Equilibria and equilibrium constants in CHEAQS Next (64 bits)

Conversions, selection criteria, and sources

Status box

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Contents

1. Introduction

This document contains the background information about the database of CHEAQS Next (64 bits), version as stated in the Status Box on page 2. For each equilibrium reaction included in the database, you can find here the source of the equilibrium constant, as well as the conversions that were made to convert from the value found in the literature to the value as entered in the CHEAQS Next 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 Next 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. 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.

Chapter 2 is organised per type of equilibrium:

1. the water equilibrium;
2. complexes
3. adsorption
4. redox equilibria
5. gases
6. solids
7. organic complexation

Chapter 3 contains the molecular weights, the selection criteria for the equilibria, information about compatibility of the different sources that were used and the radii used for the MSA-model. Literature references can also be found there.

2. Equilibria

In this chapter you will find the equilibria selected for CHEAQS, as well as any conditions (ionic strength, temperature) and conversions. This chapter is organised by (1) type of equilibrium; (2) cation. The first column gives the equilibrium reaction, where the product **is displayed in bold**. The second column contains the equilibrium constant, given as the $\log_{10}$ of the so-called β, the cumulative or overall constant. Column three gives (if available) the ΔH for the equilibrium reaction, in J/mol (note that also kJ/mol is used in the literature). Column four gives the literature reference, as a number. Full references can be found in the annex. The last column contains additional information including conversions. Ligands here are abbreviated as 'L' (without the quotes), charges are omitted here and H_2O is omitted in many reaction equations.
Data for constants and ΔH is valid for temperature = 25°C and ionic strength (I) = 0 M unless otherwise stated. If only data were available for ionic strength different from 0, those data were extrapolated to I = 0 M using the Davies-equation.

2.1. The water equilibrium

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (OH)^- \rightleftharpoons$ **H_2O**	13.997	-5.581E+4	1	

2.2. Complexes

This paragraph contains the information about complexes. For each ligand a separate sub-paragraph was created and within that sub-paragraph you find the information organised per cation.

2.2.1. Hydroxide

The formula for the ligand hydroxide is OH^-; the molecular weight is 17.007.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Li^+ + (OH)^- \rightleftharpoons$ **$Li(OH)$ *(aq)***	0.36	0	1	
$Be^{2+} + (OH)^- \rightleftharpoons$ **$Be(OH)^+$**	7.63954		1	Original data for β: $\log_{10}(\beta)$ = 8.18, at I = 3.0 M.
$Be^{2+} + 2\ (OH)^- \rightleftharpoons$ **$Be(OH)_2$ *(aq)***	16.86073		1	Original data for β: $\log_{10}(\beta)$ = 16.22, at I = 0.1 M.
$Be^{2+} + 3\ (OH)^- \rightleftharpoons$ **$Be(OH)_3^-$**	18.75		2	$Be^{2+} + 3\ H_2O \rightleftharpoons Be(OH)_3 + 3\ H^+$ $\log_{10}(\beta) = -23.25$ $3\ H^+ + 3\ OH^- \rightleftharpoons 3\ H_2O$ $\log_{10}(\beta) = 42.00$ $Be^{2+} + 3\ OH^- \rightleftharpoons Be(OH)_3$ $\log_{10}(\beta) = 18.75$
$Be^{2+} + 4\ (OH)^- \rightleftharpoons$ **$Be(OH)_4^{2-}$**	18.59		2	Similar to $Be(OH)_3^-$ (page 6)
$2\ Be^{2+} + (OH)^- \rightleftharpoons$ **$Be_2(OH)^{3+}$**	10.82	-2.7E+4	1	Original data for β: $\log_{10}(\beta)$ = 10.82, at I = 0.1 M. Original data for ΔH at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ Be^{2+} + 3\ (OH)^- \rightleftharpoons \mathbf{Be_3(OH)_3^{3+}}$	33.1	-1E+5	1	Original data for ΔH at I = 0.5 M.
$5\ Be^{2+} + 6\ (OH)^- \rightleftharpoons \mathbf{Be_5(OH)_6^{4+}}$	65.17194	-2.07E+5	1	Original data for β: $log_{10}(\beta)$ = 63.83, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$5\ Be^{2+} + 7\ (OH)^- \rightleftharpoons \mathbf{Be_5(OH)_7^{3+}}$	72.50844	-2.42E+5	1	Original data for β: $log_{10}(\beta)$ = 70.68, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$6\ Be^{2+} + 8\ (OH)^- \rightleftharpoons \mathbf{Be_6(OH)_8^{4+}}$	84.8	-2.38E+5	1	Original data for ΔH at I = 0.5 M.
$Na^+ + (OH)^- \rightleftharpoons \mathbf{Na(OH)}$ ***(aq)***	0.1	4E+3	1	
$Mg^{2+} + (OH)^- \rightleftharpoons \mathbf{Mg(OH)^+}$	2.58	1.2E+4	1	
$4\ Mg^{2+} + 4\ (OH)^- \rightleftharpoons \mathbf{Mg_4(OH)_4^{4+}}$	16.55954		1	Original data for β: $log_{10}(\beta)$ = 16.1, at I = 3.0 M when NaCl is the background electrolyte; $log_{10}(\beta)$ = 18.1 (also at I = 3.0 M) when $NaClO_4$ is the background electrolyte. The average log-value (17.1) was converted to I = 0 M.
$Al^{3+} + (OH)^- \rightleftharpoons \mathbf{Al(OH)^{2+}}$	9	-8E+3	1	
$Al^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Al(OH)_2^+}$	17.7		1	
$Al^{3+} + 3\ (OH)^- \rightleftharpoons \mathbf{Al(OH)_3}$ ***(aq)***	25.3		1	
$Al^{3+} + 4\ (OH)^- \rightleftharpoons \mathbf{Al(OH)_4^-}$	33.3	-4.35E+4	1	
$2\ Al^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Al_2(OH)_2^{4+}}$	20.3	-3.7E+4	1	Original data for ΔH at I = 1.0 M.
$3\ Al^{3+} + 4\ (OH)^- \rightleftharpoons \mathbf{Al_3(OH)_4^{5+}}$	42.1	-8.3E+4	1	Original data for ΔH at I = 1.0 M.
$13\ Al^{3+} + 32\ (OH)^- \rightleftharpoons \mathbf{Al_{13}O_4(OH)_{24}^{7+}}$	349.3	-6.69E+5	1	Original data for ΔH at I = 1.0 M.
$K^+ + (OH)^- \rightleftharpoons \mathbf{K(OH)}$ ***(aq)***	0.23787		1	Original data for β: $log_{10}(\beta)$ = 0.0, at I = 0.15 M at 37°C.
$Ca^{2+} + (OH)^- \rightleftharpoons \mathbf{Ca(OH)^+}$	1.3	8.3E+3	1	
$Sc^{3+} + (OH)^- \rightleftharpoons \mathbf{Sc(OH)^{2+}}$	9.7	8E+3	1	Original data for ΔH at I = 1.0 M.
$Sc^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Sc(OH)_2^+}$	18.3		1	
$Sc^{3+} + 3\ (OH)^- \rightleftharpoons \mathbf{Sc(OH)_3}$ ***(aq)***	23.9		1	
$Sc^{3+} + 4\ (OH)^- \rightleftharpoons \mathbf{Sc(OH)_4^-}$	30		1	
$2\ Sc^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Sc_2(OH)_2^{4+}}$	22	-5E+4	1	Original data for ΔH at I = 1.0 M.
$3\ Sc^{3+} + 5\ (OH)^- \rightleftharpoons \mathbf{Sc_3(OH)_5^{4+}}$	53.8	-1.17E+5	1	Original data for ΔH at I = 1.0 M.
$Cr(III)^{3+} + (OH)^- \rightleftharpoons \mathbf{Cr(III)(OH)^{2+}}$	10.3	-1.6E+4	1	
$Cr(III)^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Cr(III)(OH)_2^+}$	18.3		1	
$Cr(III)^{3+} + 3\ (OH)^- \rightleftharpoons \mathbf{Cr(III)(OH)_3}$ ***(aq)***	24		2	Similar to $Be(OH)_3^-$ (page 6)
$Cr(III)^{3+} + 4\ (OH)^- \rightleftharpoons \mathbf{Cr(III)(OH)_4^-}$	28.6		2	Similar to $Be(OH)_3^-$ (page 6)
$2\ Cr(III)^{3+} + 2\ (OH)^- \rightleftharpoons \mathbf{Cr(III)_2(OH)_2^{4+}}$	24.40632		1	Original data for β: $log_{10}(\beta)$ = 24.0, at I = 1.0 M.
$3\ Cr(III)^{3+} + 4\ (OH)^- \rightleftharpoons \mathbf{Cr(III)_3(OH)_4^{5+}}$	37.60948		1	Original data for β: $log_{10}(\beta)$ = 37.0, at I = 1.0 M.
$4\ Cr(III)^{3+} + 6\ (OH)^- \rightleftharpoons \mathbf{Cr(III)_4(OH)_6^{6+}}$	80.80948		1	Original data for β: $log_{10}(\beta)$ = 80.2, at I = 1.0 M.
$Mn(II)^{2+} + (OH)^- \rightleftharpoons \mathbf{Mn(II)(OH)^+}$	3.4	4E+3	1	
$Mn(II)^{2+} + 2\ (OH)^- \rightleftharpoons \mathbf{Mn(II)(OH)_2}$ ***(aq)***	5.8		2	Similar to $Be(OH)_3^-$ (page 6)
$Mn(II)^{2+} + 3\ (OH)^- \rightleftharpoons \mathbf{Mn(II)(OH)_3^-}$	7.2		2	Similar to $Be(OH)_3^-$ (page 6)
$Mn(II)^{2+} + 4\ (OH)^- \rightleftharpoons \mathbf{Mn(II)(OH)_4^{2-}}$	7.7		1	
$2\ Mn(II)^{2+} + (OH)^- \rightleftharpoons \mathbf{Mn(II)_2(OH)^{3+}}$	3.4		1	
$2\ Mn(II)^{2+} + 3\ (OH)^- \rightleftharpoons \mathbf{Mn(II)_2(OH)_3^+}$	18.1		1	
$Fe(II)^{2+} + (OH)^- \rightleftharpoons \mathbf{Fe(II)(OH)^+}$	4.6	0	1	
$Fe(II)^{2+} + 2\ (OH)^- \rightleftharpoons \mathbf{Fe(II)(OH)_2}$ ***(aq)***	7.4	8E+3	1	
$Fe(II)^{2+} + 3\ (OH)^- \rightleftharpoons \mathbf{Fe(II)(OH)_3^-}$	11	-4.1E+4	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Fe(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Fe(II)(OH)_4^{2-}$**	10		2	Similar to $Be(OH)_3^-$ (page 6)
$Fe(III)^{3+}$ + $(OH)^-$ ⇌ **$Fe(III)(OH)^{2+}$**	11.81	-1.2E+4	1	
$Fe(III)^{3+}$ + 2 $(OH)^-$ ⇌ **$Fe(III)(OH)_2^+$**	22.4		1	
$Fe(III)^{3+}$ + 3 $(OH)^-$ ⇌ **$Fe(III)(OH)_3$ *(aq)***	30.2		1	
$Fe(III)^{3+}$ + 4 $(OH)^-$ ⇌ **$Fe(III)(OH)_4^-$**	34.4		1	
2 $Fe(III)^{3+}$ + 2 $(OH)^-$ ⇌ **$Fe(III)_2(OH)_2^{4+}$**	25.1	-5.52E+4	1	
3 $Fe(III)^{3+}$ + 4 $(OH)^-$ ⇌ **$Fe(III)_3(OH)_4^{5+}$**	49.7	-1.58E+5	1	Original data for ΔH at I = 3.0 M.
$Co(II)^{2+}$ + $(OH)^-$ ⇌ **$Co(II)(OH)^+$**	4.3		1	
$Co(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Co(II)(OH)_2$ *(aq)***	9.2		1	
$Co(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Co(II)(OH)_3^-$**	10.5		1	
$Co(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Co(II)(OH)_4^{2-}$**	9.7		2	Similar to $Be(OH)_3^-$ (page 6)
4 $Co(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Co(II)_4(OH)_4^{4+}$**	25.5		1	
$Co(III)^{3+}$ + $(OH)^-$ ⇌ **$Co(III)(OH)^{2+}$**	12.72931		1	Original data for β: $log_{10}(\beta)$ = 13.54, at I = 3.0 M.
Ni^{2+} + $(OH)^-$ ⇌ **$Ni(OH)^+$**	4.1	-4E+3	1	
Ni^{2+} + 2 $(OH)^-$ ⇌ **$Ni(OH)_2$ *(aq)***	9		1	
Ni^{2+} + 3 $(OH)^-$ ⇌ **$Ni(OH)_3^-$**	12		1	
Ni^{2+} + 4 $(OH)^-$ ⇌ **$Ni(OH)_4^{2-}$**	12		2	Similar to $Be(OH)_3^-$ (page 6)
4 Ni^{2+} + 4 $(OH)^-$ ⇌ **$Ni_4(OH)_4^{4+}$**	28.3	-5.35E+4	1	Original data for ΔH at I = 3.0 M.
$Cu(II)^{2+}$ + $(OH)^-$ ⇌ **$Cu(II)(OH)^+$**	6.5	-2E+4	1	Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Cu(II)(OH)_2$ *(aq)***	10.7		2	Similar to $Be(OH)_3^-$ (page 6)
$Cu(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Cu(II)(OH)_3^-$**	14.2		2	Similar to $Be(OH)_3^-$ (page 6)
$Cu(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Cu(II)(OH)_4^{2-}$**	16.4		2	Similar to $Be(OH)_3^-$ (page 6)
2 $Cu(II)^{2+}$ + $(OH)^-$ ⇌ **$Cu(II)_2(OH)^{3+}$**	8.05	-2.5E+4	1	Original data for β: $log_{10}(\beta)$ = 7.7, at I = 3.0 M when $LiClO_4$ is the background electrolyte; $log_{10}(\beta)$ = 8.4 (also at I = 3.0 M) when $NaClO_4$ is the background electrolyte. The average log-value (8.05) was converted to I = 0 M. Original data for ΔH at I = 3.0 M.
2 $Cu(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Cu(II)_2(OH)_2^{2+}$**	17.5	-3.5E+4	1	Original data for ΔH at I = 0.1 M.
3 $Cu(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Cu(II)_3(OH)_4^{2+}$**	35.2	-1.17E+5	1	Original data for ΔH at I = 0.1 M.
Zn^{2+} + $(OH)^-$ ⇌ **$Zn(OH)^+$**	5	0	1	
Zn^{2+} + 2 $(OH)^-$ ⇌ **$Zn(OH)_2$ *(aq)***	11.1		1	
Zn^{2+} + 3 $(OH)^-$ ⇌ **$Zn(OH)_3^-$**	13.6		1	
Zn^{2+} + 4 $(OH)^-$ ⇌ **$Zn(OH)_4^{2-}$**	14.8		1	
2 Zn^{2+} + $(OH)^-$ ⇌ **$Zn_2(OH)^{3+}$**	5	8E+3	1	Original data for ΔH at I = 3.0 M.
4 Zn^{2+} + 4 $(OH)^-$ ⇌ **$Zn_4(OH)_4^{4+}$**	27.35954		1	Original data for β: $log_{10}(\beta)$ = 27.9, at I = 3.0 M.
Ga^{3+} + $(OH)^-$ ⇌ **$Ga(OH)^{2+}$**	11.1	-3.3E+4	1	Original data for ΔH at I = 0.5 M.
Ga^{3+} + 2 $(OH)^-$ ⇌ **$Ga(OH)_2^+$**	21.3		1	
Ga^{3+} + 3 $(OH)^-$ ⇌ **$Ga(OH)_3$ *(aq)***	31.7		2	Similar to $Be(OH)_3^-$ (page 6)
Ga^{3+} + 4 $(OH)^-$ ⇌ **$Ga(OH)_4^-$**	39.4		1	
2 Ga^{3+} + 2 $(OH)^-$ ⇌ **$Ga_2(OH)_2^{4+}$**	26.33678		1	Original data for β: $log_{10}(\beta)$ = 25.8, at I = 0.5 M.
Sr^{2+} + $(OH)^-$ ⇌ **$Sr(OH)^+$**	0.82	5E+3	1	
Y^{3+} + $(OH)^-$ ⇌ **$Y(OH)^{2+}$**	6.3		1	
Y^{3+} + 2 $(OH)^-$ ⇌ **$Y(OH)_2^+$**	11.6		2	Similar to $Be(OH)_3^-$ (page 6)

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Y^{3+} + 3 $(OH)^-$ ⇌ **$Y(OH)_3$** ***(aq)***	16		2	Similar to $Be(OH)_3^-$ (page 6)
Y^{3+} + 4 $(OH)^-$ ⇌ **$Y(OH)_4^-$**	19.5		2	Similar to $Be(OH)_3^-$ (page 6)
2 Y^{3+} + 2 $(OH)^-$ ⇌ **$Y_2(OH)_2^{4+}$**	13.8		1	
3 Y^{3+} + 5 $(OH)^-$ ⇌ **$Y_3(OH)_5^{4+}$**	38.4		1	
Zr^{4+} + $(OH)^-$ ⇌ **$Zr(OH)^{3+}$**	14.3		1	
Zr^{4+} + 2 $(OH)^-$ ⇌ **$Zr(OH)_2^{2+}$**	26.3		2	Similar to $Be(OH)_3^-$ (page 6)
Zr^{4+} + 3 $(OH)^-$ ⇌ **$Zr(OH)_3^+$**	36.9		2	Similar to $Be(OH)_3^-$ (page 6)
Zr^{4+} + 4 $(OH)^-$ ⇌ **$Zr(OH)_4$** ***(aq)***	49.63160		1	Original data for β: $\log_{10}(\beta)$ = 47.6, at I = 1.0 M and 20°C.
Zr^{4+} + 5 $(OH)^-$ ⇌ **$Zr(OH)_5^-$**	54		1	
3 Zr^{4+} + 4 $(OH)^-$ ⇌ **$Zr_3(OH)_4^{8+}$**	55.4		1	
4 Zr^{4+} + 8 $(OH)^-$ ⇌ **$Zr_4(OH)_8^{8+}$**	106		1	
Pd^{2+} + $(OH)^-$ ⇌ **$Pd(OH)^+$**	11.20632		1	Original data for β: $\log_{10}(\beta)$ = 10.8, at I = 1.0 M.
Ag^+ + $(OH)^-$ ⇌ **$Ag(OH)$** ***(aq)***	2		1	
Ag^+ + 2 $(OH)^-$ ⇌ **$Ag(OH)_2^-$**	3.99		1	
Cd^{2+} + $(OH)^-$ ⇌ **$Cd(OH)^+$**	3.9	-1E+3	1	Original data for ΔH at I = 3.0 M.
Cd^{2+} + 2 $(OH)^-$ ⇌ **$Cd(OH)_2$** ***(aq)***	7.7		1	
Cd^{2+} + 3 $(OH)^-$ ⇌ **$Cd(OH)_3^-$**	9.48931		1	Original data for β: $\log_{10}(\beta)$ = 10.3, at I = 3.0 M.
Cd^{2+} + 4 $(OH)^-$ ⇌ **$Cd(OH)_4^{2-}$**	8.7		1	
2 Cd^{2+} + $(OH)^-$ ⇌ **$Cd_2(OH)^{3+}$**	4.6	-1E+4	1	Original data for ΔH at I = 3.0 M.
4 Cd^{2+} + 4 $(OH)^-$ ⇌ **$Cd_4(OH)_4^{4+}$**	23.2	-5.4E+4	1	Original data for ΔH at I = 3.0 M.
In^{3+} + $(OH)^-$ ⇌ **$In(OH)^{2+}$**	10.07	-3.4E+4	1	Original data for ΔH at I = 3.0 M.
In^{3+} + 2 $(OH)^-$ ⇌ **$In(OH)_2^+$**	20.2	-5.4E+4	1	Original data for ΔH at I = 3.0 M.
In^{3+} + 3 $(OH)^-$ ⇌ **$In(OH)_3$** ***(aq)***	29.6		1	
In^{3+} + 4 $(OH)^-$ ⇌ **$In(OH)_4^-$**	33.9		1	
2 In^{3+} + 2 $(OH)^-$ ⇌ **$In_2(OH)_2^{4+}$**	22.65954	-6.69E+4	1	Original data for β: $\log_{10}(\beta)$ = 23.2, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
4 In^{3+} + 4 $(OH)^-$ ⇌ **$In_4(OH)_4^{8+}$**	45.23710		1	Original data for β: $\log_{10}(\beta)$ = 47.8, at I = 0.1 M.
4 In^{3+} + 6 $(OH)^-$ ⇌ **$In_4(OH)_6^{6+}$**	42.28931		1	Original data for β: $\log_{10}(\beta)$ = 43.1, at I = 3.0 M.
$Sn(II)^{2+}$ + $(OH)^-$ ⇌ **$Sn(II)(OH)^+$**	10.6		1	
$Sn(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Sn(II)(OH)_2$** ***(aq)***	20.9		1	
$Sn(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Sn(II)(OH)_3^-$**	25.4		1	
2 $Sn(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Sn(II)_2(OH)_2^{2+}$**	23.2		1	
3 $Sn(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Sn(II)_3(OH)_4^{2+}$**	49.12		1	
$Sn(IV)^{4+}$ + $(OH)^-$ ⇌ **$Sn(IV)(OH)^{3+}$**	15.5		2	Similar to $Be(OH)_3^-$ (page 6)
$Sn(IV)^{4+}$ + 2 $(OH)^-$ ⇌ **$Sn(IV)(OH)_2^{2+}$**	29.31		2	Similar to $Be(OH)_3^-$ (page 6)
$Sn(IV)^{4+}$ + 3 $(OH)^-$ ⇌ **$Sn(IV)(OH)_3^+$**	43.7		2	Similar to $Be(OH)_3^-$ (page 6)
$Sn(IV)^{4+}$ + 4 $(OH)^-$ ⇌ **$Sn(IV)(OH)_4$** ***(aq)***	56.51		2	Similar to $Be(OH)_3^-$ (page 6)
Ba^{2+} + $(OH)^-$ ⇌ **$Ba(OH)^+$**	0.64	5E+3	1	
La^{3+} + $(OH)^-$ ⇌ **$La(OH)^{2+}$**	5.5		1	
La^{3+} + 2 $(OH)^-$ ⇌ **$La(OH)_2^+$**	10.6		2	Similar to $Be(OH)_3^-$ (page 6)
La^{3+} + 3 $(OH)^-$ ⇌ **$La(OH)_3$** ***(aq)***	14.5		2	Similar to $Be(OH)_3^-$ (page 6)
La^{3+} + 4 $(OH)^-$ ⇌ **$La(OH)_4^-$**	17.2		2	Similar to $Be(OH)_3^-$ (page 6)

Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 La^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{La_2(OH)_2^{4+}}$	10.47112		1	Original data for β: $log_{10}(β)$ = 10.5, at I = 2.0 M.
Ce^{3+} + $(OH)^-$ ⇌ $\mathbf{Ce(OH)^{2+}}$	5.7		1	
Ce^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Ce(OH)_2^+}$	10.9		2	Similar to $Be(OH)_3^-$ (page 6)
Ce^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Ce(OH)_3}$ ***(aq)***	15.2		2	Similar to $Be(OH)_3^-$ (page 6)
Ce^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Ce(OH)_4^-}$	18.4		2	Similar to $Be(OH)_3^-$ (page 6)
2 Ce^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Ce_2(OH)_2^{4+}}$	11.15954		1	Original data for β: $log_{10}(β)$ = 11.7, at I = 3.0 M.
Pr^{3+} + $(OH)^-$ ⇌ $\mathbf{Pr(OH)^{2+}}$	6.00516		1	Original data for β: $log_{10}(β)$ = 5.2, at I = 0.5 M.
Pr^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Pr(OH)_2^+}$	11		2	Similar to $Be(OH)_3^-$ (page 6)
Pr^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Pr(OH)_3}$ ***(aq)***	15.4		2	Similar to $Be(OH)_3^-$ (page 6)
Pr^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Pr(OH)_4^-}$	18.8		2	Similar to $Be(OH)_3^-$ (page 6)
2 Pr^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Pr_2(OH)_2^{4+}}$	11.87112		1	Original data for β: $log_{10}(β)$ = 11.9, at I = 2.0 M.
Nd^{3+} + $(OH)^-$ ⇌ $\mathbf{Nd(OH)^{2+}}$	6		1	
Nd^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Nd(OH)_2^+}$	11.1		2	Similar to $Be(OH)_3^-$ (page 6)
Nd^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Nd(OH)_3}$ ***(aq)***	15.5		2	Similar to $Be(OH)_3^-$ (page 6)
Nd^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Nd(OH)_4^-}$	18.6		1	
2 Nd^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Nd_2(OH)_2^{4+}}$	14.1		1	
Sm^{3+} + $(OH)^-$ ⇌ $\mathbf{Sm(OH)^{2+}}$	6.1	-2E+4	1	Original data for ΔH at I = 3.0 M.
Sm^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Sm(OH)_2^+}$	11.4		2	Similar to $Be(OH)_3^-$ (page 6)
Sm^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Sm(OH)_3}$ ***(aq)***	16.2		2	Similar to $Be(OH)_3^-$ (page 6)
Sm^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Sm(OH)_4^-}$	20.3		2	Similar to $Be(OH)_3^-$ (page 6)
2 Sm^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Sm_2(OH)_2^{4+}}$	13.47112	-2.5E+4	1	Original data for β: $log_{10}(β)$ = 13.5, at I = 2.0 M. Original data for ΔH at I = 3.0 M.
Eu^{3+} + $(OH)^-$ ⇌ $\mathbf{Eu(OH)^{2+}}$	6.20516		1	Original data for β: $log_{10}(β)$ = 5.4, at I = 0.5 M.
Eu^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Eu(OH)_2^+}$	11.4		2	Similar to $Be(OH)_3^-$ (page 6)
Eu^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Eu(OH)_3}$ ***(aq)***	16.4		2	Similar to $Be(OH)_3^-$ (page 6)
Eu^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Eu(OH)_4^-}$	20.7		2	Similar to $Be(OH)_3^-$ (page 6)
2 Eu^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Eu_2(OH)_2^{4+}}$	13.17112		1	Original data for β: $log_{10}(β)$ = 13.2, at I = 2.0 M.
Gd^{3+} + $(OH)^-$ ⇌ $\mathbf{Gd(OH)^{2+}}$	6.20516		1	Original data for β: $log_{10}(β)$ = 5.4, at I = 0.5 M.
Gd^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Gd(OH)_2^+}$	11.6		2	Similar to $Be(OH)_3^-$ (page 6)
Gd^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Gd(OH)_3}$ ***(aq)***	16.8		2	Similar to $Be(OH)_3^-$ (page 6)
Gd^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Gd(OH)_4^-}$	21.6		2	Similar to $Be(OH)_3^-$ (page 6)
2 Gd^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Gd_2(OH)_2^{4+}}$	13.07112		1	Original data for β: $log_{10}(β)$ = 13.1, at I = 2.0 M.
Tb^{3+} + $(OH)^-$ ⇌ $\mathbf{Tb(OH)^{2+}}$	6.1		1	
Tb^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Tb(OH)_2^+}$	11.7		2	Similar to $Be(OH)_3^-$ (page 6)
Tb^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Tb(OH)_3}$ ***(aq)***	16.9		2	Similar to $Be(OH)_3^-$ (page 6)
Tb^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Tb(OH)_4^-}$	21.7		2	Similar to $Be(OH)_3^-$ (page 6)
Dy^{3+} + $(OH)^-$ ⇌ $\mathbf{Dy(OH)^{2+}}$	6.40516		1	Original data for β: $log_{10}(β)$ = 5.6, at I = 0.5 M.
Dy^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Dy(OH)_2^+}$	11.8		2	Similar to $Be(OH)_3^-$ (page 6)
Dy^{3+} + 3 $(OH)^-$ ⇌ $\mathbf{Dy(OH)_3}$ ***(aq)***	17.3		2	Similar to $Be(OH)_3^-$ (page 6)
Dy^{3+} + 4 $(OH)^-$ ⇌ $\mathbf{Dy(OH)_4^-}$	22.5		2	Similar to $Be(OH)_3^-$ (page 6)
2 Dy^{3+} + 2 $(OH)^-$ ⇌ $\mathbf{Dy_2(OH)_2^{4+}}$	13.97112		1	Original data for β: $log_{10}(β)$ = 14.0, at I = 2.0 M.
Ho^{3+} + $(OH)^-$ ⇌ $\mathbf{Ho(OH)^{2+}}$	6.50516		1	Original data for β: $log_{10}(β)$ = 5.7, at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ho^{3+} + 2 $(OH)^-$ ⇌ **$Ho(OH)_2^+$**	11.9		2	Similar to $Be(OH)_3^-$ (page 6)
Ho^{3+} + 3 $(OH)^-$ ⇌ **$Ho(OH)_3$ *(aq)***	17.4		2	Similar to $Be(OH)_3^-$ (page 6)
Ho^{3+} + 4 $(OH)^-$ ⇌ **$Ho(OH)_4^-$**	22.6		2	Similar to $Be(OH)_3^-$ (page 6)
Er^{3+} + $(OH)^-$ ⇌ **$Er(OH)^{2+}$**	6.50516		1	Original data for β: $log_{10}(\beta)$ = 5.7, at I = 0.5 M.
Er^{3+} + 2 $(OH)^-$ ⇌ **$Er(OH)_2^+$**	12.1		2	Similar to $Be(OH)_3^-$ (page 6)
Er^{3+} + 3 $(OH)^-$ ⇌ **$Er(OH)_3$ *(aq)***	17.8		2	Similar to $Be(OH)_3^-$ (page 6)
Er^{3+} + 4 $(OH)^-$ ⇌ **$Er(OH)_4^-$**	23.4		2	Similar to $Be(OH)_3^-$ (page 6)
2 Er^{3+} + 2 $(OH)^-$ ⇌ **$Er_2(OH)_2^{4+}$**	14.47112		1	Original data for β: $log_{10}(\beta)$ = 14.5, at I = 2.0 M.
Tm^{3+} + $(OH)^-$ ⇌ **$Tm(OH)^{2+}$**	6.60516		1	Original data for β: $log_{10}(\beta)$ = 5.8, at I = 0.5 M.
Tm^{3+} + 2 $(OH)^-$ ⇌ **$Tm(OH)_2^+$**	12.1		2	Similar to $Be(OH)_3^-$ (page 6)
Tm^{3+} + 3 $(OH)^-$ ⇌ **$Tm(OH)_3$ *(aq)***	17.9		2	Similar to $Be(OH)_3^-$ (page 6)
Tm^{3+} + 4 $(OH)^-$ ⇌ **$Tm(OH)_4^-$**	23.4		2	Similar to $Be(OH)_3^-$ (page 6)
Yb^{3+} + $(OH)^-$ ⇌ **$Yb(OH)^{2+}$**	6.60516		1	Original data for β: $log_{10}(\beta)$ = 5.8, at I = 0.5 M.
Yb^{3+} + 2 $(OH)^-$ ⇌ **$Yb(OH)_2^+$**	12.2		2	Similar to $Be(OH)_3^-$ (page 6)
Yb^{3+} + 3 $(OH)^-$ ⇌ **$Yb(OH)_3$ *(aq)***	17.9		2	Similar to $Be(OH)_3^-$ (page 6)
Yb^{3+} + 4 $(OH)^-$ ⇌ **$Yb(OH)_4^-$**	23.3		2	Similar to $Be(OH)_3^-$ (page 6)
2 Yb^{3+} + 2 $(OH)^-$ ⇌ **$Yb_2(OH)_2^{4+}$**	14.67112		1	Original data for β: $log_{10}(\beta)$ = 14.7, at I = 2.0 M.
Lu^{3+} + $(OH)^-$ ⇌ **$Lu(OH)^{2+}$**	6.60516		1	Original data for β: $log_{10}(\beta)$ = 5.8, at I = 0.5 M.
Lu^{3+} + 2 $(OH)^-$ ⇌ **$Lu(OH)_2^+$**	12.3		2	Similar to $Be(OH)_3^-$ (page 6)
Lu^{3+} + 3 $(OH)^-$ ⇌ **$Lu(OH)_3$ *(aq)***	18.3		2	Similar to $Be(OH)_3^-$ (page 6)
Lu^{3+} + 4 $(OH)^-$ ⇌ **$Lu(OH)_4^-$**	24.2		2	Similar to $Be(OH)_3^-$ (page 6)
Hf^{4+} + $(OH)^-$ ⇌ **$Hf(OH)^{3+}$**	13.8		1	
Hf^{4+} + 2 $(OH)^-$ ⇌ **$Hf(OH)_2^{2+}$**	25.6		2	Similar to $Be(OH)_3^-$ (page 6)
Hf^{4+} + 3 $(OH)^-$ ⇌ **$Hf(OH)_3^+$**	36		2	Similar to $Be(OH)_3^-$ (page 6)
Hf^{4+} + 4 $(OH)^-$ ⇌ **$Hf(OH)_4$ *(aq)***	45.3		2	Similar to $Be(OH)_3^-$ (page 6)
Hf^{4+} + 5 $(OH)^-$ ⇌ **$Hf(OH)_5^-$**	52.8		1	
$Pt(II)^{2+}$ + $(OH)^-$ ⇌ **$Pt(II)(OH)^+$**	24.91		12	
$Pt(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Pt(II)(OH)_2$ *(aq)***	28.81		12	
$Hg(II)^{2+}$ + $(OH)^-$ ⇌ **$Hg(II)(OH)^+$**	10.6	-3.5E+4	1	Original data for ΔH at I = 1.0 M.
$Hg(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Hg(II)(OH)_2$ *(aq)***	21.83	-7.19E+4	1	Original data for ΔH at I = 1.0 M.
$Hg(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Hg(II)(OH)_3^-$**	20.9		2	Similar to $Be(OH)_3^-$ (page 6)
2 $Hg(II)^{2+}$ + $(OH)^-$ ⇌ **$Hg(II)_2(OH)^{3+}$**	10.7		1	
3 $Hg(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Hg(II)_3(OH)_3^{3+}$**	35.6		1	
$Pb(II)^{2+}$ + $(OH)^-$ ⇌ **$Pb(II)(OH)^+$**	6.4	-3.2E+4	1	Original data for ΔH at I = 1.0 M.
$Pb(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Pb(II)(OH)_2$ *(aq)***	10.9		1	
$Pb(II)^{2+}$ + 3 $(OH)^-$ ⇌ **$Pb(II)(OH)_3^-$**	13.9		1	
2 $Pb(II)^{2+}$ + $(OH)^-$ ⇌ **$Pb(II)_2(OH)^{3+}$**	7.6		1	
3 $Pb(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Pb(II)_3(OH)_4^{2+}$**	32.1	-1.12E+5	1	Original data for ΔH at I = 1.0 M.
4 $Pb(II)^{2+}$ + 4 $(OH)^-$ ⇌ **$Pb(II)_4(OH)_4^{4+}$**	35.1	-1.38E+5	1	Original data for ΔH at I = 1.0 M.
6 $Pb(II)^{2+}$ + 8 $(OH)^-$ ⇌ **$Pb(II)_6(OH)_8^{4+}$**	68.4	-2.33E+5	1	Original data for ΔH at I = 1.0 M.
Bi^{3+} + $(OH)^-$ ⇌ **$Bi(OH)^{2+}$**	12.9		1	
Bi^{3+} + 2 $(OH)^-$ ⇌ **$Bi(OH)_2^+$**	24.51580		1	Original data for β: $log_{10}(\beta)$ = 23.5, at I = 1.0 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Bi^{3+} + 3 $(OH)^-$ ⇌ **$Bi(OH)_3$ *(aq)***	33		1	
Bi^{3+} + 4 $(OH)^-$ ⇌ **$Bi(OH)_4^-$**	34.8		1	
$(U(VI)O_2)^{2+}$ + $(OH)^-$ ⇌ **$(U(VI)O_2)(OH)^+$**	8.1	-1.2E+4	1	Original data for ΔH at I = 0.5 M.
2 $(U(VI)O_2)^{2+}$ + 2 $(OH)^-$ ⇌ **$(U(VI)O_2)_2(OH)_2^{2+}$**	22.42	-6.98E+4	1	Original data for ΔH at I = 3.0 M.
3 $(U(VI)O_2)^{2+}$ + 5 $(OH)^-$ ⇌ **$(U(VI)O_2)_3(OH)_5^+$**	54.4	-1.71E+5	1	Original data for ΔH at I = 3.0 M.

2.2.2. Borate

The formula for the ligand borate is $H_2BO_3^-$; the molecular weight is 60.823.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(H_2BO_3)^-$ ⇌ **$H(H_2BO_3)$ *(aq)***	9.236	-1.3E+4	1	
H^+ + 2 $(H_2BO_3)^-$ ⇌ **$H(H_2BO_3)_2^-$**	9.166	-1.76E+4	1	HL + L ⇌ HL_2 $\log_{10}(\beta)$ = -0.07 ΔH = -4.6E+3 H + L ⇌ HL $\log_{10}(\beta)$ = 9.236 ΔH = -1.3E+4 H + 2 L ⇌ HL_2 $\log_{10}(\beta)$ = 9.166 ΔH = -1.76E+4 Original data for ΔH at I = 1.0 M.
H^+ + 3 $(H_2BO_3)^-$ ⇌ **$H(H_2BO_3)_3^{2-}$**	10.4		3	
2 H^+ + 3 $(H_2BO_3)^-$ ⇌ **$H_2(H_2BO_3)_3^-$**	20.402	-9.6E+3	1	HL + HL_2 ⇌ H_2L_3 $\log_{10}(\beta)$ = 2.00 ΔH = 2.1E+4 H + L ⇌ HL $\log_{10}(\beta)$ = 9.236 ΔH = -1.3E+4 H + 2 L ⇌ HL_2 $\log_{10}(\beta)$ = 9.166 ΔH = -1.76E+4 2 H + 3 L ⇌ H_2L_3 $\log_{10}(\beta)$ = 20.402 ΔH = -9.6E+3 Original data for ΔH at I = 1.0 M.
2 H^+ + 4 $(H_2BO_3)^-$ ⇌ **$H_2(H_2BO_3)_4^{2-}$**	21.912	-1.6E+3	1	H_2L_3 + L ⇌ H_2L_4 $\log_{10}(\beta)$ = 1.51 ΔH = 8E+3 2 H + 3 L ⇌ H_2L_3 $\log_{10}(\beta)$ = 20.402 ΔH = -9.6E+3 2 H + 4 L ⇌ H_2L_4 $\log_{10}(\beta)$ = 21.912 ΔH = -1.6E+3 Original data for ΔH at I = 1.0 M.
4 H^+ + 5 $(H_2BO_3)^-$ ⇌ **$H_4(H_2BO_3)_5^-$**	38.8		3	
Li^+ + $(H_2BO_3)^-$ ⇌ **$Li(H_2BO_3)$ *(aq)***	0.34		1	
Na^+ + $(H_2BO_3)^-$ ⇌ **$Na(H_2BO_3)$ *(aq)***	-0.15		1	
Mg^{2+} + $(H_2BO_3)^-$ ⇌ **$Mg(H_2BO_3)^+$**	1.54	0	1	
Ca^{2+} + $(H_2BO_3)^-$ ⇌ **$Ca(H_2BO_3)^+$**	1.76	4E+3	1	
$Fe(III)^{3+}$ + $(H_2BO_3)^-$ ⇌ **$Fe(III)(H_2BO_3)^{2+}$**	7.32824		1	Original data for β: $\log_{10}(\beta)$ = 6.58, at I = 0.7 M.
$Cu(II)^{2+}$ + $(H_2BO_3)^-$ ⇌ **$Cu(II)(H_2BO_3)^+$**	3.97883		1	Original data for β: $\log_{10}(\beta)$ = 3.48, at I = 0.7 M.
$Cu(II)^{2+}$ + 2 $(H_2BO_3)^-$ ⇌ **$Cu(II)(H_2BO_3)_2$ *(aq)***	6.87824		1	Original data for β: $\log_{10}(\beta)$ = 6.13, at I = 0.7 M.
Zn^{2+} + $(H_2BO_3)^-$ ⇌ **$Zn(H_2BO_3)^+$**	1.39883		1	Original data for β: $\log_{10}(\beta)$ = 0.9, at I = 0.7 M.
Zn^{2+} + 2 $(H_2BO_3)^-$ ⇌ **$Zn(H_2BO_3)_2$ *(aq)***	4.06824		1	Original data for β: $\log_{10}(\beta)$ = 3.32, at I = 0.7 M.
Sr^{2+} + $(H_2BO_3)^-$ ⇌ **$Sr(H_2BO_3)^+$**	1.55	4E+3	1	
Ag^+ + $(H_2BO_3)^-$ ⇌ **$Ag(H_2BO_3)$ *(aq)***	0.17977		1	Original data for β: $\log_{10}(\beta)$ = 0.45, at I = 3.0 M.
Cd^{2+} + $(H_2BO_3)^-$ ⇌ **$Cd(H_2BO_3)^+$**	1.91883		1	Original data for β: $\log_{10}(\beta)$ = 1.42, at I = 0.7 M.
Cd^{2+} + 2 $(H_2BO_3)^-$ ⇌ **$Cd(H_2BO_3)_2$ *(aq)***	3.45824		1	Original data for β: $\log_{10}(\beta)$ = 2.71, at I = 0.7 M.
Ba^{2+} + $(H_2BO_3)^-$ ⇌ **$Ba(H_2BO_3)^+$**	1.49	4E+3	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+}$ + $(H_2BO_3)^-$ ⇌ **$Pb(II)(H_2BO_3)^+$**	2.69883		1	Original data for β: $log_{10}(\beta)$ = 2.2, at I = 0.7 M.
$Pb(II)^{2+}$ + 2 $(H_2BO_3)^-$ ⇌ **$Pb(II)(H_2BO_3)_2$ *(aq)***	5.15824		1	Original data for β: $log_{10}(\beta)$ = 4.41, at I = 0.7 M.
H^+ + $(H_2BO_3)^-$ + $(NO_2)^-$ ⇌ **$(B(OH)_3)(NO_2)^-$**	8.746		1	
H^+ + $(H_2BO_3)^-$ + $(acetate)^-$ ⇌ **$B(OH)_3(acetate)^-$**	8.806		1	H + H_2BO_3 ⇌ H_3BO_3 (=$B(OH)_3$) $log_{10}(\beta)$ = 9.236 $B(OH)_3$ + L ⇌ $B(OH)_3L$ $log_{10}(\beta)$ = -0.43 H + H_2BO_3 + L ⇌ $B(OH)_3L$ $log_{10}(\beta)$ = 8.806
H^+ + $(H_2BO_3)^-$ + $(phthalate)^{2-}$ ⇌ **$H(H_2BO_3)(phthalate)^{2-}$**	9.166		1	$B(OH)_3$ + (phthalate) ⇌ $B(OH)_3$(phthalate) $log_{10}(\beta)$ = -0.07 H + H_2BO_3 ⇌ H_3BO_3 $log_{10}(\beta)$ = 9.236 H + H_2BO_3 + (phthalate) ⇌ $B(OH)_3$(phthalate) $log_{10}(\beta)$ = 9.166
2 H^+ + $(H_2BO_3)^-$ + $(phthalate)^{2-}$ ⇌ **$H_2(H_2BO_3)(phthalate)^-$**	13.647		1	$B(OH)_3$ + H(phthalate) ⇌ $B(OH)_3$H(phthalate) $log_{10}(\beta)$ = -1 H + H_2BO_3 ⇌ H_3BO_3 $log_{10}(\beta)$ = 9.236 H + (phthalate) ⇌ H(phthalate) $log_{10}(\beta)$ = 5.411 2 H + H_2BO_3 + (phthalate) ⇌ $B(OH)_3$H(phthalate) $log_{10}(\beta)$ = 13.647

2.2.3. Carbonate

The formula for the ligand carbonate is CO_3^{2-}; the molecular weight is 60.008.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(CO_3)^{2-}$ ⇌ **$H(CO_3)^-$**	10.329	-1.46E+4	1	
2 H^+ + $(CO_3)^{2-}$ ⇌ **$H_2(CO_3)$ *(aq)***	16.681	-2.376E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 6.352 ΔH = -1.46E+4 H + L ⇌ HL $log_{10}(\beta)$ = 10.329 ΔH = -9.16E+3 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 16.681 ΔH = -2.376E+4
Be^{2+} + $(CO_3)^{2-}$ ⇌ **$Be(CO_3)$ *(aq)***	6.25909		1	Original data for β: $log_{10}(\beta)$ = 7.34, at I = 1.0 M.
Be^{2+} + $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Be(CO_3)(OH)^-$**	13.96632		1	BeL ⇌ BeOHL + H $log_{10}(\beta)$ = -6.56 I = 3.0 M Be + L ⇌ BeL $log_{10}(\beta)$ = 7.34 I = 3.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 14.26723 I = 3.0 M Be + L + OH ⇌ BeOHL + H_2O $log_{10}(\beta)$ = 15.04723 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 13.96632
Be^{2+} + 2 $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Be(CO_3)(OH)_2^{2-}$**	21.04377		1	BeOHL ⇌ $Be(OH)_2L$ + H $log_{10}(\beta)$ = -7.54 I = 3.0 M Be + OH + L ⇌ BeOHL $log_{10}(\beta)$ = 15.04723 I = 3.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 14.26723 I = 3.0 M Be + L + 2 OH ⇌ $Be(OH)_2L$ + H_2O $log_{10}(\beta)$ = 21.85446 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 21.04377
3 Be^{2+} + 2 $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Be_3(CO_3)(OH)_2^{2+}$**	25.63286		1	3 Be + L ⇌ $Be_3(OH)_2L$ + 2 H $log_{10}(\beta)$ = -1.01 I = 3.0 M 2 H + 2 OH ⇌ 2 H_2O $log_{10}(\beta)$ = 28.53446 I = 3.0 M 3 Be + L + 2 OH ⇌ $Be_3(OH)_2L$ + 2 H_2O $log_{10}(\beta)$ = 27.52446 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 25.63286

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ Be^{2+} + 3\ (OH)^- + 3\ (CO_3)^{2-} \rightleftharpoons \mathbf{Be_3(CO_3)_3(OH)_3^{3-}}$	47.26963		1	$3\ Be + 3\ L \rightleftharpoons Be_3(OH)_3L_3 + 3\ H$ $\log_{10}(\beta) = 6.9$ I = 3.0 M $3\ H + 3\ OH \rightleftharpoons 3\ H_2O$ $\log_{10}(\beta) = 42.80169$ I = 3.0 M $3\ Be + 3\ OH + 3\ L \rightleftharpoons Be_3(OH)_3L_3 + 3\ H_2O$ $\log_{10}(\beta) = 49.70169$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 47.26963$
$5\ Be^{2+} + 4\ (OH)^- + (CO_3)^{2-} \rightleftharpoons \mathbf{Be_5(CO_3)(OH)_4^{4+}}$	55.66755		1	$5\ Be + L \rightleftharpoons Be_5(OH)_4L + 4\ H$ $\log_{10}(\beta) = 0.22$ I = 3.0 M $4\ H + 4\ OH \rightleftharpoons 4\ H_2O$ $\log_{10}(\beta) = 57.06892$ I = 3.0 M $5\ Be + L + 4\ OH \rightleftharpoons Be_5(OH)_4L + 4\ H_2O$ $\log_{10}(\beta) = 57.28892$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 55.66755$
$6\ Be^{2+} + 5\ (OH)^- + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Be_6(CO_3)_2(OH)_5^{3+}}$	73.01295		1	$6\ Be + 2\ L \rightleftharpoons Be_6(OH)_5L_2 + 5\ H$ $\log_{10}(\beta) = 5.46$ I = 3.0 M $5\ H + 5\ OH \rightleftharpoons 5\ H_2O$ $\log_{10}(\beta) = 71.33615$ I = 3.0 M $6\ Be + 2\ L + 5\ OH \rightleftharpoons Be_6(OH)_5L_2 + 4\ H_2O$ $\log_{10}(\beta) = 76.79615$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 73.01295$
$Na^+ + (CO_3)^{2-} \rightleftharpoons \mathbf{Na(CO_3)^-}$	1.27		1	
$H^+ + Na^+ + (CO_3)^{2-} \rightleftharpoons \mathbf{NaH(CO_3)}$ ***(aq)***	10.029		1	$Na + HL \rightleftharpoons NaHL$ $\log_{10}(\beta) = -0.3$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 10.329$ $Na + H + L \rightleftharpoons NaHL$ $\log_{10}(\beta) = 10.029$
$Mg^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Mg(CO_3)}$ ***(aq)***	2.92	1E+4	1	
$H^+ + Mg^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{MgH(CO_3)^+}$	11.339	-9.6E+3	1	$Mg + HL \rightleftharpoons MgHL$ $\log_{10}(\beta) = 1.01$ ΔH = 5E+3 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 10.329$ ΔH = -1.46E+4 $Mg + H + L \rightleftharpoons MgHL$ $\log_{10}(\beta) = 11.339$ ΔH = -9.6E+3
$Al^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Al(CO_3)^+}$	8.43		2	
$2\ Al^{3+} + 2\ (OH)^- + (CO_3)^{2-} \rightleftharpoons \mathbf{Al_2(CO_3)(OH)_2^{2+}}$	32.30444		1	$2\ Al + HL \rightleftharpoons Al_2(OH)_2L + 3\ H$ $\log_{10}(\beta) = -7.3$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 9.90185$ I = 0.1 M $2\ H + 2\ OH \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.56684$ I = 0.1 M $2\ Al + L + 2\ OH \rightleftharpoons Al_2(OH)_2L$ $\log_{10}(\beta) = 30.16869$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 32.30444$
$H^+ + 3\ Al^{3+} + 4\ (OH)^- + (CO_3)^{2-} \rightleftharpoons \mathbf{Al_3H(CO_3)(OH)_4^{4+}}$	57.77128		1	$3\ Al + HL \rightleftharpoons Al_3(OH)_4HL$ $\log_{10}(\beta) = -9.4$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 9.90185$ I = 0.1 M $4\ H + 4\ OH \rightleftharpoons 4\ H_2O$ $\log_{10}(\beta) = 55.13368$ I = 0.1 M $3\ Al + 4\ OH + H + L \rightleftharpoons Al_3(OH)_4HL$ $\log_{10}(\beta) = 55.63553$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 57.77128$
$Ca^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Ca(CO_3)}$ ***(aq)***	3.22	1.5E+4	1	
$H^+ + Ca^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{CaH(CO_3)^+}$	11.529	4.4E+3	1	$Ca + HL \rightleftharpoons CaHL$ $\log_{10}(\beta) = 1.20$ ΔH = 1.9E+4 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 10.329$ ΔH = -1.46E+4 $Ca + H + L \rightleftharpoons CaHL$ $\log_{10}(\beta) = 11.529$ ΔH = 4.4E+3
$Sc^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Sc(CO_3)^+}$	10.1		2	
$Mn(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Mn(II)(CO_3)}$ ***(aq)***	4.7		1	
$H^+ + Mn(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Mn(II)H(CO_3)^+}$	11.629	-1.06E+4	1	$Mn(II) + HL \rightleftharpoons Mn(II)HL$ $\log_{10}(\beta) = 1.30$ ΔH = 4E+3 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 10.329$ ΔH = -1.46E+4 $Mn(II) + H + L \rightleftharpoons Mn(II)HL$ $\log_{10}(\beta) = 11.629$ ΔH = -1.06E+4
$Fe(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Fe(II)(CO_3)}$ ***(aq)***	4.73		2	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Fe(II)^{2+} + (CO_3)^{2-}$ ⇌ **$Fe(II)H(CO_3)^+$**	11.429		1	Fe(II) + HL ⇌ Fe(II)HL $\log_{10}(\beta)$ = 1.10 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 Fe(II) + H + L ⇌ Fe(II)HL $\log_{10}(\beta)$ = 11.429
$Fe(III)^{3+} + (CO_3)^{2-}$ ⇌ **$Fe(III)(CO_3)^+$**	9.72		2	
$Fe(III)^{3+} + (OH)^- + (CO_3)^{2-}$ ⇌ **$Fe(III)(OH)(CO_3)$ *(aq)***	11.71471		1	Fe(III) + L ⇌ Fe(III)(OH)L + H $\log_{10}(\beta)$ = -3.8 I = 0.2 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.74405 I = 0.2 M Fe(III) + L + OH ⇌ Fe(III)(OH)L $\log_{10}(\beta)$ = 9.94405 I = 0.2 M I = 0 M: $\log_{10}(\beta)$ = 11.71471
$Fe(III)^{3+} + 2\ (CO_3)^{2-}$ ⇌ **$Fe(III)(CO_3)_2^-$**	9.42361		1	Original data for β: $\log_{10}(\beta)$ = 7.4, at I = 0.2 M.
$Co(II)^{2+} + (CO_3)^{2-}$ ⇌ **$Co(II)(CO_3)$ *(aq)***	4.22355		1	Original data for β: $\log_{10}(\beta)$ = 3.15, at I = 0.5 M.
$H^+ + Co(II)^{2+} + (CO_3)^{2-}$ ⇌ **$Co(II)H(CO_3)^+$**	12.21782		1	Co(II) + HL ⇌ Co(II)HL $\log_{10}(\beta)$ = 1.39 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Co(II) + H + L ⇌ Co(II)HL $\log_{10}(\beta)$ = 11.22017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.21782
$Ni^{2+} + (CO_3)^{2-}$ ⇌ **$Ni(CO_3)$ *(aq)***	4.56765		1	Original data for β: $\log_{10}(\beta)$ = 3.57, at I = 0.7 M.
$H^+ + Ni^{2+} + (CO_3)^{2-}$ ⇌ **$NiH(CO_3)^+$**	12.41782		1	Ni + HL ⇌ NiHL $\log_{10}(\beta)$ = 1.59 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Ni + H + L ⇌ NiHL $\log_{10}(\beta)$ = 11.42017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.41782
$Cu(II)^{2+} + (CO_3)^{2-}$ ⇌ **$Cu(II)(CO_3)$ *(aq)***	6.77		1	
$H^+ + Cu(II)^{2+} + (CO_3)^{2-}$ ⇌ **$Cu(II)H(CO_3)^+$**	12.129		1	Cu(II) + HL ⇌ Cu(II)HL $\log_{10}(\beta)$ = 1.8 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 12.129
$Cu(II)^{2+} + 2\ (CO_3)^{2-}$ ⇌ **$Cu(II)(CO_3)_2^{2-}$**	10.2		1	
$Zn^{2+} + (CO_3)^{2-}$ ⇌ **$Zn(CO_3)$ *(aq)***	4.76		1	
$H^+ + Zn^{2+} + (CO_3)^{2-}$ ⇌ **$ZnH(CO_3)^+$**	11.829		1	Zn + HL ⇌ ZnHL $\log_{10}(\beta)$ = 1.5 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 11.829
$Zn^{2+} + 2\ (CO_3)^{2-}$ ⇌ **$Zn(CO_3)_2^{2-}$**	7.3		1	
$2\ Zn^{2+} + (CO_3)^{2-}$ ⇌ **$Zn_2(CO_3)^{2+}$**	3.07909		1	Original data for β: $\log_{10}(\beta)$ = 4.16, at I = 3.0 M.
$Ga^{3+} + (CO_3)^{2-}$ ⇌ **$Ga(CO_3)^+$**	8.79		2	
$Sr^{2+} + (CO_3)^{2-}$ ⇌ **$Sr(CO_3)$ *(aq)***	2.81	2.1E+4	1	
$H^+ + Sr^{2+} + (CO_3)^{2-}$ ⇌ **$SrH(CO_3)^+$**	11.539	1.04E+4	1	Sr + HL ⇌ SrHL $\log_{10}(\beta)$ = 1.21 ΔH = 2.5E+4 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 ΔH = -1.46E+4 Sr + H + L ⇌ SrHL $\log_{10}(\beta)$ = 11.539 ΔH = -1.04E+4
$Y^{3+} + (CO_3)^{2-}$ ⇌ **$Y(CO_3)^+$**	7.73		1	
$H^+ + Y^{3+} + (CO_3)^{2-}$ ⇌ **$YH(CO_3)^{2+}$**	12.729		1	Y + HL ⇌ YHL $\log_{10}(\beta)$ = 2.4 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 12.729
$Y^{3+} + 2\ (CO_3)^{2-}$ ⇌ **$Y(CO_3)_2^-$**	11.86		1	
$2\ Y^{3+} + (CO_3)^{2-}$ ⇌ **$Y_2(CO_3)^{4+}$**	8.06		1	
$Ag^+ + (CO_3)^{2-}$ ⇌ **$Ag(CO_3)^-$**	3.4		2	
$Cd^{2+} + (CO_3)^{2-}$ ⇌ **$Cd(CO_3)$ *(aq)***	4.3543		1	Original data for β: $\log_{10}(\beta)$ = 3.5, at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + Cd^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{CdH(CO_3)^{+}}$	10.68855		1	Cd + HL ⇌ CdHL $\log_{10}(\beta)$ = 0.9 I = 3.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.86946 I = 3.0 M Cd + H + L ⇌ CdHL $\log_{10}(\beta)$ = 11.76946 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 10.68855
$Cd^{2+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Cd(CO_3)_2^{2-}}$	7.2243		1	Original data for β: $\log_{10}(\beta)$ = 6.37, at I = 0.1 M at 20°C.
$In^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{In(CO_3)^{+}}$	7.6		2	
$Cs^{+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Cs(CO_3)^{-}}$	-0.29368		1	Original data for β: $\log_{10}(\beta)$ = -0.7, at I = 1.0 M.
$Ba^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Ba(CO_3)}$ ***(aq)***	2.71	1.4E+4	1	
$H^{+} + Ba^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{BaH(CO_3)^{+}}$	11.309	8.4E+3	1	Ba + HL ⇌ BaHL $\log_{10}(\beta)$ = 0.98 ΔH = 2.3E+4 H + L ⇌ HL $\log_{10}(\beta)$ = 10.329 ΔH = -1.46E+4 Ba + H + L ⇌ BaHL $\log_{10}(\beta)$ = 11.309 ΔH = 8.4E+3
$La^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{La(CO_3)^{+}}$	6.98		1	
$H^{+} + La^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{LaH(CO_3)^{2+}}$	10.92832		1	La + HL ⇌ LaHL $\log_{10}(\beta)$ = 1.41 I = 3.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.86946 I = 3.0 M La + H + L ⇌ LaHL $\log_{10}(\beta)$ = 12.27946 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 10.92832
$La^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{La(CO_3)_2^{-}}$	11.86		1	
$2\ La^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{La_2(CO_3)^{4+}}$	6.10931		1	Original data for β: $\log_{10}(\beta)$ = 6.92, at I = 3.0 M.
$Ce^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Ce(CO_3)^{+}}$	7.31		1	
$H^{+} + Ce^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{CeH(CO_3)^{2+}}$	12.67723		1	Ce + HL ⇌ CeHL $\log_{10}(\beta)$ = 1.6 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Ce + H + L ⇌ CeHL $\log_{10}(\beta)$ = 11.43017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.67723
$Ce^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Ce(CO_3)_2^{-}}$	12.32		1	
$Pr^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Pr(CO_3)^{+}}$	7.48		1	
$Pr^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Pr(CO_3)_2^{-}}$	12.63		1	
$Nd^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Nd(CO_3)^{+}}$	7.53		1	
$Nd^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Nd(CO_3)_2^{-}}$	12.73		1	
$Sm^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Sm(CO_3)^{+}}$	7.71		1	
$Sm^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Sm(CO_3)_2^{-}}$	13.09		1	
$Eu^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Eu(CO_3)^{+}}$	7.73	4E+3	1	
$H^{+} + Eu^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{EuH(CO_3)^{2+}}$	12.57723	1.44E+4	1	Eu + HL ⇌ EuHL $\log_{10}(\beta)$ = 1.5 I = 0.7 M ΔH = 2.9E+4 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M ΔH = -1.46E+4 Eu + H + L ⇌ EuHL $\log_{10}(\beta)$ = 11.33017 I = 0.7 M ΔH = 1.44E+4 I = 0 M: $\log_{10}(\beta)$ = 12.57723
$Eu^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Eu(CO_3)_2^{-}}$	13.19	2.0E+4	1	
$Gd^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Gd(CO_3)^{+}}$	7.64		1	

