_2$ | -0.29 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Eu + 2 $H_2O$ ⇆ $Eu(OH)_2$ + 2 H | -16.60 | | | Eu + 2 $H_2O$ ⇆ $Eu(OH)_2$ + 2 H -16.60<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Eu + 2 OH ⇆ $Eu(OH)_2$ 11.40 |
| Eu + 3 $H_2O$ ⇆ $Eu(OH)_3$ + 3 H | -25.60 | | | Eu + 3 $H_2O$ ⇆ $Eu(OH)_3$ + 3 H -25.60<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Eu + 3 OH ⇆ $Eu(OH)_3$ 16.40 |
| Eu + 4 $H_2O$ ⇆ $Eu(OH)_4$ + 4 H | -35.30 | | | Eu + 4 $H_2O$ ⇆ $Eu(OH)_4$ + 4 H -35.30<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Eu + 4 OH ⇆ $Eu(OH)_4$ 20.70 |
| Eu + 2 Cl ⇆ $EuCl_2$ | 0.99 | | | |
| Gd + 2 $H_2O$ ⇆ $Gd(OH)_2$ + 2 H | -16.40 | | | Gd + 2 $H_2O$ ⇆ $Gd(OH)_2$ + 2 H -16.40<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Gd + 2 OH ⇆ $Gd(OH)_2$ 11.60 |
| Gd + 3 $H_2O$ ⇆ $Gd(OH)_3$ + 3 H | -25.20 | | | Gd + 3 $H_2O$ ⇆ $Gd(OH)_3$ + 3 H -25.20<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Gd + 3 OH ⇆ $Gd(OH)_3$ 16.80 |
| Gd + 4 $H_2O$ ⇆ $Gd(OH)_4$ + 4 H | -34.40 | | | Gd + 4 $H_2O$ ⇆ $Gd(OH)_4$ + 4 H -34.40<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Gd + 4 OH ⇆ $Gd(OH)_4$ 21.60 |
| Gd + 2 Cl ⇆ $GdCl_2$ | -0.29 | | | |
| Tb + 2 $H_2O$ ⇆ $Tb(OH)_2$ + 2 H | -16.30 | | | Tb + 2 $H_2O$ ⇆ $Tb(OH)_2$ + 2 H -16.30<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Tb + 2 OH ⇆ $Tb(OH)_2$ 11.70 |
| Tb + 3 $H_2O$ ⇆ $Tb(OH)_3$ + 3 H | -25.10 | | | Tb + 3 $H_2O$ ⇆ $Tb(OH)_3$ + 3 H -25.10<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Tb + 3 OH ⇆ $Tb(OH)_3$ 16.90 |
| Tb + 4 $H_2O$ ⇆ $Tb(OH)_4$ + 4 H | -34.30 | | | Tb + 4 $H_2O$ ⇆ $Tb(OH)_4$ + 4 H -34.30<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Tb + 4 OH ⇆ $Tb(OH)_4$ 21.70 |
| Tb + 2 Cl ⇆ $TbCl_2$ | -0.29 | | | |
| Dy + 2 $H_2O$ ⇆ $Dy(OH)_2$ + 2 H | -16.20 | | | Dy + 2 $H_2O$ ⇆ $Dy(OH)_2$ + 2 H -16.20<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Dy + 2 OH ⇆ $Dy(OH)_2$ 11.80 |
| Dy + 3 $H_2O$ ⇆ $Dy(OH)_3$ + 3 H | -24.70 | | | Dy + 3 $H_2O$ ⇆ $Dy(OH)_3$ + 3 H -24.70<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Dy + 3 OH ⇆ $Dy(OH)_3$ 17.30 |
| Dy + 4 $H_2O$ ⇆ $Dy(OH)_4$ + 4 H | -33.50 | | | Dy + 4 $H_2O$ ⇆ $Dy(OH)_4$ + 4 H -33.50<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Dy + 4 OH ⇆ $Dy(OH)_4$ 22.50 |
| Dy + Cl ⇆ DyCl | 0.80 | | | |
| Dy + 2 Cl ⇆ $DyCl_2$ | -0.29 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
| --- | --- | --- | --- | --- |
| Ho + 2 $H_2O$ ⇆ $Ho(OH)_2$ + 2 H | -16.10 | | | Ho + 2 $H_2O$ ⇆ $Ho(OH)_2$ + 2 H<br>-16.10<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Ho + 2 OH ⇆ $Ho(OH)_2$ 11.90 |
| Ho + 3 $H_2O$ ⇆ $Ho(OH)_3$ + 3 H | -24.60 | | | Ho + 3 $H_2O$ ⇆ $Ho(OH)_3$ + 3 H<br>-24.60<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Ho + 3 OH ⇆ $Ho(OH)_3$ 17.40 |
| Ho + 4 $H_2O$ ⇆ $Ho(OH)_4$ + 4 H | -33.40 | | | Ho + 4 $H_2O$ ⇆ $Ho(OH)_4$ + 4 H<br>-33.40<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Ho + 4 OH ⇆ $Ho(OH)_4$ 22.60 |
| Ho + Cl ⇆ HoCl | 0.80 | | | |
| Ho + 2 Cl ⇆ $HoCl_2$ | -0.29 | | | |
| Er + 2 $H_2O$ ⇆ $Er(OH)_2$ + 2 H | -15.90 | | | Er + 2 $H_2O$ ⇆ $Er(OH)_2$ + 2 H<br>-15.90<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Er + 2 OH ⇆ $Er(OH)_2$ 12.10 |
| Er + 3 $H_2O$ ⇆ $Er(OH)_3$ + 3 H | -24.20 | | | Er + 3 $H_2O$ ⇆ $Er(OH)_3$ + 3 H<br>-24.20<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Er + 3 OH ⇆ $Er(OH)_3$ 17.80 |
| Er + 4 $H_2O$ ⇆ $Er(OH)_4$ + 4 H | -32.60 | | | Er + 4 $H_2O$ ⇆ $Er(OH)_4$ + 4 H<br>-32.60<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Er + 4 OH ⇆ $Er(OH)_4$ 23.40 |
| Er + Cl ⇆ ErCl | 0.80 | | | |
| Er + 2 Cl ⇆ $ErCl_2$ | -0.29 | | | |
| Tm + 2 $H_2O$ ⇆ $Tm(OH)_2$ + 2 H | -15.90 | | | Tm + 2 $H_2O$ ⇆ $Tm(OH)_2$ + 2 H<br>-15.90<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Tm + 2 OH ⇆ $Tm(OH)_2$ 12.10 |
| Tm + 3 $H_2O$ ⇆ $Tm(OH)_3$ + 3 H | -24.10 | | | Tm + 3 $H_2O$ ⇆ $Tm(OH)_3$ + 3 H<br>-24.10<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Tm + 3 OH ⇆ $Tm(OH)_3$ 17.90 |
| Tm + 4 $H_2O$ ⇆ $Tm(OH)_4$ + 4 H | -32.60 | | | Tm + 4 $H_2O$ ⇆ $Tm(OH)_4$ + 4 H<br>-32.60<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Tm + 4 OH ⇆ $Tm(OH)_4$ 23.40 |
| Tm + 2 Cl ⇆ $TmCl_2$ | -0.29 | | | |
| Yb + 2 $H_2O$ ⇆ $Yb(OH)_2$ + 2 H | -15.80 | | | Yb + 2 $H_2O$ ⇆ $Yb(OH)_2$ + 2 H<br>-15.80<br>2 H + 2 OH ⇆ 2 $H_2O$<br>(2*14.00) 28.00<br>Yb + 2 OH ⇆ $Yb(OH)_2$ 12.20 |
| Yb + 3 $H_2O$ ⇆ $Yb(OH)_3$ + 3 H | -24.10 | | | Yb + 3 $H_2O$ ⇆ $Yb(OH)_3$ + 3 H<br>-24.10<br>3 H + 3 OH ⇆ 3 $H_2O$<br>(3*14.00) 42.00<br>Yb + 3 OH ⇆ $Yb(OH)_3$ 17.90 |
| Yb + 4 $H_2O$ ⇆ $Yb(OH)_4$ + 4 H | -32.70 | | | Yb + 4 $H_2O$ ⇆ $Yb(OH)_4$ + 4 H<br>-32.70<br>4 H + 4 OH ⇆ 4 $H_2O$<br>(4*14.00) 56.00<br>Yb + 4 OH ⇆ $Yb(OH)_4$ 23.30 |
| Yb + 2 Cl ⇆ $YbCl_2$ | -0.29 | | | |

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Lu + 2 H_2O \leftrightarrows Lu(OH)_2 + 2 H$ | -15.70 | | | $Lu + 2 H_2O \leftrightarrows Lu(OH)_2 + 2 H$<br>-15.70<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$Lu + 2 OH \leftrightarrows Lu(OH)_2$ 12.30 |
| $Lu + 3 H_2O \leftrightarrows Lu(OH)_3 + 3 H$ | -23.70 | | | $Lu + 3 H_2O \leftrightarrows Lu(OH)_3 + 3 H$<br>-23.70<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$Lu + 3 OH \leftrightarrows Lu(OH)_3$ 18.30 |
| $Lu + 4 H_2O \leftrightarrows Lu(OH)_4 + 4 H$ | -31.80 | | | $Lu + 4 H_2O \leftrightarrows Lu(OH)_4 + 4 H$<br>-31.80<br>$4 H + 4 OH \leftrightarrows 4 H_2O$<br>(4*14.00) 56.00<br>$Lu + 4 OH \leftrightarrows Lu(OH)_4$ 24.20 |
| $Lu + 2 Cl \leftrightarrows LuCl_2$ | -0.29 | | | |
| $Hf + 2 H_2O \leftrightarrows Hf(OH)_2 + 2 H$ | -2.40 | | | $Hf + 2 H_2O \leftrightarrows Hf(OH)_2 + 2 H$<br>-2.40<br>$2 H + 2 OH \leftrightarrows 2 H_2O$<br>(2*14.00) 28.00<br>$Hf + 2 OH \leftrightarrows Hf(OH)_2$ 25.60 |
| $Hf + 3 H_2O \leftrightarrows Hf(OH)_3 + 3 H$ | -6.00 | | | $Hf + 3 H_2O \leftrightarrows Hf(OH)_3 + 3 H$<br>-6.00<br>$3 H + 3 OH \leftrightarrows 3 H_2O$<br>(3*14.00) 42.00<br>$Hf + 3 OH \leftrightarrows Hf(OH)_3$ 36.00 |
| $Hf + 4 H_2O \leftrightarrows Hf(OH)_4 + 4 H$ | -10.70 | | | $Hf + 4 H_2O \leftrightarrows Hf(OH)_4 + 4 H$<br>-10.70<br>$4 H + 4 OH \leftrightarrows 4 H_2O$<br>(4*14.00) 56.00<br>$Hf + 4 OH \leftrightarrows Hf(OH)_4$ 45.30 |
| $Hf + 5 F \leftrightarrows HfF_5$ | 36.36 | | | |
| $Hf + 6 F \leftrightarrows HfF_6$ | 39.53 | | | |
| $Hf + 2 Cl \leftrightarrows HfCl_2$ | 1.55 | | | |
| $Hf + 3 Cl \leftrightarrows HfCl_3$ | 0.88 | | | |
| $Hg(II) + 3 H_2O \leftrightarrows Hg(II)(OH)_3 + 3 H$ | -21.1 | | | $Hg(II) + 3 H_2O \leftrightarrows Hg(II)(OH)_3 + 3 H$<br>$3 H + 3 OH \leftrightarrows 3 H_2O$ -21.1<br>(3*14.00) 42.00<br>$Hg(II) + 3 OH \leftrightarrows Hg(II)(OH)_3$<br>20.9 |
| $Pb(II) + 2 SO_4 \leftrightarrows Pb(II)(SO_4)_2$ | 4.51 | | | |
| $Pb(II) + 4 Cl \leftrightarrows Pb(II)Cl_4$ | 1.40 | | | |
| $Bi + 6 Cl \leftrightarrows BiCl_6$ | 6.51 | | | |

## II.1.2 Morel

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $H + 3 (H_2BO_3) \leftrightarrows H(H_2BO_3)_3$ | 10.4 | | | |
| $4 H + 5 (H_2BO_3) \leftrightarrows H_4(H_2BO_3)_5$ | 38.8 | | | |
| $6 H + 4 (H_2SiO_4) \leftrightarrows H_6(H_2SiO_4)_4$ | 78.2 | | | |
| $H + S \leftrightarrows HS$ | 13.9 | | | |
| $Al + 3 (salicylate) \leftrightarrows Al(salicylate)_3$ | 32.8 | | | |
| $Fe(III) + 3 (salicylate) \leftrightarrows Fe(III)(salicylate)_3$ | 37.2 | | | |
| $Fe(II) + (EDTA) + (OH) \leftrightarrows Fe(II)(EDTA)(OH)$ | 20.4 | | | |
| $Fe(II) + (EDTA) + 2 (OH) \leftrightarrows Fe(II)(EDTA)(OH)_2$ | 23.7 | | | |
| $Fe(III) + (EDTA) + 2 (OH) \leftrightarrows Fe(III)(EDTA)(OH)_2$ | 37.7 | | | |
| $Ni + (CN) \leftrightarrows Ni(CN)$ | 7.7 | | | |
| $Cu(II) + 2 (CN) \leftrightarrows Cu(II)(CN)_2$ | 16.3 | | | |
| $Cu(II) + 3 (CN) \leftrightarrows Cu(II)(CN)_3$ | 21.6 | | | |
| $Cu(II) + 4 (CN) \leftrightarrows Cu(II)(CN)_4$ | 23.1 | | | |

| | | | | |
|---|---|---|---|---|
| Sr + (PO4) ⇆ Sr(PO4) | 5.5 | | | |
| Cd + S ⇆ CdS | 19.5 | | | |
| Ba + (salicylate) ⇆ Ba(salicylate) | 0.2 | | | |
| Ba + H + (EDTA) ⇆ BaH(EDTA) | 14.6 | | | |
| Hg(II) + S ⇆ Hg(II)S | 7.9 | | | |
| Hg(II) + S + (OH) ⇆ Hg(II)S(OH) | 18.5 | | | |
| Hg(II) + 3 (acetate) ⇆ Hg(II) (acetate)3 | 14.1 | | | |
| Hg(II)+ 4 (acetate) ⇆ Hg(II) (acetate)4 | 17.6 | | | |

## II.1.3 Turner & Whitfield

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| Na + H + NTA ⇆ NaHNTA | 10.808 | | | |
| Na + H + EDTA ⇆ NaH(EDTA) | 11.168 | | | |
| K + H + NTA ⇆ KHNTA | 10.788 | | | |

## II.1.4 Method of Byrne & Miller for mixed complexes

The constant for $Cu(II)(CO_3)(OH)$ was calculated after Byrne & Miller (1985) (equation 27 on page 1842):

$$\beta^*_{11} = \frac{[Cu(CO_3)(OH)^-]*[H^+]}{[Cu^{2+}]*[CO_3^{\ 2-}]} = 2(\beta^*_2\beta\ \ )^{1/2}$$

$ß^*_2$ is the constant for the equilibrium:
$Cu^{2+} + 2\ H_2O \leftrightarrows Cu(OH)_2 + 2\ H^+$ (see equation 8 in Byrne & Miller)
This constant can be obtained as follows:

Database of CHEAQS:
$Cu^{2+} + 2\ OH^- \leftrightarrows Cu(OH)_2$ 10.7
$2\ H_2O \leftrightarrows 2\ H^+ + 2\ OH^-$
(=2*-13.997) -27.994
$Cu^{2+} + 2\ H_2O \leftrightarrows Cu(OH)_2 + 2\ H^+$ -17.294 (=$ß^*_2$)

$ß_2$ is the constant for the following equilibrium:
$Cu^{2+} + 2\ CO_3^{2-} \leftrightarrows Cu(CO_3)_2^{2-}$
Database of CHEAQS: 10.2

$ß^*_{11} = 2 * (ß^*_2\ ß_2)^{1/2} = 2 * (10^{-17.294} * 10^{10.2})^{1/2}$
$= 2 * (10^{-7.094})^{1/2} = 2 * 10^{-3.547}$
$\log(ß^*_{11}) = -3.24597$

$Cu^{2+} + CO_3^{2-} \leftrightarrows Cu(CO_3)(OH)^- + H^+$ -3.24597
$H^+ + OH^- \leftrightarrows H_2O$ 13.997
$Cu^{2+} + CO_3^{2-} + OH^- \leftrightarrows Cu(CO_3)(OH)^-$ 10.75103
which was entered in CHEAQS' database.