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Gd^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{GdH(CO_3)^{2+}}$	12.97723		1	Gd + HL ⇌ GdHL $\log_{10}(\beta)$ = 1.9 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Gd + H + L ⇌ GdHL $\log_{10}(\beta)$ = 11.73017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.97723
$Gd^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Gd(CO_3)_2^-}$	13.04		1	
$Tb^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Tb(CO_3)^+}$	7.71		1	
$H^+ + Tb^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{TbH(CO_3)^{2+}}$	12.87723		1	Tb + HL ⇌ TbHL $\log_{10}(\beta)$ = 1.8 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Tb + H + L ⇌ TbHL $\log_{10}(\beta)$ = 11.63017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.87723
$Tb^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Tb(CO_3)_2^-}$	13.34		1	
$Dy^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Dy(CO_3)^+}$	7.81		1	
$Dy^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Dy(CO_3)_2^-}$	13.47		1	
$Ho^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Ho(CO_3)^+}$	7.8		1	
$Ho^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Ho(CO_3)_2^-}$	13.56		1	
$Er^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Er(CO_3)^+}$	7.86		1	
$Er^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Er(CO_3)_2^-}$	13.68		1	
$Tm^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Tm(CO_3)^+}$	7.93		1	
$Tm^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Tm(CO_3)_2^-}$	13.83		1	
$Yb^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Yb(CO_3)^+}$	8.06		1	
$H^+ + Yb^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{YbH(CO_3)^{2+}}$	12.57723		1	Yb + HL ⇌ YbHL $\log_{10}(\beta)$ = 1.5 I = 0.7 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.83017 I = 0.7 M Yb + H + L ⇌ YbHL $\log_{10}(\beta)$ = 11.33017 I = 0.7 M I = 0 M: $\log_{10}(\beta)$ = 12.57723
$Yb^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Yb(CO_3)_2^-}$	13.86		1	
$Lu^{3+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Lu(CO_3)^+}$	8		1	
$Lu^{3+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Lu(CO_3)_2^-}$	13.93		1	
$Hg(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(CO_3)}$ ***(aq)***	12.07355		1	Original data for β: $\log_{10}(\beta)$ = 11.0, at I = 0.5 M.
$H^+ + Hg(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)H(CO_3)^+}$	16.34577		1	Hg(II) + HL ⇌ Hg(II)HL $\log_{10}(\beta)$ = 5.48 I = 0.5 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.79222 I = 0.5 M Hg(II) + H + L ⇌ Hg(II)HL $\log_{10}(\beta)$ = 15.27222 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 16.34577
$Hg(II)^{2+} + (OH)^- + (CO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(CO_3)(OH)^-}$	19.20216		1	Hg(II)L ⇌ Hg(II)OHL + H $\log_{10}(\beta)$ = -6.6 I = 0.5 M Hg(II) + L ⇌ Hg(II)L $\log_{10}(\beta)$ = 11 I = 0.5 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.72861 I = 0.5 M Hg(II) + OH + L ⇌ Hg(II)OHL $\log_{10}(\beta)$ = 18.12861 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 19.20216
$Hg(II)^{2+} + 2\ (CO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(CO_3)_2^{2-}}$	15.57355		1	Original data for β: $\log_{10}(\beta)$ = 14.5, at I = 0.5 M.
$Pb(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Pb(II)(CO_3)}$ ***(aq)***	6.47355		1	Original data for β: $\log_{10}(\beta)$ = 5.40, at I = 0.5 M.
$H^+ + Pb(II)^{2+} + (CO_3)^{2-} \rightleftharpoons \mathbf{Pb(II)H(CO_3)^+}$	11.69855		1	Pb(II) + HL ⇌ Pb(II)HL $\log_{10}(\beta)$ = 1.91 I = 3.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.86946 I = 3.0 M Pb (II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 12.77946 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 11.69855

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+}$ + $(OH)^{-}$ + $(CO_3)^{2-}$ ⇌ **$Pb(II)(CO_3)(OH)^{-}$**	9.81909		1	Original data for β: $log_{10}(\beta)$ = 10.9, at I = 3.0 M.
$Pb(II)^{2+}$ + 2 $(CO_3)^{2-}$ ⇌ **$Pb(II)(CO_3)_2^{2-}$**	9.93355		1	Original data for β: $log_{10}(\beta)$ = 8.86, at I = 0.5 M.
2 $Pb(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Pb(II)_2(CO_3)^{2+}$**	6.01909		1	Original data for β: $log_{10}(\beta)$ = 7.1, at I = 3.0 M.
3 $Pb(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Pb(II)_3(CO_3)^{4+}$**	8.43		1	Original data for β: $log_{10}(\beta)$ = 8.43, at I = 3.0 M.
$(U(VI)O_2)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)(CO_3)$ *(aq)***	9.6	4E+3	1	
$(U(VI)O_2)^{2+}$ + 2 $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)(CO_3)_2^{2-}$**	16.9	-2.3E+4	1	
$(U(VI)O_2)^{2+}$ + 3 $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)(CO_3)_3^{4-}$**	21.6	-4.0E+4	1	
2 $(U(VI)O_2)^{2+}$ + 3 $(OH)^{-}$ + $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)_2(CO_3)(OH)_3^{-}$**	41.091	-2.2543E+05	1	2 (UO_2) + L ⇌ $(UO_2)_2(OH)_3L$ + 3 H $log_{10}(\beta)$ = -0.9 ΔH = 2.9E+4 3 H + 3 OH ⇌ 3 H_2O $log_{10}(\beta)$ = 41.991 ΔH = -1.6743E+05 2 (UO_2) + L + 3 (OH) ⇌ $(UO_2)_2(OH)_3L$ + 3 H_2O $log_{10}(\beta)$ = 41.091 ΔH = -2.2543E+05
3 $(U(VI)O_2)^{2+}$ + 3 $(OH)^{-}$ + $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)_3(CO_3)(OH)_3^{+}$**	42.691		1	3 (UO_2) + L ⇌ $(UO_2)_3(OH)_3L$ + 3 H $log_{10}(\beta)$ = 0.7 3 H + 3 OH ⇌ 3 H_2O $log_{10}(\beta)$ = 41.991 3 (UO_2) + L + 3 OH ⇌ $(UO_2)_3(OH)_3L$+ 3 H_2O $log_{10}(\beta)$ = 42.691
3 $(U(VI)O_2)^{2+}$ + 6 $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)_3(CO_3)_6^{6-}$**	54	-6.270E+4	1	
11 $(U(VI)O_2)^{2+}$ + 12 $(OH)^{-}$ + 6 $(CO_3)^{2-}$ ⇌ **$(U(VI)O_2)_{11}(CO_3)_6(OH)_{12}^{2-}$**	201.964		1	11 (UO_2) + 6 L ⇌ $(UO_2)_{11}(OH)_{12}L_6$ +12 H $log_{10}(\beta)$ = 34.1 12 H + 12 OH ⇌ 12 H_2O) $log_{10}(\beta)$ = 167.964 11 (UO_2) + 6 L + 12 OH ⇌ $(UO_2)_{11}(OH)_{12}L_6$ + 12 H_2O $log_{10}(\beta)$ = 201.964

2.2.4. Ammonia

The formula for the ligand ammonia is NH_3; the molecular weight is 17.031.

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

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + (NH_3) *(aq)* ⇌ **$H(NH_3)^+$**	9.244	-5.200E+4	1	
Li^+ + (NH_3) *(aq)* ⇌ **$Li(NH_3)^+$**	-0.7	-8E+2	1	Original data for ΔH at I = 2.0 M.
Mg^{2+} + (NH_3) *(aq)* ⇌ **$Mg(NH_3)^{2+}$**	0.24	-5.0E+3	1	Original data for β at I = 2.0 M.
Mg^{2+} + 2 (NH_3) *(aq)* ⇌ **$Mg(NH_3)_2^{2+}$**	0.2		1	
Ca^{2+} + (NH_3) *(aq)* ⇌ **$Ca(NH_3)^{2+}$**	0.2		1	
$Cr(III)^{3+}$ + 4 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_4^{3+}$**	9.9		1	$Cr(III)L_5$ ⇌ $Cr(III)L_4$ + L $log_{10}(\beta)$ = -1.6 I = 4.0 M Cr(III) + 5 L ⇌ $Cr(III)L_5$ $log_{10}(\beta)$ = 11.5 I = 4.0 M Cr(III) + 4 L ⇌ $Cr(III)L_4$ $log_{10}(\beta)$ = 9.9 I = 4.0 M
$Cr(III)^{3+}$ + $(OH)^{-}$ + 4 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_4(OH)$ (cis)$^{2+}$**	19.34332		1	$Cr(III)L_4$ ⇌ $Cr(III)(OH)L_4$ (cis) + H $log_{10}(\beta)$ = -4.96 I = 1.0 M Cr(III) + 4 L ⇌ $Cr(III)L_4$ $log_{10}(\beta)$ = 9.9 I = 1.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ (cis) $log_{10}(\beta)$ = 18.73384 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 19.34332

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cr(III)^{3+}$ + $(OH)^-$ + 4 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_4(OH)$ (trans)$^{2+}$**	19.92332		1	$Cr(III)L_4$ ⇌ $Cr(III)(OH)L_4$ (trans) + H $log_{10}(\beta)$ = -4.38 I = 1.0 M Cr(III) + 4 L ⇌ $Cr(III)L_4$ $log_{10}(\beta)$ = 9.9 I = 1.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ (trans) $log_{10}(\beta)$ = 19.31384 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 19.92332
$Cr(III)^{3+}$ + 2 $(OH)^-$ + 4 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_4(OH)_2$ (cis)$^+$**	26.01348		1	$Cr(III)(OH)L_4$ ⇌ $Cr(III)(OH)_2L_4$ (cis) + H $log_{10}(\beta)$ = -7.53 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ $log_{10}(\beta)$ = 18.73384 I = 1.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ (cis) $log_{10}(\beta)$ = 24.99768 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 26.01348 For the second equilibrium reaction, it is assumed that $M(OH)L_4$ (cis) reacts to $M(OH)_2L_4$ (cis).
$Cr(III)^{3+}$ + 2 $(OH)^-$ + 4 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_4(OH)_2$ (trans)$^+$**	26.34348		1	$Cr(III)(OH)L_4$ ⇌ $Cr(III)(OH)_2L_4$ (trans) + H $log_{10}(\beta)$ = -7.78 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ $log_{10}(\beta)$ = 19.31384 I = 1.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Cr(III) + 4 L + OH ⇌ $Cr(III)(OH)L_4$ (trans) $log_{10}(\beta)$ = 25.32768 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 26.34348 For the second equilibrium reaction, it is assumed that $M(OH)L_4$ (trans) reacts to $M(OH)_2L_4$ (trans).
$Cr(III)^{3+}$ + 5 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_5^{3+}$**	11.5		1	$Cr(III)L_6$ ⇌ $Cr(III)L_5$ + L $log_{10}(\beta)$ = -1.5 I = 4.0 M Cr(III) + 6 L ⇌ $Cr(III)L_6$ $log_{10}(\beta)$ = 13 I = 4.0 M Cr(III) + 5 L ⇌ $Cr(III)L_5$ $log_{10}(\beta)$ = 11.5 I = 4.0 M
$Cr(III)^{3+}$ + $(OH)^-$ + 5 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_5(OH)^{2+}$**	20.93415		1	$Cr(III)L5_4$ ⇌ $Cr(III)(OH)L_5$ + H $log_{10}(\beta)$ = -4.99 I = 0.1 M Cr(III) + 5 L ⇌ $Cr(III)L_5$ $log_{10}(\beta)$ = 11.5 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Cr(III) + 5 L + OH ⇌ $Cr(III)(OH)L_5$ $log_{10}(\beta)$ = 20.29342 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 20.93415
$Cr(III)^{3+}$ + 6 (NH_3) *(aq)* ⇌ **$Cr(III)(NH_3)_6^{3+}$**	13		1	Original data for β at I = 4.0 M.
$Mn(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Mn(II)(NH_3)^{2+}$**	0.84	-5.0E+3	1	Original data for ΔH at I = 2.0 M.
$Mn(II)^{2+}$ + 2 (NH_3) *(aq)* ⇌ **$Mn(II)(NH_3)_2^{2+}$**	1.25	-9.6E+3	1	Original data for ΔH at I = 2.0 M.
$Mn(II)^{2+}$ + 3 (NH_3) *(aq)* ⇌ **$Mn(II)(NH_3)_3^{2+}$**	1.38	-1.5E+4	1	Original data for ΔH at I = 2.0 M.
$Mn(II)^{2+}$ + 4 (NH_3) *(aq)* ⇌ **$Mn(II)(NH_3)_4^{2+}$**	1.24	-2.0E+4	1	Original data for ΔH at I = 2.0 M.
$Fe(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Fe(II)(NH_3)^{2+}$**	1.4	-7.9E+3	1	Original data for ΔH at I = 2.0 M.
$Fe(II)^{2+}$ + 2 (NH_3) *(aq)* ⇌ **$Fe(II)(NH_3)_2^{2+}$**	2.25	-1.5E+4	1	Original data for ΔH at I = 2.0 M.
$Fe(II)^{2+}$ + 3 (NH_3) *(aq)* ⇌ **$Fe(II)(NH_3)_3^{2+}$**	2.68	-2.3E+4	1	Original data for ΔH at I = 2.0 M.
$Fe(II)^{2+}$ + 4 (NH_3) *(aq)* ⇌ **$Fe(II)(NH_3)_4^{2+}$**	2.75	-3.1E+4	1	Original data for ΔH at I = 2.0 M.
$Co(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Co(II)(NH_3)^{2+}$**	2.08	-1.2E+4	1	Original data for β at I = 0.1 M. Original data for ΔH at I = 2.0 M.
$Co(II)^{2+}$ + 2 (NH_3) *(aq)* ⇌ **$Co(II)(NH_3)_2^{2+}$**	3.7	-2.3E+4	1	Original data for β at I = 1.0 M. Original data for ΔH at I = 2.0 M.
$Co(II)^{2+}$ + 3 (NH_3) *(aq)* ⇌ **$Co(II)(NH_3)_3^{2+}$**	4.8	-3.5E+4	1	Original data for β at I = 1.0 M. Original data for ΔH at I = 2.0 M.
$Co(II)^{2+}$ + 4 (NH_3) *(aq)* ⇌ **$Co(II)(NH_3)_4^{2+}$**	5.52	-4.76E+4	1	Original data for β at I = 1.0 M. Original data for ΔH at I = 2.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+}$ + 5 (NH_3) *(aq)* ⇌ **$Co(II)(NH_3)_5^{2+}$**	5.72	-5.94E+4	1	Original data for β at I = 1.0 M. Original data for ΔH at I = 2.0 M.
$Co(III)^{3+}$ + 4 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_4^{3+}$**	24.96		1	$Co(III)L_5$ ⇌ $Co(III)L_4$ + L $\log_{10}(\beta)$ = -5.07 I = 2.0 M Co(III) + 5 L ⇌ $Co(III)L_5$ $\log_{10}(\beta)$ = 30.03 I = 2.0 M Co(III) + 4 L ⇌ $Co(III)L_4$ $\log_{10}(\beta)$ = 24.96 I = 2.0 M
$Co(III)^{3+}$ + $(OH)^-$ + 4 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_4(OH)^{2+}$**	33.69415		1	$Co(III)L_4$ ⇌ $Co(III)(OH)L_4$ (cis) + H $\log_{10}(\beta)$ = -5.69 I = 0.1 M (Original data for β at T = 20°C) Co(III) + 4 L ⇌ $Co(III)L_4$ $\log_{10}(\beta)$ = 24.96 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Co(III) + OH + 4 L ⇌ $Co(III)(OH)L_4$ (cis) $\log_{10}(\beta)$ = 33.05342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 33.69415
$Co(III)^{3+}$ + 2 $(OH)^-$ + 4 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_4(OH)_2^+$**	6.86130		1	$Co(III)(OH)L_4$ ⇌ $Co(III)(OH)_2L_4$ (cis) + H $\log_{10}(\beta)$ = -7.99 I = 0.1 M (Original data for β at T = 20°C) Co(III) + OH + 4 L ⇌ $Co(III)(OH)L_4$ (cis) $\log_{10}(\beta)$ = 33.05342 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Co(III) + 2 OH + 4 L ⇌ $Co(III)(OH)_2L_4$ (cis) $\log_{10}(\beta)$ = 38.84684 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 39.91472
$Co(III)^{3+}$ + 5 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_5^{3+}$**	30.03		1	$Co(III)L_6$ ⇌ $Co(III)L_5$ + L $\log_{10}(\beta)$ = -4.33 I = 1.0 M Co(III) + 6 L ⇌ $Co(III)L_6$ $\log_{10}(\beta)$ = 34.36 I = 1.0 M Co(III) + 5 L ⇌ $Co(III)L_5$ $\log_{10}(\beta)$ = 30.03 I = 1.0 M
$Co(III)^{3+}$ + $(OH)^-$ + 5 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_5(OH)^{2+}$**	38.25415		1	$Co(III)L_5$ ⇌ $Co(III)(OH)L_5$ + H $\log_{10}(\beta)$ = -6.2 I = 0.1 M Co(III) + 5 L ⇌ $Co(III)L_5$ $\log_{10}(\beta)$ = 30.03 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Co(III) + OH + 5 L ⇌ $Co(III)(OH)L_5$ $\log_{10}(\beta)$ = 37.61342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 38.25415
$Co(III)^{3+}$ + 6 (NH_3) *(aq)* ⇌ **$Co(III)(NH_3)_6^{3+}$**	34.36		1	Original data for β at I = 1.0 M at 30°C.
Ni^{2+} + (NH_3) *(aq)* ⇌ **$Ni(NH_3)^{2+}$**	2.72	-1.5E+4	1	
Ni^{2+} + 2 (NH_3) *(aq)* ⇌ **$Ni(NH_3)_2^{2+}$**	4.88	-3.0E+4	1	
Ni^{2+} + 3 (NH_3) *(aq)* ⇌ **$Ni(NH_3)_3^{2+}$**	6.54	-4.60E+4	1	
Ni^{2+} + 4 (NH_3) *(aq)* ⇌ **$Ni(NH_3)_4^{2+}$**	7.67	-6.40E+4	1	
Ni^{2+} + 5 (NH_3) *(aq)* ⇌ **$Ni(NH_3)_5^{2+}$**	8.33	-7.69E+4	1	
Ni^{2+} + 6 (NH_3) *(aq)* ⇌ **$Ni(NH_3)_6^{2+}$**	8.3	-9.45E+4	1	
$Cu(I)^+$ + (NH_3) *(aq)* ⇌ **$Cu(I)(NH_3)^+$**	5.74	-3.3E+4	1	Original data for β at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Cu(I)^+$ + 2 (NH_3) *(aq)* ⇌ **$Cu(I)(NH_3)_2^+$**	9.9	-6.90E+4	1	Original data for β at I = 0.5 M. Original data for ΔH at I = 2.0 M.
$Cu(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Cu(II)(NH_3)^{2+}$**	4.02	-2.0E+4	1	
$Cu(II)^{2+}$ + 2 (NH_3) *(aq)* ⇌ **$Cu(II)(NH_3)_2^{2+}$**	7.4	-4.22E+4	1	
$Cu(II)^{2+}$ + 3 (NH_3) *(aq)* ⇌ **$Cu(II)(NH_3)_3^{2+}$**	10.2	-6.23E+4	1	
$Cu(II)^{2+}$ + 4 (NH_3) *(aq)* ⇌ **$Cu(II)(NH_3)_4^{2+}$**	12.3	-8.66E+4	1	
Zn^{2+} + (NH_3) *(aq)* ⇌ **$Zn(NH_3)^{2+}$**	2.21	-1.1E+4	1	Original data for ΔH at I = 2.0 M.
Zn^{2+} + 2 (NH_3) *(aq)* ⇌ **$Zn(NH_3)_2^{2+}$**	4.5	-2.4E+4	1	Original data for ΔH at I = 2.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Zn^{2+} + 3 (NH_3) *(aq)* ⇌ **$Zn(NH_3)_3^{2+}$**	6.86	-4.0E+4	1	Original data for ΔH at I = 2.0 M.
Zn^{2+} + 4 (NH_3) *(aq)* ⇌ **$Zn(NH_3)_4^{2+}$**	8.89	-6.15E+4	1	Original data for ΔH at I = 2.0 M.
Sr^{2+} + (NH_3) *(aq)* ⇌ **$Sr(NH_3)^{2+}$**	0		1	
Pd^{2+} + (NH_3) *(aq)* ⇌ **$Pd(NH_3)^{2+}$**	9.6		1	Original data for β at I = 1.0 M.
Pd^{2+} + 2 (NH_3) *(aq)* ⇌ **$Pd(NH_3)_2^{2+}$**	18.5		1	Original data for β at I = 1.0 M.
Pd^{2+} + 3 (NH_3) *(aq)* ⇌ **$Pd(NH_3)_3^{2+}$**	26		1	Original data for β at I = 1.0 M.
Pd^{2+} + 4 (NH_3) *(aq)* ⇌ **$Pd(NH_3)_4^{2+}$**	32.8		1	Original data for β at I = 1.0 M.
Ag^{+} + (NH_3) *(aq)* ⇌ **$Ag(NH_3)^{+}$**	3.31	-2.0E+4	1	
Ag^{+} + 2 (NH_3) *(aq)* ⇌ **$Ag(NH_3)_2^{+}$**	7.22	-5.60E+4	1	
Cd^{2+} + (NH_3) *(aq)* ⇌ **$Cd(NH_3)^{2+}$**	2.55	-1.2E+4	1	
Cd^{2+} + 2 (NH_3) *(aq)* ⇌ **$Cd(NH_3)_2^{2+}$**	4.56	-2.7E+4	1	
Cd^{2+} + 3 (NH_3) *(aq)* ⇌ **$Cd(NH_3)_3^{2+}$**	5.9	-3.8E+4	1	
Cd^{2+} + 4 (NH_3) *(aq)* ⇌ **$Cd(NH_3)_4^{2+}$**	6.72	-4.89E+4	1	
Ba^{2+} + (NH_3) *(aq)* ⇌ **$Ba(NH_3)^{2+}$**	-0.1		1	
$Hg(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Hg(II)(NH_3)^{2+}$**	8.75	-5.10E+4	1	Original data for β at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Hg(II)^{2+}$ + 2 (NH_3) *(aq)* ⇌ **$Hg(II)(NH_3)_2^{2+}$**	17.8	-1.02E+5	1	Original data for β at I = 1.0 M. Original data for ΔH at I = 2.0 M.
$Hg(II)^{2+}$ + 3 (NH_3) *(aq)* ⇌ **$Hg(II)(NH_3)_3^{2+}$**	18.2	-1.10E+5	1	Original data for β at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Hg(II)^{2+}$ + 4 (NH_3) *(aq)* ⇌ **$Hg(II)(NH_3)_4^{2+}$**	19.3	-1.14E+5	1	Original data for β at I = 0.1 M. Original data for ΔH at I = 2.0 M.
$Pb(II)^{2+}$ + (NH_3) *(aq)* ⇌ **$Pb(II)(NH_3)^{2+}$**	1.55		1	Original data for β at I = 5.0 M.
2 H^{+} + (NH_3) *(aq)* + $(PO_4)^{3-}$ ⇌ **$H_2(PO_4)(NH_3)^{-}$**	22.89475		1	NH_4 + $H(PO_4)$ ⇌ $NH_4H(PO_4)$ $log_{10}(\beta)$ = 0.8 I = 0.15 M (Original data for β at T = 37°C) NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 I = 0.15 M H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 11.66138 I = 0.15 M NH_3 + 2 H + (PO_4) ⇌ $NH_4H(PO_4)$ $log_{10}(\beta)$ = 21.70538 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 22.89475
3 H^{+} + (NH_3) *(aq)* + $(PO_4)^{3-}$ ⇌ **$H_3(PO_4)(NH_3)$ *(aq)***	28.95488		1	NH_4 + $H_2(PO_4)$ ⇌ $NH_4H_2(PO_4)$ $log_{10}(\beta)$ = -0.1 I = 0.15 M (Original data for β at T = 37°C) NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 I = 0.15 M 2 H + (PO_4) ⇌ $H_2(PO_4)$ $log_{10}(\beta)$ = 18.38363 I = 0.15 M NH_3 + 3 H + (PO_4) ⇌ $NH_4H_2(PO_4)$ $log_{10}(\beta)$ = 27.52763 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 28.95488
H^{+} + (NH_3) *(aq)* + $(SO_4)^{2-}$ ⇌ **$H(SO_4)(NH_3)^{-}$**	10.274			NH_4 + (SO_4) ⇌ $NH_4(SO_4)$ $log_{10}(\beta)$ = 1.03 NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 H + NH_3 + (SO_4) ⇌ $NH_4(SO_4)$ $log_{10}(\beta)$ = 10.274

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 H^+ + (NH_3) *(aq)* + 2 $(CrO_4)^{2-}$ ⇌ **$NH_4Cr_2O_7^-$**	24.664	-8.7E+4	1	NH_4 + Cr_2O_7 ⇌ $NH_4Cr_2O_7$ $log_{10}(\beta)$ = 0.88 ΔH = -2.0E+4 NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 ΔH = -5.2E+4 2 H + 2 (CrO_4) ⇌ Cr_2O_7 $log_{10}(\beta)$ = 14.54 ΔH = -1.5E+4 NH_3 + 3 H + 2 (CrO_4) ⇌ $NH_4Cr_2O_7$ $log_{10}(\beta)$ = 24.664 ΔH = -8.7E+4
H^+ + (NH_3) *(aq)* + $(phthalate)^{2-}$ ⇌ **$H(phthalate)(NH_3)^-$**	10.544		1	NH_4 + (phthalate) ⇌ NH_4(phthalate) $log_{10}(\beta)$ = 1.3 NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 H + NH_3 + (phthalate) ⇌ NH_4(phthalate) $log_{10}(\beta)$ = 10.544
H^+ + (NH_3) *(aq)* + $(citrate)^{3-}$ ⇌ **$H(NH_3)(citrate)^{2-}$**	10.90762		1	NH_4 + (citrate) ⇌ NH_4(citrate) $log_{10}(\beta)$ = 0.95 I = 0.15 M (Original data for β at T = 37°C) NH_3 + H ⇌ NH_4 $log_{10}(\beta)$ = 9.244 I = 0.15 M H + NH_3 + (citrate) ⇌ NH_4(citrate) $log_{10}(\beta)$ = 10.194 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 10.90762

2.2.5. Nitrite

The formula for the ligand nitrite is NO_2^-; the molecular weight is 46.005.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(H_2BO_3)^-$ + $(NO_2)^-$ ⇌ **$(B(OH)_3)(NO_2)^-$**	8.746		1	
H^+ + $(NO_2)^-$ ⇌ **$H(NO_2)$** ***(aq)***	3.15	-1.2E+4	1	
$Mn(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Mn(II)(NO_2)^+$**	0.85632		1	Original data for β: $log_{10}(\beta)$ = 0.45, at I = 1.0 M.
$Fe(III)^{3+}$ + $(NO_2)^-$ ⇌ **$Fe(III)(NO_2)^{2+}$**	3.19948		1	Original data for β: $log_{10}(\beta)$ = 2.59, at I = 1.0 M.
$Fe(III)^{3+}$ + 2 $(NO_2)^-$ ⇌ **$Fe(III)(NO_2)_2^+$**	4.7158		1	Original data for β: $log_{10}(\beta)$ = 3.70, at I = 1.0 M.
$Fe(III)^{3+}$ + 3 $(NO_2)^-$ ⇌ **$Fe(III)(NO_2)_3$** ***(aq)***	6.66896		1	Original data for β: $log_{10}(\beta)$ = 5.45, at I = 1.0 M.
$Co(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Co(II)(NO_2)^+$**	0.84632		1	Original data for β: $log_{10}(\beta)$ = 0.44, at I = 1.0 M.
Ni^{2+} + $(NO_2)^-$ ⇌ **$Ni(NO_2)^+$**	1.17632		1	Original data for β: $log_{10}(\beta)$ = 0.77, at I = 1.0 M.
Ni^{2+} + 2 $(NO_2)^-$ ⇌ **$Ni(NO_2)_2$** ***(aq)***	1.68948		1	Original data for β: $log_{10}(\beta)$ = 1.08, at I = 1.0 M.
$Cu(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Cu(II)(NO_2)^+$**	2.02		1	
$Cu(II)^{2+}$ + 2 $(NO_2)^-$ ⇌ **$Cu(II)(NO_2)_2$** ***(aq)***	3.03		1	
Zn^{2+} + $(NO_2)^-$ ⇌ **$Zn(NO_2)^+$**	0.77632		1	Original data for β: $log_{10}(\beta)$ = 0.37, at I = 1.0 M.
Zn^{2+} + 2 $(NO_2)^-$ ⇌ **$Zn(NO_2)_2$** ***(aq)***	1.09948		1	Original data for β: $log_{10}(\beta)$ = 0.49, at I = 1.0 M.
Ga^{3+} + $(NO_2)^-$ ⇌ **$Ga(NO_2)^{2+}$**	2.71948		1	Original data for β: $log_{10}(\beta)$ = 2.11, at I = 1.0 M.
Pd^{2+} + 4 $(NO_2)^-$ ⇌ **$Pd(NO_2)_4^{2-}$**	20.83678		1	Original data for β: $log_{10}(\beta)$ = 20.3, at I = 0.5 M.
Ag^+ + $(NO_2)^-$ ⇌ **$Ag(NO_2)$** ***(aq)***	2.32	-2.9E+4	1	
Ag^+ + 2 $(NO_2)^-$ ⇌ **$Ag(NO_2)_2^-$**	2.51	-4.6E+4	1	
Cd^{2+} + $(NO_2)^-$ ⇌ **$Cd(NO_2)^+$**	1.94632	-8.7E+3	1	Original data for β: $log_{10}(\beta)$ = 1.54, at I = 1.0 M. Original data for ΔH at I = 3.0 M.
Cd^{2+} + 2 $(NO_2)^-$ ⇌ **$Cd(NO_2)_2$** ***(aq)***	3.43948	-1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 2.83, at I = 1.0 M. Original data for ΔH at I = 3.0 M.

Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + 3 $(NO_2)^-$ ⇌ **$Cd(NO_2)_3^-$**	2.99931	-2.4E+4	1	Original data for β: $log_{10}(β)$ = 3.81, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
In^{3+} + $(NO_2)^-$ ⇌ **$In(NO_2)^{2+}$**	3.20948		1	Original data for β: $log_{10}(β)$ = 2.6, at I = 1.0 M.
In^{3+} + 2 $(NO_2)^-$ ⇌ **$In(NO_2)_2^+$**	5.0158		1	Original data for β: $log_{10}(β)$ = 4.0, at I = 1.0 M.
In^{3+} + 3 $(NO_2)^-$ ⇌ **$In(NO_2)_3$ *(aq)***	6.11896		1	Original data for β: $log_{10}(β)$ = 4.9, at I = 1.0 M.
$Pt(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Pt(II)(NO_2)^+$**	24.63678		1	Original data for β: $log_{10}(β)$ = 24.1, at I = 0.5 M.
$Hg(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Hg(II)(NO_2)^+$**	6.34632		1	Original data for β: $log_{10}(β)$ = 5.94, at I = 1.0 M.
$Hg(II)^{2+}$ + 2 $(NO_2)^-$ ⇌ **$Hg(II)(NO_2)_2$ *(aq)***	10.51948		1	Original data for β: $log_{10}(β)$ = 9.91, at I = 1.0 M.
$Hg(II)^{2+}$ + 3 $(NO_2)^-$ ⇌ **$Hg(II)(NO_2)_3^-$**	12.05948		1	Original data for β: $log_{10}(β)$ = 11.45, at I = 1.0 M.
$Hg(II)^{2+}$ + 4 $(NO_2)^-$ ⇌ **$Hg(II)(NO_2)_4^{2-}$**	12.26632		1	Original data for β: $log_{10}(β)$ = 11.86, at I = 1.0 M.
$Pb(II)^{2+}$ + $(NO_2)^-$ ⇌ **$Pb(II)(NO_2)^+$**	2.51		1	
$Pb(II)^{2+}$ + 2 $(NO_2)^-$ ⇌ **$Pb(II)(NO_2)_2$ *(aq)***	2.65669		1	Original data for β: $log_{10}(β)$ = 2.7, at I = 2.0 M.
$Pb(II)^{2+}$ + 3 $(NO_2)^-$ ⇌ **$Pb(II)(NO_2)_3^-$**	2.95669		1	Original data for β: $log_{10}(β)$ = 3.0, at I = 2.0 M.

2.2.6. Nitrate

The formula for the ligand nitrate is NO_3^-; the molecular weight is 62.004.

Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Be^{2+} + $(NO_3)^-$ ⇌ **$Be(NO_3)^+$**	-0.49368	0	1	Original data for β: $log_{10}(β)$ = -0.9, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
Na^+ + $(NO_3)^-$ ⇌ **$Na(NO_3)$ *(aq)***	-0.55		1	
K^+ + $(NO_3)^-$ ⇌ **$K(NO_3)$ *(aq)***	-0.19	-1.2E+4	1	
Ca^{2+} + $(NO_3)^-$ ⇌ **$Ca(NO_3)^+$**	0.5	-5.4E+3	1	
Sc^{3+} + $(NO_3)^-$ ⇌ **$Sc(NO_3)^{2+}$**	-1.34528		1	Original data for β: $log_{10}(β)$ = 0.28, at I = 4.0 M.
Sc^{3+} + 2 $(NO_3)^-$ ⇌ **$Sc(NO_3)_2^+$**	-3.00880		1	Original data for β: $log_{10}(β)$ = -0.3, at I = 4.0 M.
$Mn(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Mn(II)(NO_3)^+$**	0.2		1	
$Mn(II)^{2+}$ + 2 $(NO_3)^-$ ⇌ **$Mn(II)(NO_3)_2$ *(aq)***	0.6		1	
$Fe(III)^{3+}$ + $(NO_3)^-$ ⇌ **$Fe(III)(NO_3)^{2+}$**	1	-3.7E+4	1	Original data for ΔH at I = 1.0 M.
$Co(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Co(II)(NO_3)^+$**	0.2		1	
$Co(II)^{2+}$ + 2 $(NO_3)^-$ ⇌ **$Co(II)(NO_3)_2$ *(aq)***	0.50516		1	Original data for β: $log_{10}(β)$ = -0.3, at I = 0.5 M.
Ni^{2+} + $(NO_3)^-$ ⇌ **$Ni(NO_3)^+$**	0.4		1	
Ni^{2+} + 2 $(NO_3)^-$ ⇌ **$Ni(NO_3)_2$ *(aq)***	-0.54331		1	Original data for β: $log_{10}(β)$ = -0.5, at I = 2.0 M.
$Cu(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Cu(II)(NO_3)^+$**	0.5	-4.1E+3	1	Original data for ΔH at I = 1.0 M.
$Cu(II)^{2+}$ + 2 $(NO_3)^-$ ⇌ **$Cu(II)(NO_3)_2$ *(aq)***	-0.4		1	
Zn^{2+} + $(NO_3)^-$ ⇌ **$Zn(NO_3)^+$**	0.4		1	
Zn^{2+} + 2 $(NO_3)^-$ ⇌ **$Zn(NO_3)_2$ *(aq)***	-0.3	-4.6E+3	1	Original data for ΔH at I = 1.0 M.
Rb^+ + $(NO_3)^-$ ⇌ **$Rb(NO_3)$ *(aq)***	-0.08		1	
Sr^{2+} + $(NO_3)^-$ ⇌ **$Sr(NO_3)^+$**	0.6	-1.0E+4	1	Original data for ΔH at I = 0.5 M.
Zr^{4+} + $(NO_3)^-$ ⇌ **$Zr(NO_3)^{3+}$**	0.24225		1	Original data for β: $log_{10}(β)$ = 0.3, at I = 2.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Zr^{4+} + 2 $(NO_3)^-$ ⇌ **$Zr(NO_3)_2^{2+}$**	-3.69232		1	Original data for β: $log_{10}(\beta)$ = 0.1, at I = 4.0 M at 20°C.
Zr^{4+} + 3 $(NO_3)^-$ ⇌ **$Zr(NO_3)_3^{+}$**	-5.17584		1	Original data for β: $log_{10}(\beta)$ = -0.3, at I = 4.0 M at 20°C.
Zr^{4+} + 4 $(NO_3)^-$ ⇌ **$Zr(NO_3)_4$ *(aq)***	-6.21760		1	Original data for β: $log_{10}(\beta)$ = -0.8, at I = 4.0 M at 20°C.
Ag^{+} + $(NO_3)^-$ ⇌ **$Ag(NO_3)$ *(aq)***	-0.1		1	
Cd^{2+} + $(NO_3)^-$ ⇌ **$Cd(NO_3)^{+}$**	0.5	-2.1E+4	1	
Cd^{2+} + 2 $(NO_3)^-$ ⇌ **$Cd(NO_3)_2$ *(aq)***	0.2		1	
In^{3+} + $(NO_3)^-$ ⇌ **$In(NO_3)^{2+}$**	0.92824		1	Original data for β: $log_{10}(\beta)$ = 0.18, at I = 0.7 M at 20°C.
In^{3+} + 2 $(NO_3)^-$ ⇌ **$In(NO_3)_2^{+}$**	0.94706		1	Original data for β: $log_{10}(\beta)$ = -0.3, at I = 0.7 M at 20°C.
$Sn(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Sn(II)(NO_3)^{+}$**	0.84632		1	Original data for β: $log_{10}(\beta)$ = 0.44, at I = 1.0 M.
Cs^{+} + $(NO_3)^-$ ⇌ **$Cs(NO_3)$ *(aq)***	0.02		1	
Ba^{2+} + $(NO_3)^-$ ⇌ **$Ba(NO_3)^{+}$**	0.7	-1.3E+4	1	Original data for ΔH at I = 0.5 M.
La^{3+} + $(NO_3)^-$ ⇌ **$La(NO_3)^{2+}$**	0.70948		1	Original data for β: $log_{10}(\beta)$ = 0.1, at I = 1.0 M.
Ce^{3+} + $(NO_3)^-$ ⇌ **$Ce(NO_3)^{2+}$**	0.80948		1	Original data for β: $log_{10}(\beta)$ = 0.2, at I = 1.0 M.
Pr^{3+} + $(NO_3)^-$ ⇌ **$Pr(NO_3)^{2+}$**	0.80948		1	Original data for β: $log_{10}(\beta)$ = 0.2, at I = 1.0 M.
Nd^{3+} + $(NO_3)^-$ ⇌ **$Nd(NO_3)^{2+}$**	0.90948		1	Original data for β: $log_{10}(\beta)$ = 0.3, at I = 1.0 M.
Pm^{3+} + $(NO_3)^-$ ⇌ **$Pm(NO_3)^{2+}$**	1.00948		1	Original data for β: $log_{10}(\beta)$ = 0.4, at I = 1.0 M.
Sm^{3+} + $(NO_3)^-$ ⇌ **$Sm(NO_3)^{2+}$**	0.90948		1	Original data for β: $log_{10}(\beta)$ = 0.3, at I = 1.0 M.
Eu^{3+} + $(NO_3)^-$ ⇌ **$Eu(NO_3)^{2+}$**	1.22	-4.6E+3	1	Original data for ΔH at I = 0.5 M.
Gd^{3+} + $(NO_3)^-$ ⇌ **$Gd(NO_3)^{2+}$**	0.60948		1	Original data for β: $log_{10}(\beta)$ = 0.0, at I = 1.0 M.
Tb^{3+} + $(NO_3)^-$ ⇌ **$Tb(NO_3)^{2+}$**	0.88		1	
Dy^{3+} + $(NO_3)^-$ ⇌ **$Dy(NO_3)^{2+}$**	0.30948		1	Original data for β: $log_{10}(\beta)$ = -0.3, at I = 1.0 M.
Ho^{3+} + $(NO_3)^-$ ⇌ **$Ho(NO_3)^{2+}$**	0.40948		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M.
Er^{3+} + $(NO_3)^-$ ⇌ **$Er(NO_3)^{2+}$**	0.30948		1	Original data for β: $log_{10}(\beta)$ = -0.3, at I = 1.0 M.
Tm^{3+} + $(NO_3)^-$ ⇌ **$Tm(NO_3)^{2+}$**	0.35948		1	Original data for β: $log_{10}(\beta)$ = -0.25, at I = 1.0 M.
Yb^{3+} + $(NO_3)^-$ ⇌ **$Yb(NO_3)^{2+}$**	0.40948		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M.
Lu^{3+} + $(NO_3)^-$ ⇌ **$Lu(NO_3)^{2+}$**	0.40948		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M.
Hf^{4+} + $(NO_3)^-$ ⇌ **$Hf(NO_3)^{3+}$**	0.28225		1	Original data for β: $log_{10}(\beta)$ = 0.34, at I = 2.0 M.
Hf^{4+} + 2 $(NO_3)^-$ ⇌ **$Hf(NO_3)_2^{2+}$**	-0.10107		1	Original data for β: $log_{10}(\beta)$ = 0.05, at I = 2.0 M.
Hf^{4+} + 3 $(NO_3)^-$ ⇌ **$Hf(NO_3)_3^{+}$**	-0.82994		1	Original data for β: $log_{10}(\beta)$ = -0.7, at I = 2.0 M.
$Hg(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Hg(II)(NO_3)^{+}$**	-0.43046		1	Original data for β: $log_{10}(\beta)$ = 0.11, at I = 3.0 M.
$Hg(II)^{2+}$ + 2 $(NO_3)^-$ ⇌ **$Hg(II)(NO_3)_2$ *(aq)***	-0.81069		1	Original data for β: $log_{10}(\beta)$ = 0.0, at I = 3.0 M.
$Pb(II)^{2+}$ + $(NO_3)^-$ ⇌ **$Pb(II)(NO_3)^{+}$**	1.17	-2E+3	1	
$Pb(II)^{2+}$ + 2 $(NO_3)^-$ ⇌ **$Pb(II)(NO_3)_2$ *(aq)***	1.4	-6.6E+3	1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + 3 $(NO_3)^-$ ⇌ **$Pb(II)(NO_3)_3^{-}$**	0.05669	-8E+3	1	Original data for β: $log_{10}(\beta)$ = 0.1, at I = 2.0 M. Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + 4 $(NO_3)^-$ ⇌ **$Pb(II)(NO_3)_4^{2-}$**	-0.84046	-3.3E+4	1	Original data for β: $log_{10}(\beta)$ = -0.3, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Bi^{3+} + $(NO_3)^-$ ⇌ **$Bi(NO_3)^{2+}$**	1.7	1.2E+4	1	Original data for ΔH at I = 2.0 M.
Bi^{3+} + 2 $(NO_3)^-$ ⇌ **$Bi(NO_3)_2^{+}$**	2.5		1	
Bi^{3+} + 3 $(NO_3)^-$ ⇌ **$Bi(NO_3)_3$ *(aq)***	1.91896		1	Original data for β: $log_{10}(\beta)$ = 0.7, at I = 1.0 M.
Bi^{3+} + 4 $(NO_3)^-$ ⇌ **$Bi(NO_3)_4^{-}$**	0.51337		1	Original data for β: $log_{10}(\beta)$ = 0.6, at I = 2.0 M.
$(U(VI)O_2)^{2+}$ + $(NO_3)^-$ ⇌ **$(U(VI)O_2)(NO_3)^{+}$**	0.3	-1.2E+4	1	Original data for ΔH at I = 2.0 M.

2.2.7. Fluoride

The formula for the ligand fluoride is F^-; the molecular weight is 18.998.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + F^{-} \rightleftharpoons \mathbf{HF}$ ***(aq)***	3.18	1.33E+4	1	
$H^{+} + 2\ F^{-} \rightleftharpoons \mathbf{HF_2^{-}}$	3.78	1.74E+4	1	$HL + L \rightleftharpoons HL_2$ $log_{10}(\beta)$ = 0.6 ΔH = 4.1E+3 $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 3.18 ΔH = 1.33E+4 $H + 2\ L \rightleftharpoons HL_2$ $log_{10}(\beta)$ = 3.78 ΔH = 1.74E+4
$Li^{+} + F^{-} \rightleftharpoons \mathbf{LiF}$ ***(aq)***	0.31	4E+3	1	Original data for ΔH at I = 1.0 M.
$Be^{2+} + F^{-} \rightleftharpoons \mathbf{BeF^{+}}$	5.24678	0	1	Original data for β: $log_{10}(\beta)$ = 4.71, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$Be^{2+} + 2\ F^{-} \rightleftharpoons \mathbf{BeF_2}$ ***(aq)***	9.12516	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 8.32, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$Be^{2+} + 3\ F^{-} \rightleftharpoons \mathbf{BeF_3^{-}}$	11.92516	-8E+3	1	Original data for β: $log_{10}(\beta)$ = 11.12, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$Be^{2+} + 4\ F^{-} \rightleftharpoons \mathbf{BeF_4^{2-}}$	13.92678	-8E+3	1	Original data for β: $log_{10}(\beta)$ = 13.39, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$3\ Be^{2+} + 3\ (OH)^{-} + F^{-} \rightleftharpoons \mathbf{Be_3F(OH)_3^{2+}}$	37.00032		1	$3\ Be + L \rightleftharpoons Be_3(OH)_3L + 3\ H$ $log_{10}(\beta)$ = -4.18 I = 3.0 M $3\ H + 3\ OH \rightleftharpoons 3\ H_2O$ $log_{10}(\beta)$ = 42.80169 I = 3.0 M $3\ Be + 3\ OH + L \rightleftharpoons Be_3(OH)_3L$ $log_{10}(\beta)$ = 38.62169 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 37.00032
$3\ Be^{2+} + 3\ (OH)^{-} + 2\ F^{-} \rightleftharpoons \mathbf{Be_3F_2(OH)_3^{+}}$	39.93986		1	$3\ Be + 2\ L \rightleftharpoons Be_3(OH)_3L_2 + 3\ H$ $log_{10}(\beta)$ = -0.7 I = 3.0 M $3\ H + 3\ OH \rightleftharpoons 3\ H_2O$ $log_{10}(\beta)$ = 42.80169 I = 3.0 M $3\ Be + 3\ OH + 2\ L \rightleftharpoons Be_3(OH)_3L_2$ $log_{10}(\beta)$ = 42.10169 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 39.93986
$Na^{+} + F^{-} \rightleftharpoons \mathbf{NaF}$ ***(aq)***	0.02	1.2E+4	1	Original data for ΔH at I = 1.0 M.
$Mg^{2+} + F^{-} \rightleftharpoons \mathbf{MgF^{+}}$	1.9	1.3E+4	1	Original data for ΔH at I = 1.0 M.
$Al^{3+} + F^{-} \rightleftharpoons \mathbf{AlF^{2+}}$	7.01	4.6E+3	1	Original data for ΔH at I = 0.1 M.
$Al^{3+} + 2\ F^{-} \rightleftharpoons \mathbf{AlF_2^{+}}$	12.63	8.3E+3	1	Original data for ΔH at I = 0.1 M.
$Al^{3+} + 3\ F^{-} \rightleftharpoons \mathbf{AlF_3}$ ***(aq)***	16.7	8.7E+3	1	Original data for ΔH at I = 0.1 M.
$Al^{3+} + 4\ F^{-} \rightleftharpoons \mathbf{AlF_4^{-}}$	19.4	8.7E+3	1	Original data for ΔH at I = 0.1 M.
$Al^{3+} + 5\ F^{-} \rightleftharpoons \mathbf{AlF_5^{2-}}$	20.73		2	
$Al^{3+} + 6\ F^{-} \rightleftharpoons \mathbf{AlF_6^{3-}}$	20.46		2	
$K^{+} + F^{-} \rightleftharpoons \mathbf{KF}$ ***(aq)***	-0.34		1	
$Ca^{2+} + F^{-} \rightleftharpoons \mathbf{CaF^{+}}$	1.13678	1.4E+4	1	Original data for β: $log_{10}(\beta)$ = 0.6, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$Sc^{3+} + F^{-} \rightleftharpoons \mathbf{ScF^{2+}}$	7.08	1E+3	1	Original data for ΔH at I = 0.5 M.
$Sc^{3+} + 2\ F^{-} \rightleftharpoons \mathbf{ScF_2^{+}}$	12.89	5.0E+3	1	Original data for ΔH at I = 0.5 M.
$Sc^{3+} + 3\ F^{-} \rightleftharpoons \mathbf{ScF_3}$ ***(aq)***	17.4	2.3E+4	1	Original data for ΔH at I = 0.5 M.
$Sc^{3+} + 4\ F^{-} \rightleftharpoons \mathbf{ScF_4^{-}}$	20.2	1.6E+4	1	Original data for ΔH at I = 0.5 M.
$2\ Sc^{3+} + 3\ F^{-} \rightleftharpoons \mathbf{Sc_2F_3^{3+}}$	20.61033		1	Original data for β: $log_{10}(\beta)$ = 19, at I = 0.5 M.
$Cr(III)^{3+} + F^{-} \rightleftharpoons \mathbf{Cr(III)F^{2+}}$	5.2	1.0E+4	1	Original data for ΔH at I = 0.5 M.
$Cr(III)^{3+} + 2\ F^{-} \rightleftharpoons \mathbf{Cr(III)F_2^{+}}$	9.04194		1	Original data for β: $log_{10}(\beta)$ = 7.7, at I = 0.5 M.
$Cr(III)^{3+} + 3\ F^{-} \rightleftharpoons \mathbf{Cr(III)F_3}$ ***(aq)***	11.71033		1	Original data for β: $log_{10}(\beta)$ = 10.1, at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Mn(II)^{2+} + F^- \rightleftharpoons$ **$Mn(II)F^+$**	1.5	1.1E+4	1	Original data for ΔH at I = 0.5 M.
$Fe(II)^{2+} + F^- \rightleftharpoons$ **$Fe(II)F^+$**	1.20632		1	Original data for β: $log_{10}(\beta)$ = 0.8, at I = 1.0 M.
$Fe(III)^{3+} + F^- \rightleftharpoons$ **$Fe(III)F^{2+}$**	6.03	1.0E+4	1	Original data for ΔH at I = 0.5 M.
$Fe(III)^{3+} + 2\ F^- \rightleftharpoons$ **$Fe(III)F_2^+$**	10.66	1.5E+4	1	Original data for ΔH at I = 0.5 M.
$Fe(III)^{3+} + 3\ F^- \rightleftharpoons$ **$Fe(III)F_3$ *(aq)***	13.7	1.9E+4	1	Original data for ΔH at I = 0.5 M.
$Co(II)^{2+} + F^- \rightleftharpoons$ **$Co(II)F^+$**	1.4	9.2E+3	1	Original data for ΔH at I = 0.5 M.
$Ni^{2+} + F^- \rightleftharpoons$ **NiF^+**	1.3	7.1E+3	1	Original data for ΔH at I = 0.5 M.
$Cu(II)^{2+} + F^- \rightleftharpoons$ **$Cu(II)F^+$**	1.7	1.3E+4	1	Original data for ΔH at I = 0.5 M.
$Zn^{2+} + F^- \rightleftharpoons$ **ZnF^+**	1.3	1.1E+4	1	Original data for ΔH at I = 0.5 M.
$Ga^{3+} + F^- \rightleftharpoons$ **GaF^{2+}**	5.27516	1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 4.47, at I = 0.5 M. Original data for ΔH at I = 1.0 M.
$Ga^{3+} + 2\ F^- \rightleftharpoons$ **GaF_2^+**	9.34194		1	Original data for β: $log_{10}(\beta)$ = 8.00, at I = 0.5 M.
$Ga^{3+} + 3\ F^- \rightleftharpoons$ **GaF_3 *(aq)***	12.08033		1	Original data for β: $log_{10}(\beta)$ = 11.47, at I = 0.5 M.
$Rb^+ + F^- \rightleftharpoons$ **RbF *(aq)***	-0.22		1	
$Sr^{2+} + F^- \rightleftharpoons$ **SrF^+**	0.55632	1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 0.15, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$Y^{3+} + F^- \rightleftharpoons$ **YF^{2+}**	4.81	9.2E+3	1	Original data for ΔH at I = 1.0 M.
$Y^{3+} + 2\ F^- \rightleftharpoons$ **YF_2^+**	8.54		1	
$Y^{3+} + 3\ F^- \rightleftharpoons$ **YF_3 *(aq)***	12.14		1	
$Zr^{4+} + F^- \rightleftharpoons$ **ZrF^{3+}**	9.8	-5.4E+3	1	Original data for ΔH at I = 4.0 M.
$Zr^{4+} + 2\ F^- \rightleftharpoons$ **ZrF_2^{2+}**	16.25893	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 16.36, at I = 2.0 M. Original data for ΔH at I = 4.0 M.
$Zr^{4+} + 3\ F^- \rightleftharpoons$ **ZrF_3^+**	22.18006	-9.6E+3	1	Original data for β: $log_{10}(\beta)$ = 22.31, at I = 2.0 M. Original data for ΔH at I = 4.0 M.
$Zr^{4+} + 4\ F^- \rightleftharpoons$ **ZrF_4 *(aq)***	24.17240	-1.9E+4	1	Original data for β: $log_{10}(\beta)$ = 29.59, at I = 4.0 M. Original data for ΔH at I = 4.0 M.
$Zr^{4+} + 5\ F^- \rightleftharpoons$ **ZrF_5^-**	25.86		2	
$Zr^{4+} + 6\ F^- \rightleftharpoons$ **ZrF_6^{2-}**	29.83		2	
$Ag^+ + F^- \rightleftharpoons$ **AgF *(aq)***	0.4	-1.2E+4	1	Original data for ΔH at I = 0.5 M.
$Cd^{2+} + F^- \rightleftharpoons$ **CdF^+**	1.2	5.0E+3	1	Original data for ΔH at I = 1.0 M.
$Cd^{2+} + 2\ F^- \rightleftharpoons$ **CdF_2 *(aq)***	1.41		2	
$In^{3+} + F^- \rightleftharpoons$ **InF^{2+}**	4.65	1.0E+4	1	
$In^{3+} + 2\ F^- \rightleftharpoons$ **InF_2^+**	8	2.3E+4	1	
$In^{3+} + 3\ F^- \rightleftharpoons$ **InF_3 *(aq)***	10.3	2.9E+4	1	
$In^{3+} + 4\ F^- \rightleftharpoons$ **InF_4^-**	11.4	3.8E+4	1	
$Sn(II)^{2+} + F^- \rightleftharpoons$ **$Sn(II)F^+$**	4.48632		1	Original data for β: $log_{10}(\beta)$ = 4.08, at I = 1.0 M.
$Sn(II)^{2+} + 2\ F^- \rightleftharpoons$ **$Sn(II)F_2$ *(aq)***	7.28948		1	Original data for β: $log_{10}(\beta)$ = 6.68, at I = 1.0 M.
$Sn(II)^{2+} + 3\ F^- \rightleftharpoons$ **$Sn(II)F_3^-$**	10.06948		1	Original data for β: $log_{10}(\beta)$ = 9.46, at I = 1.0 M.
$Cs^+ + F^- \rightleftharpoons$ **CsF *(aq)***	-0.36		1	
$Ba^{2+} + F^- \rightleftharpoons$ **BaF^+**	0.20632	1.6E+4	1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$La^{3+} + F^- \rightleftharpoons$ **LaF^{2+}**	3.62	1.2E+4	1	Original data for ΔH at I = 1.0 M.
$La^{3+} + 2\ F^- \rightleftharpoons$ **LaF_2^+**	6.42194		1	Original data for β: $log_{10}(\beta)$ = 5.08, at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Ce^{3+} + F^- \rightleftharpoons$ **CeF^{2+}**	3.9		1	
$Pr^{3+} + F^- \rightleftharpoons$ **PrF^{2+}**	4.05	1.4E+4	1	Original data for ΔH at I = 1.0 M.
$Nd^{3+} + F^- \rightleftharpoons$ **NdF^{2+}**	4.17	1.3E+4	1	Original data for ΔH at I = 1.0 M.
$Pm^{3+} + F^- \rightleftharpoons$ **PmF^{2+}**	4.20073		1	Original data for β: $log_{10}(\beta)$ = 3.56, at I = 0.1 M.
$Pm^{3+} + 2\ F^- \rightleftharpoons$ **PmF_2^+**	6.61580		1	Original data for β: $log_{10}(\beta)$ = 5.60, at I = 1.0 M.
$Sm^{3+} + F^- \rightleftharpoons$ **SmF^{2+}**	4.19	1.0E+4	1	Original data for ΔH at I = 1.0 M.
$Eu^{3+} + F^- \rightleftharpoons$ **EuF^{2+}**	4.27	9.6E+3	1	Original data for ΔH at I = 1.0 M.
$Eu^{3+} + 2\ F^- \rightleftharpoons$ **EuF_2^+**	6.91580	1.5E+4	1	Original data for β: $log_{10}(\beta)$ = 5.90, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$Gd^{3+} + F^- \rightleftharpoons$ **GdF^{2+}**	4.32	9.2E+3	1	Original data for ΔH at I = 1.0 M.
$Tb^{3+} + F^- \rightleftharpoons$ **TbF^{2+}**	4.43	9.2E+3	1	Original data for ΔH at I = 1.0 M.
$Dy^{3+} + F^- \rightleftharpoons$ **DyF^{2+}**	4.46	9.6E+3	1	Original data for ΔH at I = 1.0 M.
$Ho^{3+} + F^- \rightleftharpoons$ **HoF^{2+}**	4.57	1.0E+4	1	Original data for ΔH at I = 1.0 M.
$Er^{3+} + F^- \rightleftharpoons$ **ErF^{2+}**	4.59	1.0E+4	1	Original data for ΔH at I = 1.0 M.
$Tm^{3+} + F^- \rightleftharpoons$ **TmF^{2+}**	4.61	1.0E+4	1	Original data for ΔH at I = 1.0 M.
$Yb^{3+} + F^- \rightleftharpoons$ **YbF^{2+}**	4.63	1.1E+4	1	Original data for ΔH at I = 1.0 M.
$Lu^{3+} + F^- \rightleftharpoons$ **LuF^{2+}**	4.66	1.1E+4	1	Original data for ΔH at I = 1.0 M.
$Hf^{4+} + F^- \rightleftharpoons$ **HfF^{3+}**	6.87296	-3E+3	1	Original data for β: $log_{10}(\beta)$ = 9.04, at I = 4.0 M. Original data for ΔH at I = 4.0 M.
$Hf^{4+} + 2\ F^- \rightleftharpoons$ **HfF_2^{2+}**	12.80768	-6.2E+3	1	Original data for β: $log_{10}(\beta)$ = 16.60, at I = 4.0 M. Original data for ΔH at I = 4.0 M.
$Hf^{4+} + 3\ F^- \rightleftharpoons$ **HfF_3^+**	18.27416	-3E+3	1	Original data for β: $log_{10}(\beta)$ = 23.15, at I = 4.0 M. Original data for ΔH at I = 4.0 M.
$Hf^{4+} + 4\ F^- \rightleftharpoons$ **HfF_4 *(aq)***	23.39240	-1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 28.81, at I = 4.0 M. Original data for ΔH at I = 4.0 M.
$Hf^{4+} + 5\ F^- \rightleftharpoons$ **HfF_5^-**	36.36		2	
$Hf^{4+} + 6\ F^- \rightleftharpoons$ **HfF_6^{2-}**	39.53		2	
$Hg(II)^{2+} + F^- \rightleftharpoons$ **$Hg(II)F^+$**	1.6	4E+3	1	
$Pb(II)^{2+} + F^- \rightleftharpoons$ **$Pb(II)F^+$**	2.14715		1	Original data for β: $log_{10}(\beta)$ = 1.72, at I = 0.1 M.
$Pb(II)^{2+} + 2\ F^- \rightleftharpoons$ **$Pb(II)F_2$ *(aq)***	3.13948		1	Original data for β: $log_{10}(\beta)$ = 2.53, at I = 1.0 M.
$Bi^{3+} + F^- \rightleftharpoons$ **BiF^{2+}**	4.43669		1	Original data for β: log10(β) = 4.48, at I = 2.0 M at 30°C.
$(U(VI)O_2)^{2+} + F^- \rightleftharpoons$ **$(U(VI)O_2)F^+$**	5.14	1E+3	1	Original data for ΔH at I = 1.0 M.
$(U(VI)O_2)^{2+} + 2\ F^- \rightleftharpoons$ **$(U(VI)O_2)F_2$ *(aq)***	8.6	2E+3	1	Original data for ΔH at I = 1.0 M.
$(U(VI)O_2)^{2+} + 3\ F^- \rightleftharpoons$ **$(U(VI)O_2)F_3^-$**	11	2E+3	1	Original data for ΔH at I = 1.0 M.
$(U(VI)O_2)^{2+} + 4\ F^- \rightleftharpoons$ **$(U(VI)O_2)F_4^{2-}$**	11.9	4E+3	1	Original data for ΔH at I = 1.0 M.

2.2.8. Silicate

The formula for the ligand silicate is $H_2SiO_4^{2-}$; the molecular weight is 94.097.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{H(H_2SiO_4)^-}$	13.2	-4.1E+4	1	Original data for ΔH at I = 0.5 M.
$2\ H^+ + (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{H_2(H_2SiO_4)}\ \mathbf{\textit{(aq)}}$	23.04	-6.1E+4	1	$H + HL \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 9.84 ΔH = -2.0E+4 (Original data for ΔH at I = 0.5 M) $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 13.2 ΔH = -4.1E+4 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 23.04 ΔH = -6.1E+4
$2\ H^+ + 2\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_2O_3(OH)_4^{2-}}$	27.27484		1	$2\ H_2L \rightleftharpoons Si_2O_3(OH)_4 + 2\ H + H_2O$ $\log_{10}(\beta)$ = -18.00 I = 0.5 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta)$ = 44.46968 I = 0.5 M $2\ H + 2\ L \rightleftharpoons Si_2O_3(OH)_4 + H_2O$ $\log_{10}(\beta)$ = 26.46968 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 27.27484
$3\ H^+ + 2\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_2O_2(OH)_5^-}$	38.06162		1	$Si_2O_3(OH)_4 + H \rightleftharpoons Si_2O_2(OH)_5$ $\log_{10}(\beta)$ = 10.25 I = 0.5 M $2\ H + 2\ L \rightleftharpoons Si_2O_3(OH)_4$ $\log_{10}(\beta)$ = 26.46968 I = 0.5 M $3\ H + 2\ L \rightleftharpoons Si_2O_2(OH)_5$ $\log_{10}(\beta)$ = 36.71968 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 38.06162
$3\ H^+ + 3\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_3O_6(OH)_3\ (cyclo)^{3-}}$	41.07968		1	$3\ H_2L \rightleftharpoons 3\ H + Si_3O_6(OH)_3$ (cyclo) $+ 3\ H_2O$ $\log_{10}(\beta)$ = -26.43 I = 0.5 M $6\ H + 3\ L \rightleftharpoons 3\ H_2L$ $\log_{10}(\beta)$ = 66.70452 I = 0.5 M $3\ H + 3\ L \rightleftharpoons Si_3O_6(OH)_3$ (cyclo) $+ H_2O$ $\log_{10}(\beta)$ = 40.27452 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 41.07968
$3\ H^+ + 3\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_3O_5(OH)_5\ (linear)^{3-}}$	42.10968		1	$3\ H_2L \rightleftharpoons 3\ H + Si_3O_5(OH)_5$ (linear) $+ 2\ H_2O$ $\log_{10}(\beta)$ = -25.40 I = 0.5 M $6\ H + 3\ L \rightleftharpoons 3\ H_2L$ $\log_{10}(\beta)$ = 66.70452 I = 0.5 M $3\ H + 3\ L \rightleftharpoons Si_3O_5(OH)_5$ (linear) $+ 2\ H_2O$ $\log_{10}(\beta)$ = 41.30452 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 42.10968
$4\ H^+ + 2\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_2O(OH)_6}\ \mathbf{\textit{(aq)}}$	47.28001		1	$2\ Si(OH)_4 \rightleftharpoons Si_2O(OH)_6$ $\log_{10}(\beta)$ = 1.2 I = 0.5 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta)$ = 44.46968 I = 0.5 M $4\ H + 2\ L \rightleftharpoons Si_2O(OH)_6$ $\log_{10}(\beta)$ = 45.66968 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 47.28001
$4\ H^+ + 4\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_4O_8(OH)_4^{4-}}$	54.68614		1	$Si_4O_7(OH)_5$ (cyclo) $\rightleftharpoons Si_4O_8(OH)_4 + H$ $\log_{10}(\beta)$ = -9.39 I = 0.5 M $5\ H + 4\ L \rightleftharpoons Si_4O_7(OH)_5$ (cyclo) $+ 4\ H_2O$ $\log_{10}(\beta)$ = 63.53936 I = 0.5 M $4\ H + 4\ L \rightleftharpoons Si_4O_8(OH)_4 + 4\ H_2O$ $\log_{10}(\beta)$ = 54.14936 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 54.68614
$5\ H^+ + 4\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Si_4O_7(OH)_5\ (cyclo)^{3-}}$	65.14969		1	$4\ H_2L \rightleftharpoons 3\ H + Si_4O_7(OH)_5$ (cyclo) $+ 4\ H_2O$ $\log_{10}(\beta)$ = -23.42 I = 0.5 M $8\ H + 4\ L \rightleftharpoons 4\ H_2L$ $\log_{10}(\beta)$ = 88.93936 I = 0.5 M $5\ H + 4\ L \rightleftharpoons Si_4O_7(OH)_5$ (cyclo) $+ 4\ H_2O$ $\log_{10}(\beta)$ = 63.53936 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 65.14969
$6\ H^+ + 4\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{H_6(H_2SiO_4)_4^{2-}}$	78.2		3	
$Mg^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Mg(H_2SiO_4)}\ \mathbf{\textit{(aq)}}$	5.38316		1	$MgHL \rightleftharpoons MgL + H$ $\log_{10}(\beta)$ = -9.06 I = 1.0 M $Mg + H + L \rightleftharpoons MgHL$ $\log_{10}(\beta)$ = 13.63052 I = 1.0 M $Mg + L \rightleftharpoons MgL$ $\log_{10}(\beta)$ = 4.57052 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 5.38316

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Mg^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$MgH(H_2SiO_4)^+$**	14.44316		1	Mg + H_2L ⇌ MgHL + H $log_{10}(\beta)$ = -8.8 I = 1.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.43052 I = 1.0 M Mg + H + L ⇌ MgHL $log_{10}(\beta)$ = 13.63052 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 14.44316
$2 H^+ + Mg^{2+} + 2 (H_2SiO_4)^{2-} \rightleftharpoons$ **$MgH_2(H_2SiO_4)_2$ *(aq)***	31.18316		1	MgHL + H_2L ⇌ MgH_2L_2 + H $log_{10}(\beta)$ = -6.3 I = 1.0 M Mg + H + L ⇌ MgHL $log_{10}(\beta)$ = 13.63052 I = 1.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.43052 I = 1.0 M Mg + 2 H + 2 L ⇌ MgH_2L_2 $log_{10}(\beta)$ = 29.76104 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 31.18316
$H^+ + Al^{3+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$AlH(H_2SiO_4)^{2+}$**	20.96715	5E+3	1	Al + H_2L ⇌ AlHL + H $log_{10}(\beta)$ = -2.5 I = 0.1 M ΔH = -6.6E+4 (Original data for ΔH at I = 0.1 M) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.39927 I = 0.1 M ΔH = -6.1E+4 Al + H + L ⇌ AlHL $log_{10}(\beta)$ = 19.89927 I = 0.1 M ΔH = -5E+3 I = 0 M: $log_{10}(\beta)$ = 20.96715
$Ca^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$Ca(H_2SiO_4)$ *(aq)***	4.25316		1	CaHL ⇌ CaL + H $log_{10}(\beta)$ = -9.89 I = 1.0 M Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 13.33052 I = 1.0 M Ca + L ⇌ CaL $log_{10}(\beta)$ = 3.44052 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 4.25316
$H^+ + Ca^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$CaH(H_2SiO_4)^+$**	14.14316		1	Ca + H_2L ⇌ CaHL + H $log_{10}(\beta)$ = -9.1 I = 1.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.43052 I = 1.0 M Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 13.33052 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 14.14316
$2 H^+ + Ca^{2+} + 2 (H_2SiO_4)^{2-} \rightleftharpoons$ **$CaH_2(H_2SiO_4)_2$ *(aq)***	30.18316		1	CaHL + H_2L ⇌ CaH_2L_2 + H $log_{10}(\beta)$ = -7.0 I = 1.0 M Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 13.33052 I = 1.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.43052 I = 1.0 M Ca + 2 H + 2 L ⇌ CaH_2L_2 $log_{10}(\beta)$ = 28.76104 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 30.18316
$H^+ + Fe(III)^{3+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$Fe(III)H(H_2SiO_4)^{2+}$**	22.86715	-4.5E+4	1	Fe(III) + H_2L ⇌ Fe(III)HL + H $log_{10}(\beta)$ = -0.6 I = 0.1 M ΔH = 1.6E+4 (Original data for ΔH at I = 0.1 M) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.39927 I = 0.1 M ΔH = -6.1E+4 Fe(III) + H + L ⇌ Fe(III)HL $log_{10}(\beta)$ = 21.79927 I = 0.1 M ΔH = -4.5E+4 I = 0 M: $log_{10}(\beta)$ = 22.86715
$H^+ + Eu^{3+} + (H_2SiO_4)^{2-} \rightleftharpoons$ **$EuH(H_2SiO_4)^{2+}$**	21.16715		1	Eu + H_2L ⇌ EuHL + H $log_{10}(\beta)$ = -2.3 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.39927 I = 0.1 M Eu + H + L ⇌ EuHL $log_{10}(\beta)$ = 20.09927 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.16715
$2 H^+ + Eu^{3+} + 2 (H_2SiO_4)^{2-} \rightleftharpoons$ **$EuH_2(H_2SiO_4)_2^+$**	39.22072		1	EuHL + H_2L ⇌ EuH_2L_2 + H $log_{10}(\beta)$ = -5.2 I = 0.1 M Eu + H + L ⇌ EuHL $log_{10}(\beta)$ = 20.09927 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.39927 I = 0.1 M Eu + 2 H + 2 L ⇌ EuH_2L_2 $log_{10}(\beta)$ = 37.29854 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 39.22072

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (U(VI)O_2)^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons$ $\mathbf{(U(VI)O_2)H(H_2SiO_4)^+}$	21.24		1	$(UO_2) + H_2L \rightleftharpoons (UO_2)HL + H$ $\log_{10}(\beta) = -1.8$ $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 23.04$ $(UO_2) + H + L \rightleftharpoons (UO_2)HL$ $\log_{10}(\beta) = 21.24$
$2\ H^+ + (H_2SiO_4)^{2-} + (SO_4)^{2-} \rightleftharpoons$ $\mathbf{H_4SiO_4(SO_4)^{2-}}$	22.5	-5.9E+4	1	$Si(OH)_4 + (SO_4) \rightleftharpoons Si(OH)_4(SO_4)$ $\log_{10}(\beta) = -0.54$ ΔH = 2E+3 $2\ H^+ + (H_2SiO_4)^{2-} \rightleftharpoons H_2(H_2SiO_4)$ $\log_{10}(\beta) = 23.04$ ΔH = -6.1E+4 $2\ H^+ + (H_2SiO_4)^{2-} + (SO_4) \rightleftharpoons H_4SiO_4(SO_4)$ $\log_{10}(\beta) = 22.50$ ΔH = -5.9E+4
$2\ H^+ + (H_2SiO_4)^{2-} + (citrate)^{3-} \rightleftharpoons$ $\mathbf{(H_4SiO_4)(citrate)^{3-}}$	23.15000		1	$H_4SiO_4 + (citrate) \rightleftharpoons H_4SiO_4(citrate)$ $\log_{10}(\beta) = 0.11$ I = 0.5 M $2\ H + H_2SiO_4 \rightleftharpoons H_4SiO_4$ $\log_{10}(\beta) = 22.23484$ I = 0.5 M $2\ H + H_2SiO_4 \rightleftharpoons H_4SiO_4(citrate)$ $\log_{10}(\beta) = 22.34484$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 23.15000$

2.2.9. Phosphate

The formula for the ligand phosphate is PO_4^{3-}; the molecular weight is 94.970.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + (NH_3)$ *(aq)* $+ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H_2(PO_4)(NH_3)^-}$	22.89475		1	$NH_4 + HL \rightleftharpoons NH_4HL$ $\log_{10}(\beta) = 0.8$ I = 0.15 M (Original data for β at T = 37°C) $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ I = 0.15 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.66138$ I = 0.15 M $NH_3 + 2\ H + L \rightleftharpoons NH_4HL$ $\log_{10}(\beta) = 21.70538$ I = 0.15 M I = 0 M: $\log_{10}(\beta) = 22.89475$
$3\ H^+ + (NH_3)$ *(aq)* $+ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H_3(PO_4)(NH_3)}$ ***(aq)***	28.95488		1	$NH_4 + H_2L \rightleftharpoons NH_4H_2L$ $\log_{10}(\beta) = -0.1$ I = 0.15 M (Original data for β at T = 37°C) $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ I = 0.15 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 18.38363$ I = 0.15 M $NH_3 + 3\ H + L \rightleftharpoons NH_4H_2L$ $\log_{10}(\beta) = 27.52763$ I = 0.15 M I = 0 M: $\log_{10}(\beta) = 28.95488$
$H^+ + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H(PO_4)^{2-}}$	12.375	-1.5E+4	1	
$2\ H^+ + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H_2(PO_4)^-}$	19.573	-1.8E+4	1	$HL + H \rightleftharpoons H_2L$ $\log_{10}(\beta) = 7.198$ ΔH = -3E+3 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ ΔH = -1.5E+4 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ ΔH = -1.8E+4
$3\ H^+ + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H_3(PO_4)}$ ***(aq)***	21.721	-1.050E+4	1	$H_2L + H \rightleftharpoons H_3L$ $\log_{10}(\beta) = 2.148$ ΔH = -7.5E+3 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ ΔH = -1.8E+4 $2\ H + L \rightleftharpoons H_3L$ $\log_{10}(\beta) = 21.721$ ΔH = -1.05E+4
$4\ H^+ + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{H_4(PO_4)^+}$	21.721		1	$H_3L + H \rightleftharpoons H_4L$ $\log_{10}(\beta) = 0.0$ I = 3.0 M $3\ H + L \rightleftharpoons H_3L$ $\log_{10}(\beta) = 23.34237$ I = 3.0 M $4\ H + L \rightleftharpoons H_4L$ $\log_{10}(\beta) = 23.34237$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 21.721$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Li^+ + (PO_4)^{3-} \rightleftharpoons$ **$Li(PO_4)^{2-}$**	1.66362		1	Original data for β: $log_{10}(\beta)$ = 0.95, at I = 0.15 M at 37°C.
$H^+ + Li^+ + (PO_4)^{3-} \rightleftharpoons$ **$LiH(PO_4)^-$**	13.53215		1	Li + HL ⇌ LiHL $log_{10}(\beta)$ = 0.73 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 11.73427 I = 0.1 M Li + H + L ⇌ LiHL $log_{10}(\beta)$ = 12.46427 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.53215
$2\ H^+ + Li^+ + (PO_4)^{3-} \rightleftharpoons$ **$LiH_2(PO_4)$ *(aq)***	20.04139		1	Li + H_2L ⇌ LiH_2L $log_{10}(\beta)$ = 0.2 I = 0.5 M (Original data for β at T = 37°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 18.23106 I = 0.5 M Li + 2 H + L ⇌ LiH_2L $log_{10}(\beta)$ = 18.43106 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 20.04139
$2\ H^+ + Be^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$BeH_2(PO_4)^+$**	20.89254		1	Be + H_2L ⇌ BeH_2L $log_{10}(\beta)$ = 1.86 I = 3.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 20.92414 I = 3.0 M Be + 2 H + L ⇌ BeH_2L $log_{10}(\beta)$ = 22.78414 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 20.89254
$4\ H^+ + Be^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$BeH_4(PO_4)_2$ *(aq)***	42.64531		1	Be + 2 H_2L ⇌ $Be(H_2L)_2$ $log_{10}(\beta)$ = 4.31 I = 3.0 M 4 H + 2 L ⇌ 2 H_2L $log_{10}(\beta)$ = 41.84828 I = 3.0 M Be + 4 H + 2 L ⇌ $Be(H_2L)_2$ $log_{10}(\beta)$ = 46.15828 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 42.64531
$5\ H^+ + 2\ Be^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$Be_2H_5(PO_4)_2^{3+}$**	43.28223		1	2 Be + 2 H_3L ⇌ $Be_2H_5L_2$ + H $log_{10}(\beta)$ = -0.43 I = 3.0 M 6 H + 2 L ⇌ 2 H_3L $log_{10}(\beta)$ = 46.68474 I = 3.0 M 2 Be + 5 H + 2 L ⇌ $Be_2H_5L_2$ $log_{10}(\beta)$ = 46.25474 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 43.28223
$15\ H^+ + 3\ Be^{2+} + 6\ (PO_4)^{3-} \rightleftharpoons$ **$Be_3H_{15}(PO_4)_6^{3+}$**	108.14599		1	$Be_3H_{17}L_6$ ⇌ $Be_3H_{15}L_6$ + 2 H $log_{10}(\beta)$ = -10.06 I = 3.0 M 3 Be + 17 H + 6 L ⇌ $Be_3H_{17}L_6$ $log_{10}(\beta)$ = 127.93422 I = 3.0 M 3 Be + 15 H + 6 L ⇌ $Be_3H_{15}L_6$ $log_{10}(\beta)$ = 117.87422 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 108.14599
$17\ H^+ + 3\ Be^{2+} + 6\ (PO_4)^{3-} \rightleftharpoons$ **$Be_3H_{17}(PO_4)_6^{5+}$**	120.09759		1	3 Be + 6 H_3L ⇌ $Be_3H_{17}L_6$+ H $log_{10}(\beta)$ = -12.12 I = 3.0 M 18 H + 6 L ⇌ 6 H_3L $log_{10}(\beta)$ = 140.05422 I = 3.0 M 3 Be + 17 H + 6 L ⇌ $Be_3H_{17}L_6$ $log_{10}(\beta)$ = 127.93422 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 120.09759
$18\ H^+ + 3\ Be^{2+} + 8\ (PO_4)^{3-} \rightleftharpoons$ **$Be_3H_{18}(PO_4)_8$ *(aq)***	174.52730		1	3 Be + 8 H_3L ⇌ $Be_3H_{18}L_8$ + 6 H $log_{10}(\beta)$ = 1.57 I = 3.0 M 24 H + 8 L ⇌ 8 H_3L $log_{10}(\beta)$ = 186.73896 I = 3.0 M 3 Be + 18 H + 8 L ⇌ $Be_3H_{18}L_8$ $log_{10}(\beta)$ = 188.30896 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 174.52730
$Na^+ + (PO_4)^{3-} \rightleftharpoons$ **$Na(PO_4)^{2-}$**	1.43	8E+3	1	
$H^+ + Na^+ + (PO_4)^{3-} \rightleftharpoons$ **$NaH(PO_4)^-$**	13.445		1	Na + HL ⇌ NaHL $log_{10}(\beta)$ = 1.07 H + L ⇌ HL $log_{10}(\beta)$ = 12.375 Na + H + L ⇌ NaHL $log_{10}(\beta)$ = 13.445
$2\ H^+ + Na^+ + (PO_4)^{3-} \rightleftharpoons$ **$NaH_2(PO_4)$ *(aq)***	19.873		1	Na + H_2L ⇌ NaH_2L $log_{10}(\beta)$ = 0.3 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 19.573 Na + 2 H + L ⇌ NaH_2L $log_{10}(\beta)$ = 19.873
$2\ Na^+ + (PO_4)^{3-} \rightleftharpoons$ **$Na_2(PO_4)^-$**	1.16		1	

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + 2\ Na^+ + (PO_4)^{3-} \rightleftharpoons$ **$Na_2H(PO_4)$ *(aq)***	13.32		1	$Na_2L + H \rightleftharpoons Na_2HL$ $\log_{10}(\beta) = 10.73$ $NaL + Na \rightleftharpoons Na_2L$ $\log_{10}(\beta) = 1.16$ $Na + L \rightleftharpoons NaL$ $\log_{10}(\beta) = 1.43$ $2\ Na + H + L \rightleftharpoons Na_2HL$ $\log_{10}(\beta) = 13.32$
$Mg^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Mg(PO_4)^-$**	4.85		2	
$H^+ + Mg^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$MgH(PO_4)$ *(aq)***	15.175	-3E+3	1	$Mg + HL \rightleftharpoons MgHL$ $\log_{10}(\beta) = 2.80$ ΔH = 1.2E+4 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ ΔH = -1.5E+4 $Mg + H + L \rightleftharpoons Mg\ iHL$ $\log_{10}(\beta) = 15.175$ ΔH = -3E+3
$2\ H^+ + Mg^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$MgH_2(PO_4)^+$**	19.19254		1	$Mg + H_2L \rightleftharpoons MgH_2L$ $\log_{10}(\beta) = 0.16$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Mg + 2\ H + L \rightleftharpoons MgH_2L$ $\log_{10}(\beta) = 21.08414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.19254$
$3\ H^+ + Mg^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$MgH_3(PO_4)_2^-$**	34.25554		1	$Mg(H_2L)_2 \rightleftharpoons MgH_3L_2 + H$ $\log_{10}(\beta) = -4.99$ I = 3.0 M $Mg + 4\ H + 2\ L \rightleftharpoons Mg(H_2L)_2$ $\log_{10}(\beta) = 42.48828$ I = 3.0 M $Mg + 3\ H + 2\ L \rightleftharpoons MgH_3L_2$ $\log_{10}(\beta) = 37.49828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 34.25554$
$4\ H^+ + Mg^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$MgH_4(PO_4)_2$ *(aq)***	38.97531		1	$Mg + 2\ H_2L \rightleftharpoons Mg(H_2L)_2$ $\log_{10}(\beta) = 0.64$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Mg + 4\ H + 2\ L \rightleftharpoons Mg(H_2L)_2$ $\log_{10}(\beta) = 42.48828$ I = 3.0 M I = 0 M: $\log_{10}(\beta)$ =38.97531
$Al^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Al(PO_4)$ *(aq)***	17.46087		1	Original data for β: log10(β) = 15.32, at I = 0.15 M at 37°C.
$H^+ + Al^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$AlH(PO_4)^+$**	20.01271		1	$Al + HL \rightleftharpoons AlHL$ $\log_{10}(\beta) = 6.12$ I = 0.2 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.61615$ I = 0.2 M $Al + H + L \rightleftharpoons AlHL$ $\log_{10}(\beta) = 17.73615$ I = 0.2 M I = 0 M: $\log_{10}(\beta) = 20.01271$
$2\ H^+ + Al^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$AlH_2(PO_4)^{2+}$**	20.78231		1	$Al + H_2L \rightleftharpoons AlH_2L$ $\log_{10}(\beta) = 2.02$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Li + 2\ H + L \rightleftharpoons LiH_2L$ $\log_{10}(\beta) = 22.94414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 20.78231$
$4\ H^+ + Al^{3+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$AlH_4(PO_4)_2^+$**	42.61485		1	$Al + 2\ H_2L \rightleftharpoons Al(H_2L)_2$ $\log_{10}(\beta) = 4.82$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Al + 4\ H + 2\ L \rightleftharpoons AlH_4L_2$ $\log_{10}(\beta) = 46.66828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 42.61485$
$2\ Al^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Al_2(PO_4)^{3+}$**	18.97656		1	Original data for β: log10(β) = 16.7, at I = 0.2 M
$2\ Al^{3+} + (OH)^- + (PO_4)^{3-} \rightleftharpoons$ **$Al_2(PO_4)(OH)^{2+}$**	31.03947		1	$Al_2L \rightleftharpoons Al_2(OH)L + H$ $\log_{10}(\beta) = -2.44$ I = 0.2 M $2\ Al + L \rightleftharpoons Al_2L$ $\log_{10}(\beta) = 16.7$ I = 0.2 M $OH + H \rightleftharpoons H_2O$ $\log_{10}(\beta) = 13.74405$ I = 0.2 M $2\ Al + OH + L \rightleftharpoons Al_2(OH)L$ $\log_{10}(\beta) = 28.00405$ I = 0.2 M I=0: 31.03947
$2\ Al^{3+} + 2\ (OH)^- + (PO_4)^{3-} \rightleftharpoons$ **$Al_2(PO_4)(OH)_2^+$**	40.93942		1	$Al_2L \rightleftharpoons Al_2(OH)_2L + 2\ H$ $\log_{10}(\beta) = -6.79$ I = 0.2 M $2\ Al + L \rightleftharpoons Al_2L$ $\log_{10}(\beta) = 16.7$ I = 0.2 M $2\ OH + 2\ H \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.48810$ I = 0.2 M $2\ Al + 2\ OH + L \rightleftharpoons Al_2(OH)_2L$ $\log_{10}(\beta) = 37.39810$ I = 0.2 M I = 0 M: $\log_{10}(\beta) = 40.93942$