### *II.2 Adsorption complexes*

The constants for the adsorption equilibria were arbitrarily (!) selected as described below. To reliably model adsorption, measurements are needed to determine the constants. CHEAQS' constants are included as examples of how to model adsorption. See also the item "Modelling adsorption" in the help file.

#### II.2.1 Acid-base-equilibria

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $=S-OH \leftrightarrows (=S-O)^- + H^+$ | -9.5 | | | |
| $=S-OH + H^+ \leftrightarrows =S-OH_2^+$ | 7.2 | | | |

Here =S represents an adsorption site. Typical examples of =S are Si, Fe, Al, Ti. Data were taken from Schindler & Stumm (1987) for =S is Al (page 95). For other =S than Al other constants have to be used (see page 97 for other examples).

#### II.2.2 Constants for metals

For the adsorption of Fe(III), Cd, Cu(II), Pb(II) and Mg on silica the following relationship has been established:
$\log {}^*K^s_1 = -0.09 + 0.62 * \log {}^*K_1$ (see page 101 in Schindler & Stumm)
$\log {}^*K_1$ is the first hydrolysis constant; it can be derived from the constant in CHEAQS' database by adding 13.997 (formation constant of $H_2O$) (symbol for constant in CHEAQS: $K_{G1}$)
So:

$$\log {}^*K^s_1 = -0.09 + 0.62 * (\log K_{G1} - 13.997)$$
$$= -0.09 + (0.62 * -13.997) + 0.62 * \log K_{G1}$$
$$= -0.09 - 8.67814 + 0.62 * \log K_{G1}$$
$$= -8.76814 + 0.62 * \log K_{G1}$$

This approach has been applied to *all* cations with a charge of 2 or more (see table below).

Similarly, for $(=S)_2$-M the constants can be derived as follows.

$$\log {}^*ß^s_2 = -0.09 + 0.62 * \log {}^*ß_2 \text{ (see page 101 in Schindler \& Stumm)}$$
$$\log {}^*ß^s_2 = -0.09 + 0.62 * (\log KG_2 - 27.994)$$
$$= -0.09 + (0.62 * -27.994) + 0.62 * \log K_{G2}$$
$$= -0.09 - 17.35628 + 0.62 * \log K_{G2}$$
$$= -17.44628 + 0.62 * \log K_{G2}$$

This approach has been applied to *all* cations with a charge of 2 or more (see table below). Note that the constant were calculated with five decimals (that's how they are given here as well) but displayed by the program with three decimals.

| cation | log $K_{compl}$ M(OH) | log $K_{compl}$ $M(OH)_2$ | log $K_{ads}$ | log $K_{ads}$ |
|---|---|---|---|---|
| $Be^{2+}$ | 7.63954 | -4.03163 | 16.86073 | -6.99263 |
| $Mg^{2+}$ | 2.58000 | -7.16854 | | |
| $Al^{3+}$ | 9.00000 | -3.18814 | 17.70000 | -6.47228 |
| $Ca^{2+}$ | 1.30000 | -7.96214 | | |
| $Sc^{3+}$ | 9.70000 | -2.75414 | 18.30000 | -6.10028 |
| $Cr(III)^{3+}$ | 10.30000 | -2.38214 | 18.30000 | -6.10028 |
| $Mn(II)^{2+}$ | 3.40000 | -6.66014 | 5.80000 | -13.85028 |
| $Fe(II)^{2+}$ | 4.60000 | -5.91614 | 7.50000 | -12.85828 |
| $Fe(III)^{3+}$ | 11.81000 | -1.44594 | 22.40000 | -3.55828 |
| $Co(II)^{2+}$ | 4.30000 | -6.10214 | 9.20000 | -11.74228 |
| $Co(III)^{3+}$ | 12.72931 | -0.87597 | | |
| $Ni^{2+}$ | 4.10000 | -6.22614 | 9.00000 | -11.86628 |
| $Cu(II)^{2+}$ | 6.50000 | -4.73814 | 10.70000 | -10.81228 |
| $Zn^{2+}$ | 5.00000 | -5.66814 | 11.10000 | -10.56428 |
| $Ga^{3+}$ | 11.10000 | -1.88614 | 21.30000 | -4.24028 |
| $Sr^{2+}$ | 0.82000 | -8.25974 | | |
| $Y^{3+}$ | 6.30000 | -4.86214 | 11.60000 | -10.25428 |
| $Zr^{4+}$ | 14.30000 | 0.09786 | 26.30000 | -1.14028 |
| $Pd^{2+}$ | 11.20632 | -1.82022 | | |
| $Cd^{2+}$ | 3.90000 | -6.35014 | 7.70000 | -12.67228 |
| $In^{3+}$ | 10.07000 | -2.52474 | 20.20000 | -4.92228 |
| $Sn(II)^{2+}$ | 10.60000 | -2.19614 | 20.90000 | -4.48828 |
| $Sn(IV)^{4+}$ | 15.50000 | 0.84186 | 29.31000 | 0.72592 |
| $Ba^{2+}$ | 0.64000 | -8.37134 | | |
| $La^{3+}$ | 5.50000 | -5.35814 | 10.60000 | -10.87428 |
| $Ce^{3+}$ | 5.70000 | -5.23414 | 10.90000 | -10.68828 |
| $Pr^{3+}$ | 6.00516 | -5.04494 | 11.00000 | -10.62628 |
| $Nd^{3+}$ | 6.00000 | -5.04814 | 11.10000 | -10.56428 |
| $Sm^{3+}$ | 6.20516 | -4.98614 | 11.40000 | -10.37828 |
| $Eu^{3+}$ | 6.20516 | -4.92094 | 11.40000 | -10.37828 |
| $Gd^{3+}$ | 6.20516 | -4.92094 | 11.60000 | -10.25428 |
| $Tb^{3+}$ | 6.40516 | -4.98614 | 11.70000 | -10.19228 |
| $Dy^{3+}$ | 6.40516 | -4.79694 | 11.80000 | -10.13028 |
| $Ho^{3+}$ | 6.50516 | -4.73494 | 11.90000 | -10.06828 |
| $Er^{3+}$ | 6.50516 | -4.73494 | 12.10000 | -9.94428 |
| $Tm^{3+}$ | 6.60516 | -4.67294 | 12.10000 | -9.94428 |
| $Yb^{3+}$ | 6.60516 | -4.67294 | 12.20000 | -9.88228 |
| $Lu^{3+}$ | 6.60516 | -4.67294 | 12.30000 | -9.82028 |
| $Hf^{4+}$ | 13.80000 | -0.21214 | 25.60000 | -1.57428 |
| $Hg(II)^{2+}$ | 10.60000 | -2.19614 | 21.83000 | -3.91168 |
| $Pb(II)^{2+}$ | 6.40000 | -4.80014 | 10.90000 | -10.68828 |
| $Bi^{3+}$ | 12.90000 | -0.77014 | 24.51580 | -2.24648 |
| $U(VI)O_2^{2+}$ | 8.10000 | -3.74614 | | |

### II.2.3 Constants for anions

Because no such straightforward relationship has been established for anions as for cations, no anion surface complexes have been entered; however, the program may be able to handle such equilibria. For advice, contact the author.

## *II.3 Saturation solids*

Some solubility constants were taken from Morel, Stumm & Morgan and Van Riemsdijk & Keizer.

### II.3.1 Morel

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| 2 Zn + Cl + 3 OH ⇆ $Zn_2Cl(OH)_3$ | 26.8 | | | |

| | | | | |
|---|---|---|---|---|
| $Hg(II) + CO_3 \leftrightarrows Hg(II)CO_3$ | 16.1 | | | |
| $Hg(II) + 2\ Br \leftrightarrows Hg(II)Br_2$ | 19.8 | | | |

## II.3.2 Stumm & Morgan

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Ca + Mg + 2\ CO_3 \leftrightarrows CaMg(CO_3)_2$ | 16.7 | | | |
| $4\ Mg + 3\ CO_3 + 2\ OH \leftrightarrows Mg_4(CO_3)_3(OH)_2{\cdot}3H_2O$ | 29.5 | | | |
| $Mg + NH_4 + PO_4 \leftrightarrows MgNH_4PO_4$ | 12.6 | | | $Mg + NH_4 + PO_4 \leftrightarrows MgNH_4PO_4$ 12.6<br>$NH_3 + H \leftrightarrows NH_4$ 9.244<br>$Mg + NH_3 + H + PO_4 \leftrightarrows MgNH_4PO_4$ 21.844 |
| $10\ Ca + 6\ PO_4 + 2\ F \leftrightarrows Ca_{10}(PO_4)_6F_2$ | 118 | | | |
| $Ca_{10}(PO_4)_6(OH)_2 + 6\ H_2O \leftrightarrows 4\ Ca_2(HPO_4)(OH)_2 + 2\ Ca + 2\ HPO_4$ | -17 | | | $Ca_{10}(PO_4)_6(OH)_2 + 6\ H_2O \leftrightarrows 4\ Ca_2(HPO_4)(OH)_2 + 2\ Ca + 2\ HPO_4$ -17<br>$10\ Ca + 6\ PO_4 + 2\ OH \leftrightarrows Ca_{10}(PO_4)_6(OH)_2$ 116.66<br>$2\ HPO_4 \leftrightarrows 2\ PO_4 + 2\ H$<br>(2*-12.375) -24.75<br>$8\ Ca + 4\ PO_4 + 2\ OH + 6\ H_2O \leftrightarrows 4\ Ca_2(HPO_4)(OH)_2 + 2\ H$ 74.91<br>$2\ OH + 2\ H \leftrightarrows 2\ H_2O$<br>(2*13.997) 27.994<br>$8\ Ca + 4\ PO_4 + 4\ OH + 4\ H_2O \leftrightarrows 4\ Ca_2(HPO_4)(OH)_2$ 102.904<br>(note: in version L05 and L06 stated as 102.906) |
| $Fe(II) + NH_4 + PO_4 \leftrightarrows Fe(II)NH_4PO_4$ | 13 | | | $Fe(II) + NH_4 + PO_4 \leftrightarrows Fe(II)NH_4PO_4$ 13<br>$NH_3 + H \leftrightarrows NH_4$ 9.244<br>$Fe(II) + NH_3 + H + PO_4 \leftrightarrows Fe(II)NH_4PO_4$ 22.244 |
| $Zn + 1.6\ H_2O + 0.4\ CO_2\ (g) \leftrightarrows Zn(OH)_{1.2}(CO_3)_{0.4} + 2\ H$ | -9.8 | | | $Zn + 1.6\ H_2O + 0.4\ CO_2\ (g) \leftrightarrows Zn(OH)_{1.2}(CO_3)_{0.4} + 2\ H$ -9.8<br>Multiply by 5:<br>$5\ Zn + 8\ H_2O + 2\ CO_2\ (g) \leftrightarrows Zn_5(OH)_6(CO_3)_2 + 10\ H$ -49<br>$4\ H + 2\ CO_3 \leftrightarrows 2\ H_2O + 2\ CO_2\ (g)$<br>(2*18.147) 36.294<br>$6\ OH + 6\ H \leftrightarrows 6\ H_2O$<br>(6*13.997) 83.982<br>$5\ Zn + 6\ OH + 2\ CO_3 \leftrightarrows Zn_5(OH)_6(CO_3)_2$ 71.276 |

## II.3.3 Van Riemsdijk & Keizer

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $Ca + 2\ H_2PO_4 + H_2O \leftrightarrows Ca(H_2PO_4)_2(H_2O)$ | 1.15 | | | $Ca + 2\ H_2PO_4 + H_2O \leftrightarrows Ca(H_2PO_4)_2(H_2O)$ 1.15<br>$4\ H + 2\ PO_4 \leftrightarrows 2\ H_2PO_4$<br>(2* 19.573) 39.146<br>$Ca + 4\ H + 2\ PO_4 \leftrightarrows CaH_4(PO_4)_2$ 40.296 |
| $Fe(III) + K + 2\ SO_4 + 6\ H_2O \leftrightarrows KFe_3(SO_4)_2(OH)_6 + 6\ H$ | 12.51 | | | $Fe(III) + K + 2\ SO_4 + 6\ H_2O \leftrightarrows KFe_3(SO_4)_2(OH)_6 + 6\ H$ 12.51<br>$6\ OH + 6\ H \leftrightarrows 6\ H_2O$<br>(6*13.997) 83.982<br>$Fe(III) + K + 2\ SO_4 + 6\ OH \leftrightarrows KFe_3(SO_4)_2(OH)_6$ 96.492 |

| | | | | |
|---|---|---|---|---|
| 5 Pb + 3 $H_2PO_4$ + $H_2O$ ⇆ $Pb_5(PO_4)_3OH$ + 7 H | 4.14 | | | 5 Pb + 3 $H_2PO_4$ + $H_2O$ ⇆ $Pb_5(PO_4)_3OH$ + 7 H 4.14<br>6 H + 3 $PO_4$ ⇆ 3 $H_2PO_4$<br>(3* 19.573) 58.719<br>OH + H ⇆ $H_2O$ 13.997<br>5 Pb + 3 $PO_4$ + OH ⇆ $Pb_5(PO_4)_3OH$ 76.856 |
| 5 Pb + 3 $H_2PO_4$ + Cl ⇆ $Pb_5(PO_4)_3Cl$ + 6 H | 25.05 | | | 5 Pb + 3 $H_2PO_4$ + Cl ⇆ $Pb_5(PO_4)_3Cl$ + 6 H 25.05<br>6 H + 3 $PO_4$ ⇆ 3$H_2PO_4$<br>(3* 19.573) 58.719<br>5 Pb + 3 $PO_4$ + Cl ⇆ $Pb_5(PO_4)_3Cl$ 83.769 |
| 3 Al + 2 $PO_4$ + 8 $H_2O$ ⇆ $Al_3(PO_4)_2(OH)_3(H_2O)_5$ + 3 H | 36.86 | | | 3 Al + 2 $PO_4$ + 8 $H_2O$ ⇆ $Al_3(PO_4)_2(OH)_3(H_2O)5$ + 3 H 36.86<br>3 OH + 3 H ⇆ 3 $H_2O$<br>(3*13.997) 41.991<br>3 Al + 2 $PO_4$ + 3 OH ⇆ $Al_3(PO_4)_2(OH)_3(H_2O)_5$ 78.851 |

## *II.4 Gas solution equilibria*

### II.4.1 Morel

| Equilibrium | Log (K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $NH_3$ (aq) ⇆ $NH_3$ (g) | -1.8 | | | Note: this value was taken from page 242; at page 130 a value of -1.87 is given. |

## *II.5 Redox couples*

Redox couples were primarily selected from the Handbook of Chemistry and Physics. In a few cases, environmentally important equilibria are missing in that source; therefore, alternative sources were included.

### II.5.1 Lide (Handbook)

Note: couples are given in volts; these can be converted to 10-base log constants by dividing by 0.0591595 and multiplying by the number of electrons involved.

| Equilibrium | E (in V) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $HCr(VI)O_4^-$ + 7 $H^+$ + 3 e ⇆ $Cr(III)^{3+}$ + 4 $H_2O$ | 1.350 | | | log(K)= (1.350 / 0.0591595) * 3 = 68.45958<br><br>$HCr(VI)O_4^-$ + 7 $H^+$ + 3 e ⇆ $Cr(III)^{3+}$ + 4 $H_2O$ 68.45958<br>$Cr(VI)O_4^{2-}$ + $H^+$ ⇆ $HCr(VI)O_4^-$ 6.51<br>$Cr(VI)O_4^{2-}$ + 8 $H^+$ + 3 e ⇆ $Cr(III)^{3+}$ + 4 $H_2O$ 74.96958 |
| $Mn(VII)O_4^-$ + 8 $H^+$ + 5 e ⇆ $Mn(II)^{2+}$ + 4 $H_2O$ | 1.507 | | | log(K)= (1.507 / 0.0591595) * 5 = 127.36862 |
| $Mn(IV)O_2$ (s) + 4 $H^+$ + 2 e ⇆ $Mn(II)^{2+}$ + 2 $H_2O$ | 1.224 | | | log(K)= (1.224 / 0.0591595) * 2 = 41.38001 |
| $Fe(III)^{3+}$ + e ⇆ $Fe(II)^{2+}$ | 0.771 | | | log(K)= (0.771 / 0.0591595) = 13.03267 |
| $Co(III)^{3+}$ + e ⇆ $Co(II)^{2+}$ | 1.92 | | | log(K)= (1.92 / 0.0591595) = 32.45491 |
| $Cu(II)^{2+}$ + e ⇆ $Cu(I)^+$ | 0.153 | | | log(K)= (0.153 / 0.0591595) = 2.58625 |