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$K^+ + (PO_4)^{3-} \rightleftharpoons$ **$K(PO_4)^{2-}$**	1.43	1.5E+4	1	
$H^+ + K^+ + (PO_4)^{3-} \rightleftharpoons$ **$KH(PO_4)^-$**	13.255		1	$K + HL \rightleftharpoons KHL$ $\log_{10}(\beta) = 0.88$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ $K + H + L \rightleftharpoons KHL$ $\log_{10}(\beta) = 13.255$
$2\ H^+ + K^+ + (PO_4)^{3-} \rightleftharpoons$ **$KH_2(PO_4)$ *(aq)***	19.873		1	$K + H_2L \rightleftharpoons KH_2L$ $\log_{10}(\beta) = 0.3$ $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $K + 2\ H + L \rightleftharpoons KH_2L$ $\log_{10}(\beta) = 19.873$
$2\ K^+ + (PO_4)^{3-} \rightleftharpoons$ **$K_2(PO_4)^-$**	0.83		1	
$H^+ + 2\ K^+ + (PO_4)^{3-} \rightleftharpoons$ **$K_2H(PO_4)$ *(aq)***	13.44		1	$K_2L + H \rightleftharpoons K_2HL$ $\log_{10}(\beta) = 11.24$ $KL + K \rightleftharpoons K_2L$ $\log_{10}(\beta) = 0.83$ $K + L \rightleftharpoons KL$ $\log_{10}(\beta) = 1.37$ $2\ K + H + L \rightleftharpoons K_2HL$ $\log_{10}(\beta) = 13.44$
$Ca^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Ca(PO_4)^-$**	6.46		2	
$H^+ + Ca^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$CaH(PO_4)$ *(aq)***	15.035	-3E+3	1	$Ca + HL \rightleftharpoons CaHL$ $\log_{10}(\beta) = 2.66$ ΔH = 1.2E+4 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ ΔH = -1.5E+4 $Ca + H + L \rightleftharpoons CaHL$ $\log_{10}(\beta) = 15.035$ ΔH = -3E+3
$2\ H^+ + Ca^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$CaH_2(PO_4)^+$**	20.923	-6E+3	1	$Ca + H_2L \rightleftharpoons CaH_2L$ $\log_{10}(\beta) = 1.35$ ΔH = 1.2E+4 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ ΔH = -1.8E+4 $Ca + 2\ H + L \rightleftharpoons CaH_2L$ $\log_{10}(\beta) = 20.923$ ΔH = -6E+3
$4\ H^+ + Ca^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$CaH_4(PO_4)_2$ *(aq)***	39.00531		1	$Ca + 2\ H_2L \rightleftharpoons Ca(H_2L)_2$ $\log_{10}(\beta) = 0.67$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Ca + 4\ H + 2\ L \rightleftharpoons Ca(H_2L)_2$ $\log_{10}(\beta) = 42.51828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 39.00531$
$H^+ + Cr(III)^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Cr(III)H(PO_4)^+$**	16.21645		1	$Cr(III) + HL \rightleftharpoons Cr(III)HL$ $\log_{10}(\beta) = 2.56$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Cr(III) + H + L \rightleftharpoons Cr(III)HL$ $\log_{10}(\beta) = 14.29427$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 16.21645$
$H^+ + Mn(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Mn(II)H(PO_4)$ *(aq)***	15.80430		1	When using tetraalkyl ammonium salt as background electrolyte, the $\log_{10}(\beta)$ of the first equilbrium reaction is 2.70; when using Na-salt as background electrolyte, the $\log_{10}(\beta)$ of the first equilbrium reaction is 2.45. The average log-value of 2.575 was used here. $Mn(II) + HL \rightleftharpoons Mn(II)HL$ $\log_{10}(\beta) = 2.575$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Mn(II) + H + L \rightleftharpoons Mn(II)HL$ $\log_{10}(\beta) = 14.30927$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 15.80430$
$H^+ + Fe(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Fe(II)H(PO_4)$ *(aq)***	13.75409		1	$Fe(II) + HL \rightleftharpoons Fe(II)HL$ $\log_{10}(\beta) = 2.46$ I = 3.0 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 13.18569$ I = 3.0 M $Fe(II) + H + L \rightleftharpoons Fe(II)HL$ $\log_{10}(\beta) = 15.64569$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 13.75409$
$2\ H^+ + Fe(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Fe(II)H_2(PO_4)^+$**	19.58254		1	$Fe(II) + H_2L \rightleftharpoons Fe(II)H_2L$ $\log_{10}(\beta) = 0.55$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Fe(II) + 2\ H + L \rightleftharpoons Fe(II)H_2L$ $\log_{10}(\beta) = 21.47414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.58254$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ H^+ + Fe(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$Fe(II)H_3(PO_4)_2^-$**	35.13554		1	$Fe(II)(H_2L)_2 \rightleftharpoons Fe(II)H_2L_3 + H$ $\log_{10}(\beta) = -5.29$ I = 3.0 M $Fe(II) + 4\ H + 2\ L \rightleftharpoons Fe(II)(H_2L)_2$ $\log_{10}(\beta) = 43.66828$ I = 3.0 M $Fe(II) + 3\ H + 2\ L \rightleftharpoons Fe(II)H_3L_2$ $\log_{10}(\beta) = 38.37828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 35.13554$
$4\ H^+ + Fe(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$Fe(II)H_4(PO_4)_2$ *(aq)***	40.15531		1	$Fe(II) + 2\ H_2L \rightleftharpoons Fe(II)(H_2L)_2$ $\log_{10}(\beta) = 1.82$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Fe(II) + 4\ H + 2\ L \rightleftharpoons Fe(II)(H_2L)_2$ $\log_{10}(\beta) = 43.66828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 40.15531$
$H^+ + Fe(III)^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Fe(III)H(PO_4)^+$**	22.28533		1	$Fe(III) + HL \rightleftharpoons Fe(III)HL$ $\log_{10}(\beta) = 8.30$ I = 0.5 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.56984$ I = 0.5 M $Fe(III) + H + L \rightleftharpoons Fe(III)HL$ $\log_{10}(\beta) = 19.86984$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 22.28533$
$2\ H^+ + Fe(III)^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Fe(III)H_2(PO_4)^{2+}$**	23.84817		1	$Fe(III) + H_2L \rightleftharpoons Fe(III)H_2L$ $\log_{10}(\beta) = 3.47$ I = 0.5 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 18.23106$ I = 0.5 M $Fe(III) + 2\ H + L \rightleftharpoons Fe(III)H_2L$ $\log_{10}(\beta) = 21.70106$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 23.84817$
$3\ H^+ + Fe(III)^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Fe(III)H_3(PO_4)^{3+}$**	24.98863		1	$Fe(III)H_2L + H \rightleftharpoons Fe(III)H_3L$ $\log_{10}(\beta) = 0.6$ I = 3.0 M $Fe(III) + 2\ H + L \rightleftharpoons Fe(III)H_2L$ $\log_{10}(\beta) = 26.01$ I = 3.0 M $Fe(III) + 3\ H + L \rightleftharpoons Fe(III)H_3L$ $\log_{10}(\beta) = 26.61$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 24.98863$
$4\ H^+ + Fe(III)^{3+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$Fe(III)H_4(PO_4)_2^+$**	43.82485		1	$Fe(III) + 2\ H_2L \rightleftharpoons Fe(III)(H_2L)_2$ $\log_{10}(\beta) = 6.03$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Fe(III) + 4\ H + 2\ L \rightleftharpoons Fe(III)(H_2L)_2$ $\log_{10}(\beta) = 47.87828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 43.82485$
$6\ H^+ + Fe(III)^{3+} + 3\ (PO_4)^{3-} \rightleftharpoons$ **$Fe(III)H_6(PO_4)_3$ *(aq)***	65.19762		1	$Fe(III) + 3\ H_2L \rightleftharpoons Fe(III)(H_2L)_3$ $\log_{10}(\beta) = 8.1$ I = 3.0 M $6\ H + 3\ L \rightleftharpoons 3\ H_2L$ $\log_{10}(\beta) = 62.77242$ I = 3.0 M $Fe(III) + 6\ H + 3\ L \rightleftharpoons Fe(III)(H_2L)_3$ $\log_{10}(\beta) = 70.87242$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 65.19762$
$H^+ + Co(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Co(II)H(PO_4)$ *(aq)***	15.4293		1	$Co(II) + HL \rightleftharpoons Co(II)HL$ $\log_{10}(\beta) = 2.20$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Co(II) + H + L \rightleftharpoons Co(II)HL$ $\log_{10}(\beta) = 13.93427$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 15.42930$
$2\ H^+ + Co(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Co(II)H_2(PO_4)^+$**	19.54254		1	$Co(II) + H_2L \rightleftharpoons Co(II)H_2L$ $\log_{10}(\beta) = 0.51$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Co(II) + 2\ H + L \rightleftharpoons Co(II)H_2L$ $\log_{10}(\beta) = 21.43414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.54254$
$4\ H^+ + Co(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$Co(II)H_4(PO_4)_2$ *(aq)***	39.36531		1	$Co(II) + 2\ H_2L \rightleftharpoons Co(II)(H_2L)_2$ $\log_{10}(\beta) = 1.03$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Co(II) + 4\ H + 2\ L \rightleftharpoons Co(II)(H_2L)_2$ $\log_{10}(\beta) = 42.87828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 39.36531$
$H^+ + Ni^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$NiH(PO_4)$ *(aq)***	15.32930		1	$Ni + HL \rightleftharpoons NiHL$ $\log_{10}(\beta) = 2.10$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Ni + H + L \rightleftharpoons NiHL$ $\log_{10}(\beta) = 13.83427$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 15.32930$

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + Ni^{2+} + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{NiH_2(PO_4)^+}$	20.50015		1	$Ni + H_2L \rightleftharpoons NiH_2L$ $\log_{10}(\beta)$ = 0.5 I = 0.1 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 18.50512 I = 0.1 M $Ni + 2\ H + L \rightleftharpoons NiH_2L$ $\log_{10}(\beta)$ = 19.00512 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.50015
$2\ H^+ + Cu(I)^+ + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(I)H_2(PO_4)}$ ***(aq)***	19.80277		1	$Cu(I) + H_2L \rightleftharpoons Cu(I)H_2L$ $\log_{10}(\beta)$ = 0.5 I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 20.92414 I = 3.0 M $Cu(I) + 2\ H + L \rightleftharpoons Cu(I)H_2L$ $\log_{10}(\beta)$ = 21.42414 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 19.80277
$4\ H^+ + Cu(I)^+ + 2\ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(I)H_4(PO_4)_2^-}$	40.35577		1	$Cu(I) + 2\ H_2L \rightleftharpoons Cu(I)(H_2L)_2$ $\log_{10}(\beta)$ = 1.48 I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta)$ = 41.84828 I = 3.0 M $Cu(I) + 4\ H + 2\ L \rightleftharpoons Cu(I)(H_2L)_2$ $\log_{10}(\beta)$ = 43.32828 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 40.35577
$H^+ + Cu(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(II)H(PO_4)}$ ***(aq)***	16.49930		1	$Cu(II) + HL \rightleftharpoons Cu(II)HL$ $\log_{10}(\beta)$ = 3.27 I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 11.73427 I = 0.1 M $Cu(II) + H + L \rightleftharpoons Cu(II)HL$ $\log_{10}(\beta)$ = 15.00427 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 16.49930
$2\ H^+ + Cu(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(II)H_2(PO_4)^+}$	19.67254		1	$Cu(II) + H_2L \rightleftharpoons Cu(II)H_2L$ $\log_{10}(\beta)$ = 0.64 I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 20.92414 I = 3.0 M $Cu(II) + 2\ H + L \rightleftharpoons Cu(II)H_2L$ $\log_{10}(\beta)$ = 21.56414 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 19.67254
$2\ H^+ + Cu(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(II)H_2(PO_4)_2^{2-}}$	31.57599		1	$Cu(II)H_3L_2 \rightleftharpoons Cu(II)H_2L_2 + H$ $\log_{10}(\beta)$ = -4.8 I = 3.0 M $Cu(II) + 3\ H + 2\ L \rightleftharpoons Cu(II)H_3L_2$ $\log_{10}(\beta)$ = 39.07828 I = 3.0 M $Cu(II) + 2\ H + 2\ L \rightleftharpoons Cu(II)H_2L_2$ $\log_{10}(\beta)$ = 34.27828 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 31.57599
$3\ H^+ + Cu(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(II)H_3(PO_4)_2^-}$	35.83554		1	$Cu(II)(H_2L)_2 \rightleftharpoons Cu(II)H_3L_2 + H$ $\log_{10}(\beta)$ = -3.80 I = 3.0 M $Cu(II) + 4\ H + 2\ L \rightleftharpoons Cu(II)(H_2L)_2$ $\log_{10}(\beta)$ = 42.87828 I = 3.0 M $Cu(II) + 3\ H + 2\ L \rightleftharpoons Cu(II)H_3L_2$ $\log_{10}(\beta)$ = 39.07828 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 35.83554
$4\ H^+ + Cu(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{Cu(II)H_4(PO_4)_2}$ ***(aq)***	39.36531		1	$Cu(II) + 2\ H_2L \rightleftharpoons Cu(II)(H_2L)_2$ $\log_{10}(\beta)$ = 1.03 I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta)$ = 41.84828 I = 3.0 M $Cu(II) + 4\ H + 2\ L \rightleftharpoons Cu(II)(H_2L)_2$ $\log_{10}(\beta)$ = 42.87828 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 39.36531
$H^+ + Zn^{2+} + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{ZnH(PO_4)}$ ***(aq)***	15.68930		1	$Zn + HL \rightleftharpoons ZnHL$ $\log_{10}(\beta)$ = 2.46 I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 11.73427 I = 0.1 M $Zn + H + L \rightleftharpoons ZnHL$ $\log_{10}(\beta)$ = 14.19427 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 15.68930
$2\ H^+ + Zn^{2+} + (PO_4)^{3-} \rightleftharpoons$ $\mathbf{ZnH_2(PO_4)^+}$	19.40254		1	$Zn + H_2L \rightleftharpoons ZnH_2L$ $\log_{10}(\beta)$ = 0.37 I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 20.92414 I = 3.0 M $Zn + 2\ H + L \rightleftharpoons ZnH_2L$ $\log_{10}(\beta)$ = 21.29414 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 19.40254
$H^+ + Zn^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ $\mathbf{ZnH(PO_4)_2^{3-}}$	27.09668		1	$ZnH_2L_2 \rightleftharpoons ZnHL_2 + H$ $\log_{10}(\beta)$ = -5.76 I = 3.0 M $Zn + 2\ H + 2\ L \rightleftharpoons ZnH_2L_2$ $\log_{10}(\beta)$ = 34.74828 I = 3.0 M $Zn + H + 2\ L \rightleftharpoons ZnHL_2$ $\log_{10}(\beta)$ = 28.98828 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 27.09668

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + Zn^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$ZnH_2(PO_4)_2^{2-}$**	32.04599		1	$ZnH_3L_2 \rightleftharpoons ZnH_2L_2 + H$ $log_{10}(\beta) = -3.3$ I = 3.0 M $Zn + 3\ H + 2\ L \rightleftharpoons ZnH_3L_2$ $log_{10}(\beta) = 38.04828$ I = 3.0 M $Zn + 2\ H + 2\ L \rightleftharpoons ZnH_2L_2$ $log_{10}(\beta) = 34.74828$ I = 3.0 M I = 0 M: $log_{10}(\beta) = 32.04599$
$3\ H^+ + Zn^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$ZnH_3(PO_4)_2^-$**	34.80554		1	$Zn(H_2L)_2 \rightleftharpoons ZnH_3L_2 + H$ $log_{10}(\beta) = -4.90$ I = 3.0 M $Zn + 4\ H + 2\ L \rightleftharpoons Zn(H_2L)_2$ $log_{10}(\beta) = 42.87828$ I = 3.0 M $Zn + 3\ H + 2\ L \rightleftharpoons ZnH_3L_2$ $log_{10}(\beta) = 38.04828$ I = 3.0 M I = 0 M: $log_{10}(\beta) = 34.80554$
$4\ H^+ + Zn^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$ZnH_4(PO_4)_2$ *(aq)***	39.43531		1	$Zn + 2\ H_2L \rightleftharpoons Zn(H_2L)_2$ $log_{10}(\beta) = 1.10$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $log_{10}(\beta) = 41.84828$ I = 3.0 M $Zn + 4\ H + 2\ L \rightleftharpoons Zn(H_2L)_2$ $log_{10}(\beta) = 42.94828$ I = 3.0 M I = 0 M: $log_{10}(\beta) = 39.43531$
$H^+ + Ga^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$GaH(PO_4)^+$**	20.76396		1	$Ga + HL \rightleftharpoons GaHL$ $log_{10}(\beta) = 7.26$ I = 1.0 M $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 11.67552$ I = 1.0 M $Ga + H + L \rightleftharpoons GaHL$ $log_{10}(\beta) = 18.93552$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 20.76396$
$2\ H^+ + Ga^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$GaH_2(PO_4)^{2+}$**	21.66248		1	$Ga + H_2L \rightleftharpoons GaH_2L$ $log_{10}(\beta) = 1.48$ I = 1.0 M $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 18.55720$ I = 1.0 M $Ga + 2\ H + L \rightleftharpoons GaH_2L$ $log_{10}(\beta) = 20.03720$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 21.66248$
$Sr^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Sr(PO_4)^-$**	5.5		3	
$H^+ + Sr^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$SrH(PO_4)$ *(aq)***	14.73930		1	When using tetraalkyl ammonium salt as background electrolyte, the $log_{10}(\beta)$ of the first equilbrium reaction is 1.64; when using Na-salt as background electrolyte, the $log_{10}(\beta)$ of the first equilbrium reaction is 1.38. The average log-value of 1.51 was used here. $Sr + HL \rightleftharpoons SrHL$ $log_{10}(\beta) = 1.51$ I = 0.1 M $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 11.73427$ I = 0.1 M $Sr + H + L \rightleftharpoons SrHL$ $log_{10}(\beta) = 13.24427$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 14.73930$
$2\ H^+ + Sr^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$SrH_2(PO_4)^+$**	20.40015		1	$Sr + H_2L \rightleftharpoons SrH_2L$ $log_{10}(\beta) = 0.4$ I = 0.1 M (Original data for β at T = 20°C) $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 18.50512$ I = 0.1 M $Sr + 2\ H + L \rightleftharpoons SrH_2L$ $log_{10}(\beta) = 18.90512$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 20.40015$
$2\ H^+ + Y^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$YH_2(PO_4)^{2+}$**	22.223		1	$Y + H_2L \rightleftharpoons YH_2L$ $log_{10}(\beta) = 2.65$ $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 19.573$ $Y + 2\ H + L \rightleftharpoons YH_2L$ $log_{10}(\beta) = 22.223$
$H^+ + Ag^+ + (PO_4)^{3-} \rightleftharpoons$ **$AgH(PO_4)^-$**	14.013		1	$AgH_2L \rightleftharpoons AgHL + H$ $log_{10}(\beta) = -5.39$ I = 3.0 M $Ag + 2\ H + L \rightleftharpoons AgH_2L$ $log_{10}(\beta) = 20.75414$ I = 3.0 M $Ag + H + L \rightleftharpoons AgHL$ $log_{10}(\beta) = 15.36414$ I = 3.0 M I = 0 M: $log_{10}(\beta) = 14.01300$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + Ag^+ + (PO_4)^{3-} \rightleftharpoons$ **$AgH_2(PO_4)$ *(aq)***	19.13277		1	$Ag + H_2L \rightleftharpoons AgH_2L$ $\log_{10}(\beta) = -0.17$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Ag + 2\ H + L \rightleftharpoons AgH_2L$ $\log_{10}(\beta) = 20.75414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.13277$
$4\ H^+ + Ag^+ + 2\ (PO_4)^{3-} \rightleftharpoons$ **$AgH_4(PO_4)_2^-$**	38.77577		1	$Ag + 2\ H_2L \rightleftharpoons Ag(H_2L)_2$ $\log_{10}(\beta) = -0.1$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Ag + 4\ H + 2\ L \rightleftharpoons Ag(H_2L)_2$ $\log_{10}(\beta) = 41.74828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 38.77577$
$H^+ + Cd^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$CdH(PO_4)$ *(aq)***	16.07930		1	$Cd + HL \rightleftharpoons CdHL$ $\log_{10}(\beta) = 2.85$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Cd + H + L \rightleftharpoons CdHL$ $\log_{10}(\beta) = 14.58427$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 16.07930$
$2\ H^+ + Cd^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$CdH_2(PO_4)^+$**	19.79254		1	$Cd + H_2L \rightleftharpoons CdH_2L$ $\log_{10}(\beta) = 0.76$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Cd + 2\ H + L \rightleftharpoons CdH_2L$ $\log_{10}(\beta) = 21.68414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.79254$
$2\ H^+ + Cd^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$CdH_2(PO_4)_2^{2-}$**	30.45599		1	$CdH_3L_2 \rightleftharpoons CdH_2L_2 + H$ $\log_{10}(\beta) = -5.67$ I = 3.0 M $Cd + 3\ H + 2\ L \rightleftharpoons CdH_3L_2$ $\log_{10}(\beta) = 38.82828$ I = 3.0 M $Cd + 2\ H + 2\ L \rightleftharpoons CdH_2L_2$ $\log_{10}(\beta) = 33.15828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 30.45599$
$3\ H^+ + Cd^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$CdH_3(PO_4)_2^-$**	35.58554		1	$Cd(H_2L)_2 \rightleftharpoons CdH_3L_2 + H$ $\log_{10}(\beta) = -4.03$ I = 3.0 M $Cd + 4\ H + 2\ L \rightleftharpoons Cd(H_2L)_2$ $\log_{10}(\beta) = 42.85828$ I = 3.0 M $Cd + 3\ H + 2\ L \rightleftharpoons CdH_3L_2$ $\log_{10}(\beta) = 38.82828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 35.58554$
$4\ H^+ + Cd^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons$ **$CdH_4(PO_4)_2$ *(aq)***	39.34531		1	$Cd + 2\ H_2L \rightleftharpoons Cd(H_2L)_2$ $\log_{10}(\beta) = 1.01$ I = 3.0 M $4\ H + 2\ L \rightleftharpoons 2\ H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Cd + 4\ H + 2\ L \rightleftharpoons Cd\ (H_2L)_2$ $\log_{10}(\beta) = 42.85828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 39.34531$
$2\ H^+ + In^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$InH_2(PO_4)^{2+}$**	22.61248		1	$In + H_2L \rightleftharpoons InH_2L$ $\log_{10}(\beta) = 2.43$ I = 1.0 M (Original data for β at T = 20°C) $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 18.55720$ I = 1.0 M $In + 2\ H + L \rightleftharpoons InH_2L$ $\log_{10}(\beta) = 20.98700$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 22.61248$
$H^+ + Ba^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$BaH(PO_4)$ *(aq)***	14.58930		1	$Ba + HL \rightleftharpoons BaHL$ $\log_{10}(\beta) = 1.36$ I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 11.73427$ I = 0.1 M $Ba + H + L \rightleftharpoons BaHL$ $\log_{10}(\beta) = 13.09427$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 14.58930$
$2\ H^+ + Ba^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$BaH_2(PO_4)^+$**	19.03254		1	$Ba + H_2L \rightleftharpoons BaH_2L$ $\log_{10}(\beta) = 0.00$ I = 3.0 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M $Ba + 2\ H + L \rightleftharpoons BaH_2L$ $\log_{10}(\beta) = 20.92414$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 19.03254$

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$4 H^+ + Ba^{2+} + 2 (PO_4)^{3-} \rightleftharpoons$ **$BaH_4(PO_4)_2$ *(aq)***	38.32531		1	$Ba + 2 H_2L \rightleftharpoons Ba(H_2L)_2$ $\log_{10}(\beta) = -0.01$ I = 3.0 M $4 H + 2 L \rightleftharpoons 2 H_2L$ $\log_{10}(\beta) = 41.84828$ I = 3.0 M $Ba + 4 H + 2 L \rightleftharpoons Ba(H_2L)_2$ $\log_{10}(\beta) = 41.83828$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 38.32531$
$2 H^+ + La^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$LaH_2(PO_4)^{2+}$**	21.98817		1	$La + H_2L \rightleftharpoons LaH_2L$ $\log_{10}(\beta) = 1.61$ I = 0.5 M $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 18.23106$ I = 0.5 M $La + 2 H + L \rightleftharpoons LaH_2L$ $\log_{10}(\beta) = 19.84106$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 21.98817$
$Ce^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Ce(PO_4)$ *(aq)***	11.73		1	
$2 H^+ + Ce^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$CeH_2(PO_4)^{2+}$**	21.903		1	$Ce + H_2L \rightleftharpoons CeH_2L$ $\log_{10}(\beta) = 2.33$ $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $Ce + 2 H + L \rightleftharpoons CeH_2L$ $\log_{10}(\beta) = 21.903$
$2 H^+ + Pm^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$PmH_2(PO_4)^{2+}$**	22.083		1	$Pm + H_2L \rightleftharpoons PmH_2L$ $\log_{10}(\beta) = 2.51$ $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $Pm + 2 H + L \rightleftharpoons PmH_2L$ $\log_{10}(\beta) = 22.083$
$Gd^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$Gd(PO_4)$ *(aq)***	12.19		1	
$H^+ + Gd^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$GdH(PO_4)^+$**	18.285		1	$Gd + HL \rightleftharpoons GdHL$ $\log_{10}(\beta) = 5.91$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ $Gd + H + L \rightleftharpoons GdHL$ $\log_{10}(\beta) = 18.285$
$2 H^+ + Gd^{3+} + (PO_4)^{3-} \rightleftharpoons$ **$GdH_2(PO_4)^{2+}$**	22.313		1	$Gd + H_2L \rightleftharpoons GdH_2L$ $\log_{10}(\beta) = 2.74$ $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $Gd + 2 H + L \rightleftharpoons GdH_2L$ $\log_{10}(\beta) = 22.313$
$2 H^+ + Gd^{3+} + 2 (PO_4)^{3-} \rightleftharpoons$ **$GdH_2(PO_4)_2^-$**	34.72		1	$Gd + 2 HL \rightleftharpoons GdH_2L_2$ $\log_{10}(\beta) = 9.97$ $2 H + 2 L \rightleftharpoons 2 HL$ $\log_{10}(\beta) = 24.750$ $Gd + 2 H + 2 L \rightleftharpoons GdH_2L_2$ $\log_{10}(\beta) = 34.720$
$Hg(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Hg(II)(PO_4)^-$**	12.37863		1	Original data for β: $\log_{10}(\beta) = 14.0$, at I = 3.0 M.
$H^+ + Hg(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Hg(II)H(PO_4)$ *(aq)***	20.09409		1	$Hg(II) + HL \rightleftharpoons Hg(II)HL$ $\log_{10}(\beta) = 8.8$ I = 3.0 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 13.18569$ I = 3.0 M $Hg(II) + H + L \rightleftharpoons Hg(II)HL$ $\log_{10}(\beta) = 21.98569$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 20.09409$
$H^+ + Pb(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Pb(II)H(PO_4)$ *(aq)***	15.475		1	$Pb(II) + HL \rightleftharpoons Pb(II)HL$ $\log_{10}(\beta) = 3.1$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ $Pb(II) + H + L \rightleftharpoons Pb(II)HL$ $\log_{10}(\beta) = 15.475$
$2 H^+ + Pb(II)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$Pb(II)H_2(PO_4)^+$**	21.073		1	$Pb(II) + H_2L \rightleftharpoons Pb(II)H_2L$ $\log_{10}(\beta) = 1.5$ $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $Pb(II) + 2 H + L \rightleftharpoons Pb(II)H_2L$ $\log_{10}(\beta) = 21.073$
$(U(VI)O_2)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$(U(VI)O_2)(PO_4)^-$**	13.25		1	
$H^+ + (U(VI)O_2)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$(U(VI)O_2)H(PO_4)$ *(aq)***	19.575		1	$(UO_2) + HL \rightleftharpoons (UO_2)HL$ $\log_{10}(\beta) = 7.2$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ $(UO_2) + H + L \rightleftharpoons (UO_2)HL$ $\log_{10}(\beta) = 19.575$
$2 H^+ + (U(VI)O_2)^{2+} + (PO_4)^{3-} \rightleftharpoons$ **$(U(VI)O_2)H_2(PO_4)^+$**	22.833		1	$(UO_2) + H_2L \rightleftharpoons (UO_2)H_2L$ $\log_{10}(\beta) = 3.26$ $2 H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 19.573$ $(UO_2) + 2 H + L \rightleftharpoons (UO_2)H_2L$ $\log_{10}(\beta) = 22.833$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 H^+ + $(U(VI)O_2)^{2+}$ + $(PO_4)^{3-}$ ⇌ **$(U(VI)O_2)H_3(PO_4)^{2+}$**	23.633		1	$(UO_2)H_2L$ + H ⇌ $(UO_2)H_2L$ $log_{10}(\beta)$ = 0.8 (UO_2) + 2 H + L ⇌ $(UO_2)H_2L$ $log_{10}(\beta)$ = 22.833 (UO_2) + 3 H + L ⇌ $(UO_2)H_3L$ $log_{10}(\beta)$ = 23.633