| | | | | |
|---|---|---|---|---|
| Cu(II)$^{2+}$ + 2 e ⇆ Cu (s) | 0.3419 | | | log(K)= (0.3419 / 0.0591595) * 2 = 11.55868 |
| Sn(IV)$^{4+}$ + 2 e ⇆ Sn(II)$^{2+}$ | 0.151 | | | log(K)= (0.151 / 0.0591595) * 2 = 5.10489 |
| Pb(IV)$O_2$ + 4 $H^+$ + 2 e ⇆ Pb(II)$^{2+}$ + 2 $H_2O$ | 1.455 | | | log(K)= (1.455 / 0.0591595) * 2 = 49.18947 |
| $NO_3^-$ + 3 $H^+$ + 2 e ⇆ $HNO_2$ + $H_2O$ | 0.934 | | | log(K)= (0.934 / 0.0591595) * 2 = 31.57592<br>$NO_3^-$ + 3 $H^+$ + 2 e ⇆ $HNO_2$ + $H_2O$ 31.57592<br>$HNO_2$ ⇆ $H^+$ + $NO_2^-$ -3.15<br>$NO_3^-$ + 2 $H^+$ + 2 e ⇆ $NO_2^-$ + $H_2O$ 28.42592<br>(see next couple) |
| $NO_3^-$ + $H_2O$ + 2e ⇆ $NO_2^-$ + 2 $OH^-$ | 0.01 | | | log(K)= (0.01 / 0.0591595) * 2 = 0.3380<br>$NO_3^-$ + $H_2O$ + 2e ⇆ $NO_2^-$ + 2 $OH^-$ 0.33807<br>2 $H^+$ + 2 $OH^-$ ⇆ 2 $H_2O$<br>(2*13.997) 27.994<br>$NO_3^-$ + 2 $H^+$ 2e ⇆ $H_2O$ + $NO_2^-$ 28.33207<br>Average of this one and the previous one: (28.42592 + 28.33207)/2= 28.379 which was entered. |
| $SO_4^{2-}$ + 4 $H^+$ + 2e ⇆ $H_2SO_3$ + $H_2O$ | 0.172 | | | log(K)= (0.172 / 0.0591595) * 2 = 5.81484<br>$SO_4^{2-}$ + 4 $H^+$ + 2e ⇆ $H_2SO_3$ + $H_2O$ 5.81484<br>$H_2SO_3$ ⇆ 2 $H^+$ + $SO_3^{2-}$ -9.05<br>$SO_4^{2-}$ + 2 $H^+$ + 2e ⇆ $SO_3^{2-}$ + $H_2O$ -3.23516<br>(see next couple) |
| $SO_4^{2-}$ + $H_2O$ + 2 e ⇆ $SO_3^{2-}$ + 2 $OH^-$ | -0.93 | | | log(K)= (-0.93 / 0.0591595) * 2 = 31.44069<br>$SO_4^{2-}$ + $H_2O$ + 2 e ⇆ $SO_3^{2-}$ + 2 $OH^-$ -31.44069<br>2 $H^+$ + 2 $OH^-$ ⇆ 2 $H_2O$<br>(2*13.997) 27.994<br>$SO_4^{2-}$ + 2 $H^+$ + 2e ⇆ $SO_3^{2-}$ + $H_2O$ -3.44669<br>Average of this one and the previous one: (-3.23516 + -3.44669)/2= -3.340925 which was entered. |
| $H_3AsO_4$ + 2 $H^+$ + 2 e ⇆ $HAsO_2$ + 2 $H_2O$ | 0.560 | | | log(K)= (0.560 / 0.0591595) * 2 = 19.93203<br>$H_3AsO_4$ + 2 $H^+$ + 2 e ⇆ $HAsO_2$ + 2 $H_2O$ 18.93203<br>$AsO_4^{3-}$ + 3 $H^+$ ⇆ $H_3AsO_4$ 20.70<br>$HAsO_2$ ⇆ $H^+$ + $AsO_2^-$ -9.29<br>$AsO_4^{3-}$ + 4 $H^+$ + 2 e ⇆ $AsO_2^-$ +2 $H_2O$ 30.34203<br>(see next couple) |
| $AsO_4^{3-}$ + 2 $H_2O$ + 2 e ⇆ $AsO_2^-$ + 4 $OH^-$ | -0.71 | | | log(K)= (-0.71 / 0.0591595) * 2 = -24.00311<br>$AsO_4^{3-}$ + 2 $H_2O$ + 2 e ⇆ $AsO_2^-$ + 4 $OH^-$ -24.00311<br>4 $OH^-$ + 4 $H^+$ ⇆ 4 $H_2O$<br>(4*13.997) 55.988<br>$AsO_4^{3-}$ + 4 $H^+$ + 2 e⇆ $AsO_2^-$ + 2 $H_2O$ 31.98489<br>Average of this one and the previous one: (30.34203 + 31.98489)/2= 31.16346 which was entered. |

| | | | | |
|---|---|---|---|---|
| $Se(VI)O_4^{2-} + 4\ H^+ + 2e \leftrightarrows H_2Se(IV)O_3 + H_2O$ | 1.151 | | | log(K)= (1.151 / 0.0591595) * 2 = 38.91208<br>$Se(VI)O_4^{2-} + 4\ H^+ + 2e \leftrightarrows H_2Se(IV)O_3 + H_2O$ 38.91208<br>$H_2Se(IV)O_3 \leftrightarrows 2\ H + Se(IV)O_3^{2-}$ -11.03<br>$Se(VI)O_4^{2-} + 2\ H^+ + 2e \leftrightarrows Se(IV)O_3^{2-}$ 27.88208<br>(see next couple) |
| $Se(VI)O_4^{2-} + H_2O + 2e \leftrightarrows Se(IV)O_3^{2-} + 2\ OH^-$ | 0.05 | | | log(K)= (0.05 / 0.0591595) * 2 = 1.69036<br>$Se(VI)O_4^{2-} + H_2O + 2e \leftrightarrows Se(IV)O_3^{2-} + 2\ OH^-$ 1.69036<br>2 H+ + 2 OH- ⇆ 2 $H_2O$<br>(2*13.997) 27.994<br>$Se(VI)O_4^{2-} + 2\ H^+ + 2e \leftrightarrows Se(IV)O_3^{2-}$ 29.68436<br>Average of this one and the previous one: (27.88208 + 29.68436)/2= 28.78322 which was entered. |

### II.5.2 Morel

| Equilibrium | Log(K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $1/8\ NO_3^- + 5/4\ H^+ + e \leftrightarrows 1/8\ NH_4^+ + 3/8\ H_2O$ | 14.9 | | | multiply by 8:<br>$NO_3^- + 10\ H^+ + 8\ e \leftrightarrows NH_4^+ + 3\ H_2O$ 119.2<br>$NH_4^+ \leftrightarrows NH_3 + H$ -9.244<br>$NO_3^- + 9\ H^+ + 8\ e \leftrightarrows NH_3 + 3H_2O$ 109.956 |
| $1/8\ S(VI)O_4^{2-} + 5/4\ H^+ + e \leftrightarrows 1/8\ H_2S(-II)\ (aq) + 1/2\ H_2O$ | 5.13 | | | multiply by 8:<br>$S(VI)O_4^{2-} + 10\ H^+ + 8\ e \leftrightarrows H_2S(-II)\ (aq) + 4\ H_2O$ 41.04<br>$H_2S \leftrightarrows 2\ H + S$ -20.92<br>$S(VI)O_4^{2-} + 8\ H^+ + 8\ e \leftrightarrows S(-II)^{2-}$ 20.12 |

### II.5.3 Stumm & Morgan

| Equilibrium | Log(K) | I | T | Conversion or remarks |
|---|---|---|---|---|
| $S(s) + 2\ H^+ + 2\ e \leftrightarrows H_2S$ | 4.8 | | | invert:<br>$H_2S\ (aq) \leftrightarrows S(s) + 2\ H^+ + 2\ e$ -4.8<br>From Morel:<br>$S(VI)O_4^{2-} + 10\ H^+ + 8\ e \leftrightarrows H_2S(-II)\ (aq) + 4\ H_2O$<br>41.04<br>$SO_4^{2-} + 8\ H^+ + 6\ e \leftrightarrows S(s)$ 36.24 |

## *II.6 Organic complexation*

Since version Pro 2012.4, four models for organic complexation are included, one published by Cabaniss and Shuman[3] (1988a, 1988b), one by Tipping and Hurley (Model V or WHAM-W, 1992, 1994), one by Tipping (Model VI or WHAM 6; 1998), one by Tipping *et al.* (2011). This document contains the values of the equilibrium constants used in the models.
The help file of the program contains information about how to use and interpret the models. Please DO read that section before (and after) including organic complexation.
This document does not include that information.

[3]In CHEAQS Next 2015.1, this model is not included yet.

### II.6.1 Model of Cabaniss and Shuman

The model of Cabaniss and Shuman (1988a, 1988b) was derived for Cu(II). The constants are given below. CHEAQS offers the option to extrapolate these equilibria and constants to other metals. This extrapolation, including a discussion of the background and drawbacks, was discussed by Janssen & Verweij (2003).

| Equilibrium | Log(K) |
|---|---|
| $Cu^{2+} + DOC^{5-} \leftrightarrows Cu(II)DOC^{3-}$ | 3.900 |
| $Cu^{2+} + HDOC^{4-} \leftrightarrows Cu(II)DOC^{3-} + H^{+}$ | 1.494 |
| $Cu^{2+} + HDOC^{4-} \leftrightarrows Cu(II)DOC^{3-} + H^{+}$ | -0.364 |
| $Cu^{2+} + H_2DOC^{3-} \leftrightarrows Cu(II)DOC^{3-} + 2\ H^{+}$ | -7.483 |
| $Cu^{2+} + H_2DOC^{3-} \leftrightarrows Cu(II)DOC^{3-} + 2\ H^{+}$ | -10.050 |

### II.6.2 Model of Tipping and Hurley

CHEAQS includes ‘Model V’, also known as WHAM-W(ater). In the table below, the ‘basic’ constants are given for each metal or metal hydroxides. These constants are used to calculate values for eight monodentate sites and twelve bidentate sites, for fulvic acids and humic acids. Details are given in Tipping & Hurley (1992) and Tipping (1994). The help file of CHEAQS also contains a summary of the model.

In the table the complexes with their constants are given in the following order. For each metal:

- complex of metal with fulvic acid (FA);
- complex of metal hydroxide with fulvic acid (FA);
- complex of metal with humic acid (HA);
- complex of metal hydroxide with humic acid (HA).

Note: for some metals, no constants for the metal hydroxides are given (e.g. Mg and Ca). Charges are omitted for clarity.

| | Log(K) for: | | | |
|---|---|---|---|---|
| Metal | M-FA | M(OH)-FA | M-HA | M(OH)-HA |
| Be | 0.4 | 0.4 | 1.7 | 1.7 |
| Mg | 2.2 | | 3.3 | |
| Al | 0.4 | 0.4 | 1.3 | 1.3 |
| Ca | 2.2 | | 3.2 | |
| Cr(III) | 0.1 | 0.1 | 0.5 | 0.5 |
| Mn(II) | 1.7 | 1.7 | 3.4 | 3.4 |
| Fe(II) | 1.3 | 1.3 | 2.1 | 2.1 |
| Fe(III) | -0.2 | -0.2 | 0.8 | 0.8 |
| Co(II) | 1.7 | 1.7 | 2.7 | 2.7 |
| Ni | 1.4 | 1.4 | 2.7 | 2.7 |
| Cu(II) | 0.8 | 0.8 | 1.5 | 1.5 |
| Zn | 1.3 | 1.3 | 2.3 | 2.3 |
| Sr | 2.3 | | 2.8 | |
| Cd | 1.5 | 1.5 | 2.7 | 2.7 |
| Ba | 2.6 | | 3.6 | |
| Hg(II) | -0.3 | -0.3 | 0.2 | 0.2 |
| Pb(II) | 0.9 | 0.9 | 1.7 | 1.7 |
| $(U(VI)O_2)$ | 0.9 | 0.9 | 1.3 | 1.3 |

### II.6.3 Tipping's Model VI (WHAM 6)

Since CHEAQS Pro 2011, CHEAQS also includes 'Model VI', also known as WHAM-6. In the table below, the 'basic' constants are given for each metal or metal hydroxides. These constants are used to calculate values for eight monodentate sites, eight bidentate sites (each with three sub-sites) and 16 tridentate sites (also each with three sub-sites), for fulvic acids and humic acids. Details are given in Tipping (1998). The help file of CHEAQS also contains a summary of the model.

In the table the complexes with their constants are given in the following order. For each metal:

- complex of metal with fulvic acid (FA);
- complex of metal hydroxide with fulvic acid (FA);
- complex of metal with humic acid (HA);
- complex of metal hydroxide with humic acid (HA).

Note: for some metals, no constants for the metal hydroxides are given (e.g. Mg and Ca). Charges are omitted for clarity.

| | Log(K) for: | | | |
|---|---|---|---|---|
| Metal | M-FA | M(OH)-FA | M-HA | M(OH)-HA |
| Mg | 1.1 | | 0.7 | |
| Al | 2.5 | 2.5 | 2.6 | 2.6 |
| Ca | 1.3 | | 0.7 | |
| Cr(III) | 2.2 | 2.2 | 2.2 | 2.2 |
| Mn(II) | 1.7 | 1.7 | 0.6 | 0.6 |
| Fe(II) | 1.6 | 1.6 | 1.3 | 1.3 |
| Fe(III) | 2.4 | 2.4 | 2.5 | 2.5 |
| Co(II) | 1.4 | 1.4 | 1.1 | 1.1 |
| Ni | 1.4 | 1.4 | 1.1 | 1.1 |
| Cu(II) | 2.1 | 2.1 | 2.0 | 2.0 |
| Zn | 1.6 | 1.6 | 1.5 | 1.5 |
| Sr | 1.2 | | 1.1 | |
| Cd | 1.6 | 1.6 | 1.3 | 1.3 |
| Ba | 0.6 | | -0.2 | |
| Eu | 2.4 | 2.4 | 2.1 | 2.1 |
| Hg(II) | 3.5 | 3.5 | 3.5 | 3.5 |
| Pb(II) | 2.2 | 2.2 | 2.0 | 2.0 |
| $(U(VI)O_2)$ | 2.1 | 2.1 | 2.2 | 2.2 |

### II.6.3 Tipping's Model VII (7)

Since CHEAQS Pro 2012.4, CHEAQS also includes 'Model VII'. In the table below, the 'basic' constants are given for each metal or metal hydroxides. These constants are used to calculate values for eight monodentate sites, six bidentate sites (each with three sub-sites) and eight tridentate sites (also each with three sub-sites), for fulvic acids and humic acids. Details are given in Tipping *et al.* (2011). The help file of CHEAQS also contains a summary of the model.

In the table the complexes with their constants are given in the following order. For each metal:

- complex of metal with fulvic acid (FA);
- complex of metal hydroxide with fulvic acid (FA);
- complex of metal with humic acid (HA);

- complex of metal hydroxide with humic acid (HA).