2.2.10. Sulfide

The formula for the ligand sulfide is S^{2-}; the molecular weight is 32.06.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + S^{2-} ⇌ **HS^-**	13.9		3	
2 H^+ + S^{2-} ⇌ **H_2S *(aq)***	20.92	-2.2E+4	1	H + L ⇌ HL $log_{10}(\beta)$ = 13.9 HL + H ⇌ H_2L $log_{10}(\beta)$ = 7.02 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 20.92
H^+ + Na^+ + S^{2-} ⇌ **NaHS *(aq)***	13.1		1	Na + HL ⇌ NaHL $log_{10}(\beta)$ = -0.8 H + L ⇌ HL $log_{10}(\beta)$ = 13.9 Na + H + L ⇌ NaHL $log_{10}(\beta)$ = 13.1
Zn^{2+} + S^{2-} ⇌ **ZnS *(aq)***	19.30632		1	Zn + HL ⇌ ZnHL $log_{10}(\beta)$ = 5.0 I = 1.0 M H + L ⇌ HL $log_{10}(\beta)$ = 13.49368 I = 1.0 M Zn + H + L ⇌ ZnHL $log_{10}(\beta)$ = 18.49368 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 19.30632
Ag^+ + S^{2-} ⇌ **AgS^-**	19.2		1	AgHL ⇌ AgL + H $log_{10}(\beta)$ = -8.3 I = 0.1 M (Original data for β at T = 20°C) Ag + H + L ⇌ AgHL $log_{10}(\beta)$ = 27.07285 I = 0.1 M Ag + L ⇌ AgL $log_{10}(\beta)$ = 18.77285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.2
H^+ + Ag^+ + S^{2-} ⇌ **AgHS *(aq)***	27.71358		1	Ag + HL ⇌ AgHL $log_{10}(\beta)$ = 13.6 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 13.47285 I = 0.1 M Ag + H + L ⇌ AgHL $log_{10}(\beta)$ = 27.07285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 27.71358
H^+ + Ag^+ + 2 S^{2-} ⇌ **$AgHS_2^{2-}$**	35.78643		1	AgH_2L_2 ⇌ $AgHL_2$ + H $log_{10}(\beta)$ = -9.5 I = 0.1 M (Original data for β at T = 20°C) Ag + 2 H + 2 L ⇌ AgH_2L_2 $log_{10}(\beta)$ = 44.64570 I = 0.1 M Ag + H + 2 L ⇌ $AgHL_2$ $log_{10}(\beta)$ = 35.14570 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 35.78643

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^{+} + Ag^{+} + 2\ S^{2-} \rightleftharpoons$ $\mathbf{AgH_2S_2^{-}}$	45.71358		1	$Ag + 2\ HL \rightleftharpoons AgH_2L_2$, $log_{10}(\beta) = 17.7$, I = 0.1 M (Original data for β at T = 20°C) $2\ H + 2\ L \rightleftharpoons 2\ HL$, $log_{10}(\beta) = 26.94570$, I = 0.1 M $Ag + 2\ H + 2\ L \rightleftharpoons AgH_2L_2$, $log_{10}(\beta) = 44.64570$, I = 0.1 M I = 0 M: $log_{10}(\beta) = 45.71358$
$Cd^{2+} + S^{2-} \rightleftharpoons$ **CdS *(aq)***	19.5		3	
$H^{+} + Cd^{2+} + S^{2-} \rightleftharpoons$ $\mathbf{CdHS^{+}}$	21.90632		1	$Cd + HL \rightleftharpoons CdHL$, $log_{10}(\beta) = 7.6$, I = 1.0 M $H + L \rightleftharpoons HL$, $log_{10}(\beta) = 13.49368$, I = 1.0 M $Cd + H + L \rightleftharpoons CdHL$, $log_{10}(\beta) = 21.09368$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 21.90632$
$2\ H^{+} + Cd^{2+} + 2\ S^{2-} \rightleftharpoons$ $\mathbf{CdH_2S_2}$ ***(aq)***	43.00948		1	$Cd + 2\ HL \rightleftharpoons CdH_2L_2$, $log_{10}(\beta) = 14.6$, I = 1.0 M $2\ H + 2\ L \rightleftharpoons 2\ HL$, $log_{10}(\beta) = 26.98736$, I = 1.0 M $Cd + 2\ H + 2\ L \rightleftharpoons CdH_2L_2$, $log_{10}(\beta) = 41.58736$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 43.00948$
$3\ H^{+} + Cd^{2+} + 3\ S^{2-} \rightleftharpoons$ $\mathbf{CdH_3S_3^{-}}$	58.80948		1	$Cd + 3\ HL \rightleftharpoons CdH_3L_3$, $log_{10}(\beta) = 16.5$, I = 1.0 M $3\ H + 3\ L \rightleftharpoons 3\ HL$, $log_{10}(\beta) = 40.48104$, I = 1.0 M $Cd + 3\ H + 3\ L \rightleftharpoons CdH_3L_3$, $log_{10}(\beta) = 56.98104$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 58.80948$
$4\ H^{+} + Cd^{2+} + 4\ S^{2-} \rightleftharpoons$ $\mathbf{CdH_4S_4^{2-}}$	74.90632		1	$Cd + 4\ HL \rightleftharpoons CdH_4L_4$, $log_{10}(\beta) = 18.9$, I = 1.0 M $4\ H + 4\ L \rightleftharpoons 4\ HL$, $log_{10}(\beta) = 53.97472$, I = 1.0 M $Cd + 4\ H + 4\ L \rightleftharpoons CdH_4L_4$, $log_{10}(\beta) = 72.87472$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 74.90632$
$H^{+} + In^{3+} + S^{2-} \rightleftharpoons$ $\mathbf{InHS^{2+}}$	25.50948		1	$In + HL \rightleftharpoons InHL$, $log_{10}(\beta) = 11$, I = 1.0 M (Original data for β at T = 20°C) $H + L \rightleftharpoons HL$, $log_{10}(\beta) = 13.49368$, I = 1.0 M $In + H + L \rightleftharpoons InHL$, $log_{10}(\beta) = 24.49368$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 25.50948$
$2\ H^{+} + In^{3+} + 2\ S^{2-} \rightleftharpoons$ $\mathbf{InH_2S_2^{+}}$	45.81580		1	$In + 2\ HL \rightleftharpoons InHL$, $log_{10}(\beta) = 17$, I = 1.0 M (Original data for β at T = 20°C) $2\ H + 2\ L \rightleftharpoons 2\ HL$, $log_{10}(\beta) = 26.98736$, I = 1.0 M $In + 2\ H + 2\ L \rightleftharpoons InH_2L_2$, $log_{10}(\beta) = 43.98736$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 45.81580$
$Hg(II)^{2+} + S^{2-} \rightleftharpoons$ **Hg(II)S *(aq)***	7.9		3	
$Hg(II)^{2+} + (OH)^{-} + S^{2-} \rightleftharpoons$ $\mathbf{Hg(II)S(OH)^{-}}$	18.5		3	
$Hg(II)^{2+} + 2\ S^{2-} \rightleftharpoons$ $\mathbf{Hg(II)S_2^{2-}}$	51.02		1	$Hg(II)HL_2 \rightleftharpoons Hg(II)L_2 + H$, $log_{10}(\beta) = -8.30$, I = 1.0 M (Original data for β for 20°C) $Hg(II) + H + 2\ L \rightleftharpoons Hg(II)HL_2$, $log_{10}(\beta) = 58.50736$, I = 1.0 M $Hg(II) + 2\ L \rightleftharpoons Hg(II)L_2$, $log_{10}(\beta) = 50.20736$, I = 1.0 M I = 0 M: $log_{10}(\beta) = 51.02$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Hg(II)^{2+} + 2\ S^{2-} \rightleftharpoons$ **$Hg(II)HS_2^-$**	59.72632		1	$Hg(II)H_2L_2 \rightleftharpoons Hg(II)HL_2 + H$ $\log_{10}(\beta) = -6.19$ I = 1.0 M (Original data for β for 20°C) $Hg(II) + 2\ H + 2\ L \rightleftharpoons Hg(II)H_2L_2$ $\log_{10}(\beta) = 64.69736$ I = 1.0 M $Hg(II) + H + 2\ L \rightleftharpoons Hg(II)HL_2$ $\log_{10}(\beta) = 58.50736$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 59.72632$
$2\ H^+ + Hg(II)^{2+} + 2\ S^{2-} \rightleftharpoons$ **$Hg(II)H_2S_2$ *(aq)***	66.11948		1	$Hg(II) + 2\ HL \rightleftharpoons Hg(II)H_2L_2$ $\log_{10}(\beta) = 37.71$ I = 1.0 M (Original data for β for 20°C) $2\ H + 2\ L \rightleftharpoons 2\ HL$ $\log_{10}(\beta) = 26.98736$ I = 1.0 M $Hg(II) + 2\ H + 2\ L \rightleftharpoons Hg(II)H_2L_2$ $\log_{10}(\beta) = 64.69736$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 66.11948$

2.2.11. Sulfite

The formula for the ligand sulfite is SO_3^{2-}; the molecular weight is 80.057.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (SO_3)^{2-} \rightleftharpoons$ **$H(SO_3)^-$**	7.19	3.6E+3	1	
$2\ H^+ + (SO_3)^{2-} \rightleftharpoons$ **$H_2(SO_3)$ *(aq)***	9.04	2.14E+4	1	$HL + H \rightleftharpoons H_2L$ $\log_{10}(\beta) = 1.85$ ΔH = 1.78E+4 $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 7.19$ ΔH = 3.6E+3 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 9.04$ ΔH = 2.14E+4
$2\ H^+ + 2\ (SO_3)^{2-} \rightleftharpoons$ **$H_2(SO_3)_2^{2-}$**	15.87	1.12E+4	1	$2\ HL \rightleftharpoons S_2O_5$ $\log_{10}(\beta) = 1.49$ ΔH = 4E+3 (Original data for ΔH at I = 2.0 M) $2\ H + 2\ L \rightleftharpoons 2\ HL$ $\log_{10}(\beta) = 14.38$ ΔH = 7.2E+3 $2\ H + 2\ L \rightleftharpoons S_2O_5$ $\log_{10}(\beta) = 15.87$ ΔH = 1.12E+4
$Na^+ + (SO_3)^{2-} \rightleftharpoons$ **$Na(SO_3)^-$**	0.82632		1	Original data for β: $\log_{10}(\beta) = 0.42$, at I = 1.0 M.
$Mg^{2+} + (SO_3)^{2-} \rightleftharpoons$ **$Mg(SO_3)$ *(aq)***	2.36		1	
$K^+ + (SO_3)^{2-} \rightleftharpoons$ **$K(SO_3)^-$**	0.62632		1	Original data for β: $\log_{10}(\beta) = 0.22$, at I = 1.0 M.
$Ca^{2+} + (SO_3)^{2-} \rightleftharpoons$ **$Ca(SO_3)$ *(aq)***	2.62		1	
$Mn(II)^{2+} + (SO_3)^{2-} \rightleftharpoons$ **$Mn(II)(SO_3)$ *(aq)***	3.00		1	
$Fe(III)^{3+} + (SO_3)^{2-} \rightleftharpoons$ **$Fe(III)(SO_3)^+$**	8.21033		1	Original data for β: $\log_{10}(\beta) = 6.6$, at I = 0.5 M at 20°C.
$Fe(III)^{3+} + (OH)^- + (SO_3)^{2-} \rightleftharpoons$ **$Fe(III)(SO_3)(OH)$ *(aq)***	20.18356		1	$Fe(III)(OH) + L \rightleftharpoons Fe(III)(OH)L$ $\log_{10}(\beta) = 7.3$ I = 0.5 M (Original data for β for 20°C) $Fe(III) + (OH) \rightleftharpoons Fe(III)(OH)$ $\log_{10}(\beta) = 11.00484$ I = 0.5 M $Fe(III) + (OH) + L \rightleftharpoons Fe(III)(OH)L$ $\log_{10}(\beta) = 18.30484$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 20.18356$
$Co(II)^{2+} + (SO_3)^{2-} \rightleftharpoons$ **$Co(II)(SO_3)$ *(aq)***	3.08		1	
$Co(II)^{2+} + 2\ (SO_3)^{2-} \rightleftharpoons$ **$Co(II)(SO_3)_2^{2-}$**	4.28225		1	Original data for β: $\log_{10}(\beta) = 4.34$, at I = 2.0 M.
$Co(II)^{2+} + 3\ (SO_3)^{2-} \rightleftharpoons$ **$Co(II)(SO_3)_3^{4-}$**	6.48		1	Original data for β: $\log_{10}(\beta) = 6.48$, at I = 2.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Ni^{2+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Ni(SO_3)}$ ***(aq)***	2.88		1	
$Cu(I)^{+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Cu(I)(SO_3)^{-}}$	8.25632		1	Original data for β: $log_{10}(\beta)$ = 7.85, at I = 1.0 M.
$Cu(I)^{+} + 2\ (SO_3)^{2-} \rightleftharpoons \mathbf{Cu(I)(SO_3)_2^{3-}}$	8.7		1	Original data for β: $log_{10}(\beta)$ = 8.7, at I = 1.0 M.
$Cu(I)^{+} + 3\ (SO_3)^{2-} \rightleftharpoons \mathbf{Cu(I)(SO_3)_3^{5-}}$	8.18104		1	Original data for β: $log_{10}(\beta)$ = 9.4, at I = 1.0 M.
$Cu(II)^{2+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Cu(II)(SO_3)}$ ***(aq)***	5.33355		1	Original data for β: $log_{10}(\beta)$ = 4.26, at I = 0.5 M at 20°C.
$Pd^{2+} + 4\ (SO_3)^{2-} \rightleftharpoons \mathbf{Pd(SO_3)_4^{6-}}$	27.10470		1	Original data for β: $log_{10}(\beta)$ = 29.1, at I = 0.7 M.
$Ag^{+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Ag(SO_3)^{-}}$	5.6		1	
$Ag^{+} + 2\ (SO_3)^{2-} \rightleftharpoons \mathbf{Ag(SO_3)_2^{3-}}$	8.68		1	
$Ag^{+} + 3\ (SO_3)^{2-} \rightleftharpoons \mathbf{Ag(SO_3)_3^{5-}}$	9		1	
$Cd^{2+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Cd(SO_3)}$ ***(aq)***	3.29		1	
$Cd^{2+} + 2\ (SO_3)^{2-} \rightleftharpoons \mathbf{Cd(SO_3)_2^{2-}}$	5.01264		1	Original data for β: $log_{10}(\beta)$ = 4.2, at I = 1.0 M.
$Ce^{3+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Ce(SO_3)^{+}}$	8.04		1	
$Pt(II)^{2+} + 4\ (SO_3)^{2-} \rightleftharpoons \mathbf{Pt(II)(SO_3)_4^{6-}}$	35.905		1	Original data for β: $log_{10}(\beta)$ = 37.9, at I = 0.7 M.
$Hg(II)^{2+} + 2\ (SO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(SO_3)_2^{2-}}$	23.40355	-8.3E+4	1	Original data for β: $log_{10}(\beta)$ = 22.33, at I = 0.5 M. Original data for ΔH at I = 0.5 M
$Hg(II)^{2+} + 3\ (SO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(SO_3)_3^{4-}}$	24.1		1	Original data for β: $log_{10}(\beta)$ = 24.1, at I = 0.5 M.
$(U(VI)O_2)^{2+} + (SO_3)^{2-} \rightleftharpoons \mathbf{(U(VI)O_2)(SO_3)}$ ***(aq)***	6.7		1	

2.2.12. Sulfate

The formula for the ligand sulfate is SO_4^{2-}; the molecular weight is 96.056.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + (NH_3)$ *(aq)* $+ (SO_4)^{2-} \rightleftharpoons \mathbf{H(SO_4)(NH_3)^{-}}$	10.274			$NH_4 + SO_4 \rightleftharpoons NH_4\ SO_4$ — $log_{10}(\beta)$ = 1.03 $NH_3 + H \rightleftharpoons NH_4$ — $log_{10}(\beta)$ = 9.244 $H + NH_3 + SO_4 \rightleftharpoons NH_4\ SO_4$ — $log_{10}(\beta)$ = 10.274
$2\ H^{+} + (H_2SiO_4)^{2-} + (SO_4)^{2-} \rightleftharpoons \mathbf{H_4SiO_4(SO_4)^{2-}}$	22.50	-5.9E+4	1	$Si(OH)_4 + SO_4 \rightleftharpoons Si(OH)_4\ SO_4$ — $log_{10}(\beta)$ = -0.54 — ΔH = 2E+3 $2\ H^{+} + (H_2SiO_4)^{2-} \rightleftharpoons H_2(H_2SiO_4)$ — $log_{10}(\beta)$ = 23.04 — ΔH = -6.1E+4 $2\ H^{+} + (H_2SiO_4)^{2-} + SO_4 \rightleftharpoons H_4SiO_4\ SO_4$ — $log_{10}(\beta)$ = 22.50 — ΔH = -5.9E+4
$H^{+} + (SO_4)^{2-} \rightleftharpoons \mathbf{H(SO_4)^{-}}$	1.99	2.2E+4	1	
$Li^{+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Li(SO_4)^{-}}$	0.64	0	1	
$Be^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Be(SO_4)}$ ***(aq)***	2.19	2.9E+4	1	
$Be^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons \mathbf{Be(SO_4)_2^{2-}}$	2.59264		1	Original data for β: $log_{10}(\beta)$ = 1.78, at I = 1.0 M.
$Be^{2+} + 3\ (SO_4)^{2-} \rightleftharpoons \mathbf{Be(SO_4)_3^{4-}}$	2.08		1	Original data for β: $log_{10}(\beta)$ = 2.08, at I = 1.0 M.
$Na^{+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Na(SO_4)^{-}}$	0.74	1E+3	1	
$Mg^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Mg(SO_4)}$ ***(aq)***	2.26	5.8E+3	1	
$Al^{3+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Al(SO_4)^{+}}$	3.89	2.8E+4	1	Original data for ΔH at I = 3.0 M.
$K^{+} + (SO_4)^{2-} \rightleftharpoons \mathbf{K(SO_4)^{-}}$	0.85	4.1E+3	1	
$Ca^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Ca(SO_4)}$ ***(aq)***	2.36	7.1E+3	1	
$Sc^{3+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Sc(SO_4)^{+}}$	4.18	3.1E+4	1	
$Sc^{3+} + 2\ (SO_4)^{2-} \rightleftharpoons \mathbf{Sc(SO_4)_2^{-}}$	5.6	5.4E+4	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cr(III)^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$Cr(III)(SO_4)^{+}$**	3.81896	3.1E+4	1	Original data for β: $log_{10}(\beta)$ = 2.60, at I = 1.0 M at 50°C. Original data for ΔH at I = 0.5 M.
$Cr(III)^{3+} + (OH)^{-} + (SO_4)^{2-} \rightleftharpoons$ **$Cr(III)(SO_4)(OH)$ *(aq)***	13.16596		1	$Cr(III)L \rightleftharpoons Cr(III)L(OH) + H$ $log_{10}(\beta)$ = -4.65 I = 0.1 M $Cr(III) + L \rightleftharpoons Cr(III)L$ $log_{10}(\beta)$ = 2.53751 I = 0.1 M $OH + H \rightleftharpoons H_2O$ $log_{10}(\beta)$ = 13.78342 I = 0.1 M $Cr(III) + OH + L \rightleftharpoons Cr(III)OHL$ $log_{10}(\beta)$ = 11.67093 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.16596
$Mn(II)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Mn(II)(SO_4)$ *(aq)***	2.25	8.7E+3	1	
$Fe(II)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Fe(II)(SO_4)$ *(aq)***	2.39	8E+3	1	
$Fe(III)^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$Fe(III)(SO_4)^{+}$**	4.05	2.5E+4	1	Original data for ΔH at I = 0.5 M.
$Fe(III)^{3+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Fe(III)(SO_4)_2^{-}$**	5.38		2	
$Co(II)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Co(II)(SO_4)$ *(aq)***	2.3	6.2E+3	1	
$Ni^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Ni(SO_4)$ *(aq)***	2.3	5.8E+3	1	
$Ni^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Ni(SO_4)_2^{2-}$**	3.2		2	
$Cu(II)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Cu(II)(SO_4)$ *(aq)***	2.36	8.7E+3	1	
$Zn^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Zn(SO_4)$ *(aq)***	2.34	6.2E+3	1	
$Zn^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Zn(SO_4)_2^{2-}$**	3.63		2	
$Zn^{2+} + 3\ (SO_4)^{2-} \rightleftharpoons$ **$Zn(SO_4)_3^{4-}$**	2.7		2	
$Zn^{2+} + 4\ (SO_4)^{2-} \rightleftharpoons$ **$Zn(SO_4)_4^{6-}$**	-0.82		2	
$Rb^{+} + (SO_4)^{2-} \rightleftharpoons$ **$Rb(SO_4)^{-}$**	0.94		1	Original data for β at 37°C.
$Sr^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Sr(SO_4)$ *(aq)***	2.3	8E+3	1	
$Y^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$Y(SO_4)^{+}$**	3.48	2.0E+4	1	
$Y^{3+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Y(SO_4)_2^{-}$**	5.2	2.9E+4	1	
$Zr^{4+} + (SO_4)^{2-} \rightleftharpoons$ **$Zr(SO_4)^{2+}$**	3.55449		1	Original data for β: $log_{10}(\beta)$ = 3.67, at I = 2.0 M.
$Zr^{4+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Zr(SO_4)_2$ *(aq)***	6.22674		1	Original data for β: $log_{10}(\beta)$ = 6.40, at I = 2.0 M.
$Zr^{4+} + 3\ (SO_4)^{2-} \rightleftharpoons$ **$Zr(SO_4)_3^{2-}$**	7.22674		1	Original data for β: $log_{10}(\beta)$ = 7.4, at I = 2.0 M.
$Pd^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Pd(SO_4)$ *(aq)***	2.09264		1	Original data for β: $log_{10}(\beta)$ = 1.28, at I = 1.0 M.
$Ag^{+} + (SO_4)^{2-} \rightleftharpoons$ **$Ag(SO_4)^{-}$**	1.3	6.2E+3	1	
$Ag^{+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Ag(SO_4)_2^{3-}$**	0.57		2	
$Ag^{+} + 3\ (SO_4)^{2-} \rightleftharpoons$ **$Ag(SO_4)_3^{5-}$**	-1.51		2	
$Cd^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Cd(SO_4)$ *(aq)***	2.37	8.7E+3	1	
$Cd^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Cd(SO_4)_2^{2-}$**	3.44		2	
$Cd^{2+} + 3\ (SO_4)^{2-} \rightleftharpoons$ **$Cd(SO_4)_3^{4-}$**	3.09		2	
$Cd^{2+} + 4\ (SO_4)^{2-} \rightleftharpoons$ **$Cd(SO_4)_4^{6-}$**	-0.72		2	
$In^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$In(SO_4)^{+}$**	3.01896		1	Original data for β: $log_{10}(\beta)$ = 1.80, at I = 1.0 M at 20°C.
$In^{3+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$In(SO_4)_2^{-}$**	4.17528		1	Original data for β: $log_{10}(\beta)$ = 2.55, at I = 1.0 M at 20°C.
$In^{3+} + 3\ (SO_4)^{2-} \rightleftharpoons$ **$In(SO_4)_3^{3-}$**	4.21896		1	Original data for β: $log_{10}(\beta)$ = 3.0, at I = 1.0 M at 20°C.
$Cs^{+} + (SO_4)^{2-} \rightleftharpoons$ **$Cs(SO_4)^{-}$**	1.04		1	Original data for β at 37°C.
$Ba^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Ba(SO_4)$ *(aq)***	2.13		1	
$Ba^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$Ba(SO_4)_2^{2-}$**	3.2		2	
$La^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$La(SO_4)^{+}$**	3.64	1.8E+4	1	
$La^{3+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$La(SO_4)_2^{-}$**	5.3	3.5E+4	1	
$Ce^{3+} + (SO_4)^{2-} \rightleftharpoons$ **$Ce(SO_4)^{+}$**	3.64	1.9E+4	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ce^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Ce(SO_4)_2^-$**	5.1	3.3E+4	1	
Pr^{3+} + $(SO_4)^{2-}$ ⇌ **$Pr(SO_4)^+$**	3.64	1.9E+4	1	
Pr^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Pr(SO_4)_2^-$**	4.9	4.35E+4	1	
Nd^{3+} + $(SO_4)^{2-}$ ⇌ **$Nd(SO_4)^+$**	3.66	2.0E+4	1	
Nd^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Nd(SO_4)_2^-$**	5.1	3.5E+4	1	
Pm^{3+} + $(SO_4)^{2-}$ ⇌ **$Pm(SO_4)^+$**	1.25337	1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 1.34, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
Pm^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Pm(SO_4)_2^-$**	1.78449		1	Original data for β: $log_{10}(\beta)$ = 1.9, at I = 2.0 M.
Sm^{3+} + $(SO_4)^{2-}$ ⇌ **$Sm(SO_4)^+$**	3.67	2.0E+4	1	
Sm^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Sm(SO_4)_2^-$**	5.1	2.7E+4	1	
Eu^{3+} + $(SO_4)^{2-}$ ⇌ **$Eu(SO_4)^+$**	3.67	2.0E+4	1	
Eu^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Eu(SO_4)_2^-$**	5.4	2.9E+4	1	
Gd^{3+} + $(SO_4)^{2-}$ ⇌ **$Gd(SO_4)^+$**	3.66	2.0E+4	1	
Gd^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Gd(SO_4)_2^-$**	5.2	3.0E+4	1	
Tb^{3+} + $(SO_4)^{2-}$ ⇌ **$Tb(SO_4)^+$**	3.64	1.9E+4	1	
Tb^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Tb(SO_4)_2^-$**	5.1	3.2E+4	1	
Dy^{3+} + $(SO_4)^{2-}$ ⇌ **$Dy(SO_4)^+$**	3.61	2.0E+4	1	
Dy^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Dy(SO_4)_2^-$**	4.8	4.1E+4	1	
Ho^{3+} + $(SO_4)^{2-}$ ⇌ **$Ho(SO_4)^+$**	3.59	2.0E+4	1	
Ho^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Ho(SO_4)_2^-$**	4.9	3.7E+4	1	
Er^{3+} + $(SO_4)^{2-}$ ⇌ **$Er(SO_4)^+$**	3.59	2.0E+4	1	
Er^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Er(SO_4)_2^-$**	5.1	3.3E+4	1	
Tm^{3+} + $(SO_4)^{2-}$ ⇌ **$Tm(SO_4)^+$**	3.59	2.0E+4	1	
Tm^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Tm(SO_4)_2^-$**	5.1	2.9E+4	1	
Yb^{3+} + $(SO_4)^{2-}$ ⇌ **$Yb(SO_4)^+$**	3.55	1.9E+4	1	
Yb^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Yb(SO_4)_2^-$**	5.2	2.9E+4	1	
Lu^{3+} + $(SO_4)^{2-}$ ⇌ **$Lu(SO_4)^+$**	3.52	1.9E+4	1	
Lu^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Lu(SO_4)_2^-$**	5.2	2.5E+4	1	
Hf^{4+} + $(SO_4)^{2-}$ ⇌ **$Hf(SO_4)^{2+}$**	2.92449		1	Original data for β: $log_{10}(\beta)$ = 3.04, at I = 2.0 M.
Hf^{4+} + 2 $(SO_4)^{2-}$ ⇌ **$Hf(SO_4)_2$ *(aq)***	5.26674		1	Original data for β: $log_{10}(\beta)$ = 5.44, at I = 2.0 M.
$Pt(II)^{2+}$ + $(SO_4)^{2-}$ ⇌ **$Pt(II)(SO_4)$ *(aq)***	0.56		12	
$Pt(II)^{2+}$ + 2 $(SO_4)^{2-}$ ⇌ **$Pt(II)(SO_4)_2^{2-}$**	2.38		12	
$Pt(II)^{2+}$ + 3 $(SO_4)^{2-}$ ⇌ **$Pt(II)(SO_4)_3^{4-}$**	3.67		12	
$Hg(II)^{2+}$ + $(SO_4)^{2-}$ ⇌ **$Hg(II)(SO_4)$ *(aq)***	2.41355		1	Original data for β: $log_{10}(\beta)$ = 1.34, at I = 0.5 M.
$Hg(II)^{2+}$ + 2 $(SO_4)^{2-}$ ⇌ **$Hg(II)(SO_4)_2^{2-}$**	3.47355		1	Original data for β: $log_{10}(\beta)$ = 2.4, at I = 0.5 M.
$Pb(II)^{2+}$ + $(SO_4)^{2-}$ ⇌ **$Pb(II)(SO_4)$ *(aq)***	2.69		1	
$Pb(II)^{2+}$ + 2 $(SO_4)^{2-}$ ⇌ **$Pb(II)(SO_4)_2^{2-}$**	4.51		2	
Bi^{3+} + $(SO_4)^{2-}$ ⇌ **$Bi(SO_4)^+$**	0.35863	1.2E+4	1	Original data for β: $log_{10}(\beta)$ = 1.98, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Bi^{3+} + 2 $(SO_4)^{2-}$ ⇌ **$Bi(SO_4)_2^-$**	1.24817	2.9E+4	1	Original data for β: $log_{10}(\beta)$ = 3.41, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Bi^{3+} + 3 $(SO_4)^{2-}$ ⇌ **$Bi(SO_4)_3^{3-}$**	2.45863	4.6E+4	1	Original data for β: $log_{10}(\beta)$ = 4.08, at I = 3.0 M. Original data for ΔH at I = 3.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Bi^{3+} + 4\ (SO_4)^{2-} \rightleftharpoons$ **$Bi(SO_4)_4^{5-}$**	4.34	5.4E+4	1	Original data for β: $log_{10}(\beta)$ = 4.34, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Bi^{3+} + 5\ (SO_4)^{2-} \rightleftharpoons$ **$Bi(SO_4)_5^{7-}$**	7.30229		1	Original data for β: $log_{10}(\beta)$ = 4.60, at I = 3.0 M.
$(U(VI)O_2)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)(SO_4)$ *(aq)***	3.18	2.0E+4	1	
$(U(VI)O_2)^{2+} + 2\ (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)(SO_4)_2^{2-}$**	4.3	3.8E+4	1	
$2\ (U(VI)O_2)^{2+} + 2\ (OH)^- + 2\ (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)_2(OH)_2(SO_4)_2^{2-}$**	23.24088		1	$2\ U(VI)O_2 + 2\ L \rightleftharpoons (U(VI)O_2)_2(OH)_2L_2 + 2\ H$ $log_{10}(\beta)$ = -2.73 I = 3.5 M $2\ H + 2\ OH \rightleftharpoons 2\ H_2O$ $log_{10}(\beta)$ = 28.80326 I = 3.5 M $2\ U(VI)O_2 + 2\ L + 2\ OH \rightleftharpoons (U(VI)O_2)_2(OH)_2L_2$ $log_{10}(\beta)$ = 26.07326 I = 3.5 M I = 0 M: $log_{10}(\beta)$ = 23.24088
$3\ (U(VI)O_2)^{2+} + 4\ (OH)^- + 3\ (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)_3(OH)_4(SO_4)_3^{4-}$**	46.97877		1	$3\ U(VI)O_2 + 3\ L \rightleftharpoons (U(VI)O_2)_3(OH)_4L_3 + 4\ H$ $log_{10}(\beta)$ = -8.2 I = 3.5 M $4\ H + 4\ OH \rightleftharpoons 4\ H_2O$ $log_{10}(\beta)$ = 57.60652 I = 3.5 M $3\ U(VI)O_2 + 3\ L + 4\ OH \rightleftharpoons (U(VI)O_2)_3(OH)_4L_3$ $log_{10}(\beta)$ = 49.40652 I = 3.5 M I = 0 M: $log_{10}(\beta)$ = 46.97877
$3\ (U(VI)O_2)^{2+} + 4\ (OH)^- + 4\ (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)_3(OH)_4(SO_4)_4^{6-}$**	50.61577		1	$3\ U(VI)O_2 + 4\ L \rightleftharpoons (U(VI)O_2)_3(OH)_4L_4 + 4\ H$ $log_{10}(\beta)$ = -7.8 I = 3.5 M $4\ H + 4\ OH \rightleftharpoons 4\ H_2O$ $log_{10}(\beta)$ = 57.60652 I = 3.5 M $3\ U(VI)O_2 + 4\ L + 4\ OH \rightleftharpoons (U(VI)O_2)_3(OH)_4L_4$ $log_{10}(\beta)$ = 49.80652 I = 3.5 M I = 0 M: $log_{10}(\beta)$ = 50.61577
$5\ (U(VI)O_2)^{2+} + 8\ (OH)^- + 6\ (SO_4)^{2-} \rightleftharpoons$ **$(U(VI)O_2)_5(OH)_8(SO_4)_6^{10-}$**	106.42404		1	$5\ U(VI)O_2 + 6\ L \rightleftharpoons (U(VI)O_2)_5(OH)_8L_6 + 8\ H$ $log_{10}(\beta)$ =-18.5 I = 3.5 M $8\ H + 8\ OH \rightleftharpoons 8\ H_2O$ $log_{10}(\beta)$ =115.21304 I = 3.5 M $5\ U(VI)O_2 + 6\ L + 8\ OH \rightleftharpoons (U(VI)O_2)_5(OH)_8L_6$ $log_{10}(\beta)$ =96.71304 I = 3.5 M I = 0 M: $log_{10}(\beta)$ = 106.42404