Note: for some metals, no constants for the metal hydroxides are given (e.g. Mg and Ca). Charges are omitted for clarity.

| | Log(K) for: | | | |
|---|---|---|---|---|
| Metal | M-FA | M(OH)-FA | M-HA | M(OH)-HA |
| Be | 2.02 | 2.02 | 2.27 | 2.27 |
| Mg | 0.99 | | 1.14 | |
| Al | 2.57 | 2.57 | 2.82 | 2.82 |
| Ca | 1.13 | | 1.26 | |
| Sc | 3.28 | 3.28 | 3.61 | 3.61 |
| Cr(III) | 2.89 | 2.89 | 3.07 | 3.07 |
| Mn(II) | 1.76 | 1.76 | 1.98 | 1.98 |
| Fe(II) | 1.46 | 1.46 | 1.76 | 1.76 |
| Fe(III) | 3.12 | 3.12 | 3.37 | 3.37 |
| Co(II) | 1.35 | 1.35 | 1.5 | 1.5 |
| Ni | 1.43 | 1.43 | 1.6 | 1.6 |
| Cu(II) | 2.16 | 2.16 | 2.38 | 2.38 |
| Zn | 1.68 | 1.68 | 1.87 | 1.87 |
| Sr | 1.13 | | 1.32 | |
| Y | 2.76 | 2.76 | 3.03 | 3.03 |
| Ag | 1.27 | 1.27 | 1.44 | 1.44 |
| Cd | 1.51 | 1.51 | 1.67 | 1.67 |
| Ba | 0.97 | | 1.3 | |
| La | 2.36 | 2.36 | 2.62 | 2.62 |
| Ce | 2.41 | 2.41 | 2.66 | 2.66 |
| Pr | 2.59 | 2.59 | 2.85 | 2.85 |
| Nd | 2.57 | 2.57 | 2.83 | 2.83 |
| Sm | 2.66 | 2.66 | 2.93 | 2.93 |
| Eu | 2.62 | 2.62 | 2.89 | 2.89 |
| Gd | 2.68 | 2.68 | 2.95 | 2.95 |
| Tb | 2.76 | 2.76 | 3.04 | 3.04 |
| Dy | 2.91 | 2.91 | 3.2 | 3.2 |
| Ho | 2.82 | 2.82 | 3.1 | 3.1 |
| Er | 2.92 | 2.92 | 3.21 | 3.21 |
| Tm | 2.94 | 2.94 | 3.23 | 3.23 |
| Yb | 2.94 | 2.94 | 3.24 | 3.24 |
| Lu | 2.99 | 2.99 | 3.29 | 3.29 |
| Hg(II) | 3.51 | 3.51 | 3.84 | 3.84 |
| Pb(II) | 2.15 | 2.15 | 2.37 | 2.37 |
| (U(VI)$O_2$) | 2.38 | 2.38 | 2.61 | 2.61 |

## Part III: molecular weights

Part III contains the molecular weights that are included in the file COMPON.DAT. In the selection and calculation of the molecular weights some arbitrary choices were made. For the cations and inorganic ligands, the weight of the total ion was entered (note that this is different from CHEAQS Pro and the beta-releases of CHEAQS Next). For the organic ligands (including $CN^-$), the weight of the completely deprotonated anion was entered. Please check your own data before entering concentrations in $g.L^{-1}$.
Atomic weights were taken from Wieser (2010) except where stated otherwise.

| Component | Molecular weight | Conversion or remarks |
|---|---|---|
| H | 1.007975 | |
| Li | 6.9675 | |
| Be | 9.012182 | |
| Na | 22.98976928 | |
| Mg | 24.3050 | |
| Al | 26.9815386 | |
| K | 39.0983 | |
| Ca | 40.078 | |
| Sc | 44.955912 | |
| Cr(III) | 51.9961 | |
| Mn(II) | 54.938045 | |
| Fe(II) | 55.845 | |
| Fe(III) | 55.845 | |
| Co(II) | 58.933195 | |
| Co(III) | 58.933195 | |
| Ni | 58.6934 | |
| Cu(I) | 63.546 | |
| Cu(II) | 63.546 | |
| Zn | 65.38 | |
| Ga | 69.723 | |
| Rb | 85.4678 | |
| Sr | 87.62 | |
| Y | 88.90585 | |
| Zr | 91.224 | |
| Pd | 106.42 | |
| Ag | 107.8682 | |
| Cd | 112.411 | |
| In | 114.818 | |
| Sn(II) | 118.710 | |
| Sn(IV) | 118.710 | |
| Cs | 132.9054519 | |
| Ba | 137.327 | |
| La | 138.90547 | |
| Ce | 140.116 | |
| Pr | 140.90765 | |
| Nd | 144.242 | |
| Pm | 145 | taken from Lide (1999) |
| Sm | 150.36 | |
| Eu | 151.964 | |
| Gd | 157.25 | |
| Tb | 158.92535 | |
| Dy | 162.500 | |
| Ho | 164.93032 | |
| Er | 167.259 | |
| Tm | 168.93421 | |
| Yb | 173.054 | |
| Lu | 174.9668 | |
| Hf | 178.49 | |
| Hg(II) | 200.59 | |
| Pb(II) | 207.2 | |
| Bi | 208.9804 | |
| $(U(VI)O_2)$ | 270.02771 | is atomic weight of U (238.02891) + 2 x O (15.9994) |
| e | | (not relevant; not used in the calculations) |

| Component | Molecular weight | Conversion or remarks |
|---|---|---|
| (OH) | 17.007375 | is atomic weight of O + H |
| $(H_2BO_3)$ | 60.82765 | is atomic weight of B (10.8135) + 2 x H + 3 x O |
| $(CO_3)$ | 60.0088 | is atomic weight of C (12.0106) + 3 x O |
| $(NH_3)$ | 17.03078 | is atomic weight of N (14.006855) + 3 x H |
| $(NO_2)$ | 46.005655 | is atomic weight of N + 2 x O |
| $(NO_3)$ | 62.005055 | is atomic weight of N + 3 x O |
| F | 18.9984032 | |
| $(H_2SiO_4)$ | 94.09855 | is atomic weight of Si (28.085) + 2 x H + 4 x O |
| $(PO_4)$ | 94.971362 | is atomic weight of P (30.973762) + 4 x O |
| S | 32.0675 | |
| $(SO_3)$ | 80.0657 | is atomic weight of S (32.0675) + 3 x O |
| $(SO_4)$ | 96.0651 | is atomic weight of S + 4 x O |
| Cl | 35.4515 | |
| $(VO_4)$ | 114.9391 | is atomic weight of V (50.9415) + 4 x O |
| $(CrO_4)$ | 115.9937 | is atomic weight of Cr + 4 x O |
| $(MnO_4)$ | 118.935645 | is atomic weight of Mn + 4 x O |
| $(H_2AsO_3)$ | 124.93575 | is atomic weight of As (74.92160) + 2 x H + 3 x O |
| $(AsO_4)$ | 138.9192 | is atomic weight of As + 4 x O |
| $(SeO_3)$ | 126.9582 | is atomic weight of Se (78.96) + 3 x O |
| $(SeO_4)$ | 142.9576 | is atomic weight of Se + 4 x O |
| Br | 79.904 | |
| $(MoO_4)$ | 159.9576 | is atomic weight of Mo (95.96) + 4 x O |
| I | 126.90447 | |
| $(WO_4)$ | 247.8376 | is atomic weight of W (183.84) + 4 x O |
| (CN) | 26.017455 | is atomic weight of C + N |
| (acetate) | 59.043925 | is atomic weight of 2 x C + 3 x H + 2 x O |
| (catechol) | 108.0943 | is atomic weight of 6 x C + 4 x H + 2 x O |
| (salicylate) | 136.1043 | is atomic weight of 7 x C + 4 x H + 3 x O |
| (phthalate) | 164.1143 | is atomic weight of 8 x C + 4 x H + 4 x O |
| (NTA) | 188.114705 | is atomic weight of 6 x C + 6 x H + N + 7 x O |
| (HEDTA) | 275.235135 | is atomic weight of 10 x C + 15 x H + 2 x N + 7 x O |
| (EDTA) | 288.21061 | is atomic weight of 10 x C + 12 x H + 2 x N + 8 x O |
| (=S-OH) | 10000 | this is an arbitrary number |
| $MnO_2$ (s) | 86.936845 | is atomic weight of Mn + 2 x O |
| Cu (s) | 63.546 | |
| $PbO_2$ (s) | 239.1988 | is atomic weight of Pb + 2 x O |
| S (s) | 32.0675 | |
| $CO_2$ (g) | | (molecular weights of gases are not used by the program, but for consistency reasons they do occur in the datafile COMPON.DAT) |
| $NH_3$ (g) | | |
| $H_2S$ (g) | | |
| $SO_2$ (g) | | |

## Appendix: compatibility of datasources

It is not trivial that data taken from different sources are comparable: many, sometimes undocumented conversions are done and assumptions made. As stated on page 96, some data were taken from other sources than the NIST database as well. In this appendix it is shown that the other sources are compatible with the NIST database. In addition, it is shown that redox couples taken from different sources are compatible with Lide (1999), the "default" source for redox couples.
Section A1 to A3 deal with complexes, A4 and A5 with solids and A6 and A7 with redox couples.
Note: for redox couples and solids one can not be as stringent as for complexes because for solids there often is a considerable range of data even within one source; for solids this is mainly caused by differences in cristalline forms.
Values are given with no more than three decimals (and rounded if necessary).

A.1 Turner *et al.*
Two cations were taken (the first two in Turner) with the first five complexes.
Note: M(OH)-data have been converted (see section II.1.1 for details).

| Complex | NIST 46 v8 | Turner et al. |
|---|---|---|
| Ag(OH) | 2.000 | 2.00 |
| $Ag(OH)_2$ | 3.990 | 4.00 |
| AgF | 0.400 | 0.40 |
| AgCl | 3.310 | 3.27 |
| $AgCl_2$ | 5.250 | 5.23 |
| Al(OH) | 9.000 | 9.03 |
| $Al(OH)_2$ | 17.700 | 18.70 |
| $Al(OH)_3$ | 25.300 | 27.00 |
| $Al(OH)_4$ | 33.300 | 33.00 |
| AlF | 7.010 | 7.01 |

A.2 Morel

| Complex | NIST 46 v8 | Morel |
|---|---|---|
| Ca(OH) | 1.3 | 1.15 |
| Mg(OH) | 2.58 | 2.56 |
| $Mg_4(OH)_4$ | 16.55954 | 16.28 |
| Cr(III)(OH) | 10.3 | 10.0 |
| $H(CO_3)$ | 10.329 | 10.33 |
| $H_2(CO_3)$ | 16.681 | 16.68 |
| $Na(CO_3)$ | 1.27 | 1.27 |
| $H(SO_4)$ | 1.99 | 1.99 |
| $Na(SO_4)$ | 0.74 | 1.06 |
| $K(SO_4)$ | 0.85 | 0.96 |

A.3 Turner & Whitfield

| Complex | NIST 46 v8 | Turner & Whitfield |
|---|---|---|
| HEDTA | 10.948 | 11.094 |
| $H_2EDTA$ | 17.221 | 17.807 |
| NaEDTA | 2.7143 | 2.544 |
| KEDTA | 1.6543 | 1.504 |
| MgEDTA | 10.5836 | 10.70 |
| HNTA | 10.29406 | 10.389 |
| NaNTA | 1.84073 | 1.899 |
| KNTA | 1.24073 | 1.339 |
| MgNTA | 6.78145 | 6.70 |
| CaNTA | 7.74145 | 7.67 |

## A.4 Stumm & Morgan

| Solid | NIST 46 v8 | Stumm & Morgan |
| --- | --- | --- |
| Fe(III)(OH)$_3$ | 38.6<br>39.3 (aged)<br>41.5 (FeOOH; alpha)<br>42.7 ($Fe_2O_3$; alpha) | 41.5 |
| Fe(II)(OH)$_2$ | 14.5 (amorf)<br>15.1 (crystalline) | 14.43 |

## A.5 Van Riemsdijk & Keizer

| Solid | NIST 46 v8 | Van Riemsdijk & Keizer |
| --- | --- | --- |
| $CaSO_4$ | 4.61 | 4.64 |
| CdS | 27.92 | 27.07 |
| Cu(II)S | 36.12 | 36.10 |

## A.6 Morel

| Couple | Lide | | Morel |
| --- | --- | --- | --- |
| | E (V) | Log(K) | Log(K) |
| Fe(III)/Fe(II) | 0.771 | 13.03267 | 13.0 |
| Cu(II)/Cu(I) | 0.153 | 2.58625 | 2.6 |

## A.7 Stumm & Morgan

| Couple | Lide | | Stumm & Morgan |
| --- | --- | --- | --- |
| | E (V) | Log(K) | Log(K) |
| Co(III)/Co(II) | 1.92 | 32.45491 | 31 |
| Cu(II)/$Cu^0$ *(s)* | 0.3419 | 11.55868 | 11.4 |

## References

This section contains two types of references; the first type gives details about the sources of constants as they are referred to in the database. This information can be found in the on-line help as well. The second part consists of the "normal" bibliographic references.

### *Part I: sources of the database*

| Abbreviation used in CHEAQS | Bibiographic reference |
|---|---|
| after Byrne & Miller | Byrne, R.H. & W.L. Miller (1985). Copper(II) carbonate complexation in seawater. Geochimica et Cosmochimica Acta *49*, 1837 - 1844. |
| after Schindler & Stumm | Schindler, P.W. & W. Stumm (1987). The surface chemistry of oxides, hydroxides, and oxide minerals. In: Aquatic surface chemistry, W. Stumm (ed.), John Wiley & Sons, New York. |
| Cabaniss & Shuman | Cabaniss, S.E. & M.S. Shuman (1988).<br>a) Copper binding by dissolved organic matter: I. Suwannee River fulvic acid equilibria. Geochimica Cosmochimica Acta *52*, 185 - 193.<br>b) Copper binding by dissolved organic matter: II. Variation in type and source of organic matter. Geochimica Cosmochimica Acta *52*, 195 - 200. |
| extrapolated from Cabaniss & Shuman | See help file, topic "Organic complexation" |
| Lide (Handbook) | Lide, D.R. (ed.) (1999). CRC Handbook of Chemistry and Physics, electronic version of the 79$^{th}$ edition. CRC Press LLC. |
| Morel | Morel, F.M.M. (1983). Principles of aquatic chemistry. John Wiley & Sons, New York. |
| NIST Database 46 Version 8.0 | NIST Standard Reference Database 46 Version 8.0 (2004). A.E. Martell & R.M. Smith (eds.), NIST, Gaithersburg, USA. |
| Stumm & Morgan | Stumm, W. & J.J. Morgan (1981). Aquatic chemistry. John Wiley & Sons, New York. |
| Tipping (1994) | Tipping, E. (1994). WHAM - A chemical equilibrium model and computer code for waters, sediments, and soils incorporating a discrete site/electrostatic model of ion-binding by humic substances. Computers & Geosciences *20*, 973 - 1023. |
| Tipping (1998) | Tipping, E. (1998). Humic Ion-Binding Model VI: An Improved Description of the Interactions of Protons and Metal Ions with Humic Substances. Aquatic Geochemistry *4*, 3 - 48. |

| Abbreviation used in CHEAQS | Bibiographic reference |
|---|---|
| Tipping et al. (2011) | Tipping, E., S. Lofts & J.E. Sonke (2011). Humic Ion-Binding Model VII: a revised parameterisation of cation-binding by humic substances. Environmental Chemistry *8*, 228 - 235. |
| Turner et al. | Turner, D.R., M. Whitfield & A.G. Dickson (1981). The equilibrium speciation of dissolved components in freshwater and seawater at 25°C and 1 atm pressure. Geochimica et Cosmochimica Acta *45*, 855 - 881. |
| Turner & Whitfield | Turner, D.R. & M. Whitfield (1987). An equilibrium speciation model for copper in sea and estuarine waters at 25°C including complexation with glycine, EDTA and NTA. Geochimica et Cosmochimica Acta *51*, 3231 - 3239. |
| Van Riemsdijk & Keizer | Van Riemsdijk, W.H. & M.G. Keizer (1984). Computer assisted education. Chemical equilibria in soil-water-sediment (in Dutch). Department of Soil Science and Plant Nutrition, Agricultural University of Wageningen, The Netherlands. |


### *Part II: other bibliographic references*


Giesy, J.P & J.J. Alberts (1989). Conditional stability constants and binding capacities for copper(II) by ultrafilterable material isolated from six surface waters of Wyoming, USA. Hydrobiologia *188/189*, 659 - 679.

Janssen, R.P.T. & W. Verweij (2003). Geochemistry of some rare earth elements in groundwater, Vierlingsbeek, The Netherlands. Water Research *37*, 1320–1350.

Martell, A.E. & R.M. Smith (1974). Critical stability constants. Volume 1. Amino acids. Plenum Press, New York.

Martell, A.E. & R.M. Smith (1977). Critical stability constants. Volume 3. Other organic ligands. Plenum Press, New York.

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The structural formulas were created using a Java applet called 'Marvin', available at
http://www.chemaxon.com/marvin
Accessed late November 2014.