2.2.13. Chloride

The formula for the ligand chloride is Cl^-; the molecular weight is 35.45.
Some chloride complexes are not included in the CHEAQS' database because the details as laid out in earlier works by Smith and Martell, suggest that these complexes are not found in practice.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)		Literature reference	Remarks / conversions
$Li^+ + Cl^- \rightleftharpoons$ **$LiCl$ *(aq)***					Present in NIST but not included in CHEAQS' database
$Be^{2+} + Cl^- \rightleftharpoons$ **$BeCl^+$**	-1.93352			1	Original data for β: $log_{10}(\beta)$ = -0.85, at I = 4.0 M.
$Be^{2+} + 2\ Cl^- \rightleftharpoons$ **$BeCl_2$ *(aq)***	-0.54			2	
$Na^+ + Cl^- \rightleftharpoons$ **$NaCl$ *(aq)***					Present in NIST but not included in CHEAQS' database
$Mg^{2+} + Cl^- \rightleftharpoons$ **$MgCl^+$**					Present in NIST but not included in CHEAQS' database
$Al^{3+} + Cl^- \rightleftharpoons$ **$AlCl^{2+}$**	-0.39052			1	Original data for β: $log_{10}(\beta)$ = -1.0 , at I = 1.0 M.
$K^+ + Cl^- \rightleftharpoons$ **KCl *(aq)***					Present in NIST but not included in CHEAQS' database
$Ca^{2+} + Cl^- \rightleftharpoons$ **$CaCl^+$**					Present in NIST but not included in CHEAQS' database
$Sc^{3+} + Cl^- \rightleftharpoons$ **$ScCl^{2+}$**	-1.74528			1	Original data for β: $log_{10}(\beta)$ = -0.12, at I = 4.0 M.
$Sc^{3+} + 2\ Cl^- \rightleftharpoons$ **$ScCl_2^+$**	1.57			2	
$Cr(III)^{3+} + Cl^- \rightleftharpoons$ **$Cr(III)Cl^{2+}$**	-0.39052	2.6E+4		1	Original data for β: $log_{10}(\beta)$ = -1.0, at I = 1.0 M. Original data for ΔH at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)		Literature reference	Remarks / conversions
$Mn(II)^{2+} + Cl^{-} \rightleftharpoons \mathbf{Mn(II)Cl^{+}}$	0			1	
$Fe(II)^{2+} + Cl^{-} \rightleftharpoons \mathbf{Fe(II)Cl^{+}}$	-0.3			1	
$Fe(III)^{3+} + Cl^{-} \rightleftharpoons \mathbf{Fe(III)Cl^{2+}}$	1.4	2.3E+4		1	
$Fe(III)^{3+} + 2\ Cl^{-} \rightleftharpoons \mathbf{Fe(III)Cl_2^{+}}$	2.44			2	
$Fe(III)^{3+} + 3\ Cl^{-} \rightleftharpoons \mathbf{Fe(III)Cl_3}\ \mathbf{\textit{(aq)}}$	0.99			2	
$Co(II)^{2+} + Cl^{-} \rightleftharpoons \mathbf{Co(II)Cl^{+}}$	-0.35	2E+3		1	Original data for ΔH at I = 2.0 M.
$Co(III)^{3+} + Cl^{-} \rightleftharpoons \mathbf{Co(III)Cl^{2+}}$	2.30516	1.6E+4		1	Original data for β: $log_{10}(\beta)$ = 1.5 , at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Ni^{2+} + Cl^{-} \rightleftharpoons \mathbf{NiCl^{+}}$	-0.43	2E+3		1	
$Cu(I)^{+} + Cl^{-} \rightleftharpoons \mathbf{Cu(I)Cl}\ \mathbf{\textit{(aq)}}$	3.1			1	
$Cu(I)^{+} + 2\ Cl^{-} \rightleftharpoons \mathbf{Cu(I)Cl_2^{-}}$	5.42			1	
$Cu(I)^{+} + 3\ Cl^{-} \rightleftharpoons \mathbf{Cu(I)Cl_3^{2-}}$	4.75			1	$Cu(I)L_2 + L \rightleftharpoons Cu(I)L_3$ $log_{10}(\beta)$ = -0.67 ΔH = -20E+3 (Original data for ΔH at I = 5.0 M) $Cu(I) + 2\ L \rightleftharpoons Cu(I)L_2$ $log_{10}(\beta)$ = 5.42 ΔH = ? $Cu(I) + 3\ L \rightleftharpoons Cu(I)L_3$ $log_{10}(\beta)$ = 4.75 ΔH = ?
$2\ Cu(I)^{+} + 4\ Cl^{-} \rightleftharpoons \mathbf{Cu(I)_2Cl_4^{2-}}$	12.17820			1	Original data for β: $log_{10}(\beta)$ = 13.0, at I = 5.0 M.
$Cu(II)^{2+} + Cl^{-} \rightleftharpoons \mathbf{Cu(II)Cl^{+}}$	0.3	8.3E+3		1	Original data for ΔH at I = 2.0 M.
$Zn^{2+} + Cl^{-} \rightleftharpoons \mathbf{ZnCl^{+}}$	0.46	5.4E+3		1	Original data for ΔH at I = 3.0 M.
$Zn^{2+} + 2\ Cl^{-} \rightleftharpoons \mathbf{ZnCl_2}\ \mathbf{\textit{(aq)}}$	0.62			2	
$Zn^{2+} + 3\ Cl^{-} \rightleftharpoons \mathbf{ZnCl_3^{-}}$	0.51			2	
$Zn^{2+} + 4\ Cl^{-} \rightleftharpoons \mathbf{ZnCl_4^{2-}}$	0.2			2	
$Ga^{3+} + Cl^{-} \rightleftharpoons \mathbf{GaCl^{2+}}$	0.60948			1	Original data for β: $log_{10}(\beta)$ = 0.00, at I = 1.0 M.
$Rb^{+} + Cl^{-} \rightleftharpoons \mathbf{RbCl}\ \mathbf{\textit{(aq)}}$					Present in NIST but not included in CHEAQS' database
$Sr^{2+} + Cl^{-} \rightleftharpoons \mathbf{SrCl^{+}}$					Present in NIST but not included in CHEAQS' database
$Y^{3+} + Cl^{-} \rightleftharpoons \mathbf{YCl^{2+}}$	0.57948			1	Original data for β: $log_{10}(\beta)$ = -0.03, at I = 1.0 M.
$Zr^{4+} + Cl^{-} \rightleftharpoons \mathbf{ZrCl^{3+}}$	0.14225			1	Original data for β: $log_{10}(\beta)$ = 0.2, at I = 2.0 M.
$Zr^{4+} + 2\ Cl^{-} \rightleftharpoons \mathbf{ZrCl_2^{2+}}$	1.47			2	
$Zr^{4+} + 3\ Cl^{-} \rightleftharpoons \mathbf{ZrCl_3^{+}}$	0.8			2	
$Pd^{2+} + Cl^{-} \rightleftharpoons \mathbf{PdCl^{+}}$	6.1	-1.2E+4		1	Original data for ΔH at I = 1.0 M.
$Pd^{2+} + 2\ Cl^{-} \rightleftharpoons \mathbf{PdCl_2}\ \mathbf{\textit{(aq)}}$	10.7	-2.3E+4		1	Original data for ΔH at I = 1.0 M.
$Pd^{2+} + 3\ Cl^{-} \rightleftharpoons \mathbf{PdCl_3^{-}}$	13.1	-3.4E+4		1	Original data for ΔH at I = 1.0 M.
$Pd^{2+} + 4\ Cl^{-} \rightleftharpoons \mathbf{PdCl_4^{2-}}$	15.4	-4.85E+4		1	Original data for ΔH at I = 1.0 M.
$Ag^{+} + Cl^{-} \rightleftharpoons \mathbf{AgCl}\ \mathbf{\textit{(aq)}}$	3.31	-1.2E+4		1	
$Ag^{+} + 2\ Cl^{-} \rightleftharpoons \mathbf{AgCl_2^{-}}$	5.25	-1.6E+4		1	
$Ag^{+} + 3\ Cl^{-} \rightleftharpoons \mathbf{AgCl_3^{2-}}$	5.2	-3.8E+4		1	Original data for ΔH at I = 5.0 M.
$Ag^{+} + 4\ Cl^{-} \rightleftharpoons \mathbf{AgCl_4^{3-}}$	6.96360	-5.8E+4		1	Original data for β: $log_{10}(\beta)$ = 5.32, at I = 5.0 M. Original data for ΔH at I = 5.0 M.
$Cd^{2+} + Cl^{-} \rightleftharpoons \mathbf{CdCl^{+}}$	1.98	2E+3		1	
$Cd^{2+} + 2\ Cl^{-} \rightleftharpoons \mathbf{CdCl_2}\ \mathbf{\textit{(aq)}}$	2.6	4.6E+3		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)		Literature reference	Remarks / conversions
Cd^{2+} + 3 Cl^- ⇌ **$CdCl_3^-$**	2.00169	7.9E+3		1	Original data for β: $log_{10}(\beta)$ = 1.96, at I = 2.0 M when $NaClO_4$ is the background electrolyte; $log_{10}(\beta)$ = 2.13 (also at I = 2.0 M) when $LiClO_4$ is the background electrolyte. The average log-value (2.045) was converted to I = 0 M. Original data for ΔH at I = 2.0 M.
Cd^{2+} + 4 Cl^- ⇌ **$CdCl_4^{2-}$**	1.47			2	
In^{3+} + Cl^- ⇌ **$InCl^{2+}$**	2.93948	5.0E+3		1	Original data for β: $log_{10}(\beta)$ = 2.33, at I = 1.0 M. Original data for ΔH at I = 2.0 M.
In^{3+} + $(OH)^-$ + Cl^- ⇌ **$In(OH)Cl^+$**	12.76626			1	InL ⇌ InOHL + H $log_{10}(\beta)$ = -3.9 I = 3.0 M In + L ⇌ InL $log_{10}(\beta)$ = 3.75017 I = 3.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 14.26723 I = 3.0 M In + OH + L ⇌ InOHL $log_{10}(\beta)$ = 14.11740 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 12.76626
In^{3+} + 2 Cl^- ⇌ **$InCl_2^+$**	4.41580	3E+3		1	Original data for β: $log_{10}(\beta)$ = 3.4, at I = 1.0 M. Original data for ΔH at I = 2.0 M.
In^{3+} + 3 Cl^- ⇌ **$InCl_3$ *(aq)***	5.01896	3.3E+4		1	Original data for β: $log_{10}(\beta)$ = 3.8, at I = 1.0 M. Original data for ΔH at I = 2.0 M.
2 In^{3+} + $(OH)^-$ + Cl^- ⇌ **$In_2(OH)Cl^{4+}$**	15.17694			1	InOHL + In ⇌ In_2OHL $log_{10}(\beta)$ = 1.6 I = 3.0 M In + OH + L ⇌ InOHL $log_{10}(\beta)$ = 14.11740 I = 3.0 M 2 In + OH + L ⇌ In_2OHL $log_{10}(\beta)$ = 15.71740 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 15.17694
$Sn(II)^{2+}$ + Cl^- ⇌ **$Sn(II)Cl^+$**	1.64	9.2E+3		1	
$Sn(II)^{2+}$ + 2 Cl^- ⇌ **$Sn(II)Cl_2$ *(aq)***	2.4	1.6E+4		1	Original data for ΔH at I = 3.0 M.
$Sn(II)^{2+}$ + 3 Cl^- ⇌ **$Sn(II)Cl_3^-$**	1.25669	2.5E+4		1	Original data for β: $log_{10}(\beta)$ = 1.3, at I = 2.0 M. Original data for ΔH at I = 3.0 M.
Cs^+ + Cl^- ⇌ **CsCl *(aq)***	-0.1			1	
Ba^{2+} + Cl^- ⇌ **$BaCl^+$**					Present in NIST but not included in CHEAQS' database
La^{3+} + Cl^- ⇌ **$LaCl^{2+}$**	0.52948	5.0E+3		1	Original data for β: $log_{10}(\beta)$ = -0.04, at I = 1.0 M when $HClO_4$ is the background electrolyte; $log_{10}(\beta)$ = -0.12 (also at I = 1.0 M) when $NaClO_4$ is the background electrolyte. The average log-value (-0.08) was converted to I = 0 M.
La^{3+} + 2 Cl^- ⇌ **$LaCl_2^+$**	-0.29			2	
Ce^{3+} + Cl^- ⇌ **$CeCl^{2+}$**	0.56948			1	Original data for β: $log_{10}(\beta)$ = -0.04, at I = 1.0 M.
Ce^{3+} + 2 Cl^- ⇌ **$CeCl_2^+$**	1.19			2	
Pr^{3+} + Cl^- ⇌ **$PrCl^{2+}$**	0.56948			1	Original data for β: $log_{10}(\beta)$ = -0.04, at I = 1.0 M.
Pr^{3+} + 2 Cl^- ⇌ **$PrCl_2^+$**	-0.29			2	
Nd^{3+} + Cl^- ⇌ **$NdCl^{2+}$**	0.8			2	
Nd^{3+} + 2 Cl^- ⇌ **$NdCl_2^+$**	-0.29			2	
Sm^{3+} + Cl^- ⇌ **$SmCl^{2+}$**	-1.20069			1	Original data for β: $log_{10}(\beta)$ = -0.39, at I = 3.0 M at 20°C.
Sm^{3+} + 2 Cl^- ⇌ **$SmCl_2^+$**	-0.29			2	
Eu^{3+} + Cl^- ⇌ **$EuCl^{2+}$**	0.56948	0		1	Original data for β: $log_{10}(\beta)$ = -0.04, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
Eu^{3+} + 2 Cl^- ⇌ **$EuCl_2^+$**	0.99			2	
Gd^{3+} + Cl^- ⇌ **$GdCl^{2+}$**	-1.06069			1	Original data for β: $log_{10}(\beta)$ = -0.25, at I = 3.0 M at 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)		Literature reference	Remarks / conversions
$Gd^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{GdCl_2^+}$	-0.29			2	
$Tb^{3+} + Cl^- \rightleftharpoons \mathbf{TbCl^{2+}}$	-1.16069			1	Original data for β: $log_{10}(\beta)$ = -0.35, at I = 3.0 M at 20°C.
$Tb^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{TbCl_2^+}$	-0.29			2	
$Dy^{3+} + Cl^- \rightleftharpoons \mathbf{DyCl^{2+}}$	0.8			2	
$Dy^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{DyCl_2^+}$	-0.29			2	
$Ho^{3+} + Cl^- \rightleftharpoons \mathbf{HoCl^{2+}}$	0.8			2	
$Ho^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{HoCl_2^+}$	-0.29			2	
$Er^{3+} + Cl^- \rightleftharpoons \mathbf{ErCl^{2+}}$	0.8			2	
$Er^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{ErCl_2^+}$	-0.29			2	
$Tm^{3+} + Cl^- \rightleftharpoons \mathbf{TmCl^{2+}}$	0.50948			1	Original data for β: $log_{10}(\beta)$ = -0.1, at I = 1.0 M at 20°C.
$Tm^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{TmCl_2^+}$	-0.29			2	
$Yb^{3+} + Cl^- \rightleftharpoons \mathbf{YbCl^{2+}}$	0.40948			1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M at 20°C.
$Yb^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{YbCl_2^+}$	-0.29			2	
$Lu^{3+} + Cl^- \rightleftharpoons \mathbf{LuCl^{2+}}$	-1.97528			1	Original data for β: $log_{10}(\beta)$ = -0.35, at I = 4.0 M.
$Lu^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{LuCl_2^+}$	-0.29			2	
$Hf^{4+} + Cl^- \rightleftharpoons \mathbf{HfCl^{3+}}$	-0.74091			1	Original data for β: $log_{10}(\beta)$ = 0.34, at I = 3.0 M at 20°C.
$Hf^{4+} + 2\ Cl^- \rightleftharpoons \mathbf{HfCl_2^{2+}}$	1.55			2	
$Hf^{4+} + 3\ Cl^- \rightleftharpoons \mathbf{HfCl_3^+}$	0.88			2	
$Pt(II)^{2+} + Cl^- \rightleftharpoons \mathbf{Pt(II)Cl^+}$	6.33			12	
$Pt(II)^{2+} + 2\ Cl^- \rightleftharpoons \mathbf{Pt(II)Cl_2}$ ***(aq)***	13.14			12	
$Pt(II)^{2+} + 3\ Cl^- \rightleftharpoons \mathbf{Pt(II)Cl_3^-}$	16.14			12	
$Pt(II)^{2+} + 4\ Cl^- \rightleftharpoons \mathbf{Pt(II)Cl_4^{2-}}$	17.66			12	
$Hg(II)^{2+} + Cl^- \rightleftharpoons \mathbf{Hg(II)Cl^+}$	7.30	-2.1E+4		1	
$Hg(II)^{2+} + (OH)^- + Cl^- \rightleftharpoons \mathbf{Hg(II)Cl(OH)}$ ***(aq)***	18.247			1	Hg(II)L ⇌ Hg(II)OHL+ H $log_{10}(\beta)$ = -3.05 I = 1.0 M ΔH = -20E+3 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M ΔH = ? Hg(II) + L ⇌ Hg(II)L $log_{10}(\beta)$ = 6.89368 I = 1.0 M ΔH = ? Hg(II) + L + OH ⇌ Hg(II)OHL $log_{10}(\beta)$ = 17.63752 I = 1.0 M ΔH = ? I = 0 M: $log_{10}(\beta)$ = 18.247
$Hg(II)^{2+} + 2\ Cl^- \rightleftharpoons \mathbf{Hg(II)Cl_2}$ ***(aq)***	14	-5.14E+4		1	
$Hg(II)^{2+} + 3\ Cl^- \rightleftharpoons \mathbf{Hg(II)Cl_3^-}$	15	-5.10E+4		1	
$Hg(II)^{2+} + 4\ Cl^- \rightleftharpoons \mathbf{Hg(II)Cl_4^{2-}}$	15.6	-5.94E+4		1	
$Hg(II)Cl_2$ ***(aq)*** + $(glycine)^- \rightleftharpoons$ **Hg(II)Cl(glycine)** ***(aq)*** + Cl^-	17.42	-7.64E+4		1	$Hg(II)Cl_2$ + (glycine) ⇌ Hg(II)Cl(glycine) + Cl $log_{10}(\beta)$ = 3.42 ΔH = -2.5E+4 Hg(II) + 2 Cl ⇌ $Hg(II)Cl_2$ $log_{10}(\beta)$ = 14 ΔH = -5.14E+04 Hg(II) + Cl + (glycine) ⇌ Hg(II)Cl(glycine) $log_{10}(\beta)$ = 17.42 ΔH = -7.64E+04
$Pb(II)^{2+} + Cl^- \rightleftharpoons \mathbf{Pb(II)Cl^+}$	1.56	8.7E+3		1	
$Pb(II)^{2+} + 2\ Cl^- \rightleftharpoons \mathbf{Pb(II)Cl_2}$ ***(aq)***	1.9	1.2E+4		1	
$Pb(II)^{2+} + 3\ Cl^- \rightleftharpoons \mathbf{Pb(II)Cl_3^-}$	1.8	1.2E+4		1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+} + 4\ Cl^- \rightleftharpoons \mathbf{Pb(II)Cl_4^{2-}}$	1.4			2	
$Bi^{3+} + Cl^- \rightleftharpoons \mathbf{BiCl^{2+}}$	3.6	1.6E+4		1	
$Bi^{3+} + 2\ Cl^- \rightleftharpoons \mathbf{BiCl_2^+}$	5.5	2.6E+4		1	Original data for ΔH at I = 4.0 M.
$Bi^{3+} + 3\ Cl^- \rightleftharpoons \mathbf{BiCl_3}$ ***(aq)***	7.1	-1.9E+4		1	Original data for ΔH at I = 4.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)		Literature reference	Remarks / conversions
Bi^{3+} + 4 Cl^{-} ⇌ **$BiCl_4^{-}$**	8.1	1.7E+4		1	Original data for ΔH at I = 4.0 M.
Bi^{3+} + 5 Cl^{-} ⇌ **$BiCl_5^{2-}$**	6.62781	-3.0E+4		1	Original data for β: $log_{10}(\beta)$ = 6.7, at I = 2.0 M. Original data for ΔH at I = 4.0 M.
Bi^{3+} + 6 Cl^{-} ⇌ **$BiCl_6^{3-}$**	6.51			2	
$(U(VI)O_2)^{2+}$ + Cl^{-} ⇌ **$(U(VI)O_2)Cl^{+}$**	0.3	8E+3		1	Original data for ΔH at I = 1.0 M.

2.2.14. Vanadate

The formula for the ligand vanadate is VO_4^{3-}; the molecular weight is 114.938.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + $(VO_4)^{3-}$ ⇌ **$H(VO_4)^{2-}$**	14.3	-2.7E+4	1	Original data for ΔH at I = 1.0 M.
2 H^{+} + $(VO_4)^{3-}$ ⇌ **$H_2(VO_4)^{-}$**	22.85	-3.62E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 8.55 ΔH = -9.2E+3 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 14.3 ΔH = -2.7E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.85 ΔH = -3.62E+4 Note: ΔH for the original equilibrium is at I = 1.0 M.
4 H^{+} + $(VO_4)^{3-}$ ⇌ **VO_2^{+}**	30.15	-6.92E+04	1	H_2L + 2 H ⇌ VO_2 $log_{10}(\beta)$ = 7.3 ΔH = -3.3E+4 (Original data for ΔH at I = 1.0 M) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.85 ΔH = -3.62E+04 4 H + L ⇌ VO_2 $log_{10}(\beta)$ = 30.15 ΔH = -6.92E+04 Note: ΔH for the original equilibrium is at I = 1.0 M.
H^{+} + Na^{+} + $(VO_4)^{3-}$ ⇌ **$NaH(VO_4)^{-}$**	15.46		2	Na + HVO_4 ⇌ $NaHVO_4$ $log_{10}(\beta)$ = 1.16 H + VO_4 ⇌ HVO_4 $log_{10}(\beta)$ = 14.3 Na + H + VO_4 ⇌ $NaHVO_4$ $log_{10}(\beta)$ = 15.46
H^{+} + K^{+} + $(VO_4)^{3-}$ ⇌ **$KH(VO_4)^{-}$**	15.2		2	K + HVO_4 ⇌ $KHVO_4$ $log_{10}(\beta)$ = 0.90 H + VO_4 ⇌ HVO_4 $log_{10}(\beta)$ = 14.3 K + H + VO_4 ⇌ $KHVO_4$ $log_{10}(\beta)$ = 15.20

2.2.15. Chromate

The formula for the ligand chromate is CrO_4^{2-}; the molecular weight is 115.992.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ H^+ + (NH_3)$ *(aq)* $+ 2\ (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{NH_4Cr_2O_7^-}$	24.664	-8.7E+4	1	$NH_4 + Cr_2O_7 \rightleftharpoons NH_4Cr_2O_7$ $\log_{10}(\beta) = 0.88$ ΔH = -2.0E+4 $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ ΔH = -5.2E+4 $2\ H + 2\ L \rightleftharpoons Cr_2O_7$ $\log_{10}(\beta) = 14.54$ ΔH = -1.5E+4 $NH_3 + 3\ H + 2\ L \rightleftharpoons NH_4Cr_2O_7$ $\log_{10}(\beta) = 24.664$ ΔH = -8.7E+4
$H^+ + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{H(CrO_4)^-}$	6.51	2E+3	1	
$2\ H^+ + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{H_2(CrO_4)}$ ***(aq)***	6.01316	3.9E+4	1	$HL + H \rightleftharpoons H_2L$ $\log_{10}(\beta) = -0.7$ I = 1.0 ΔH = 3.7E+4 (Original data for ΔH at I = 1.0 M) $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 6.10368$ I = 1.0 ΔH = 2E+3 $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 5.40368$ I = 1.0 ΔH = 3.9E+4 I = 0 M: $\log_{10}(\beta) = 6.01316$
$2\ H^+ + 2\ (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{Cr_2O_7^{2-}}$	14.54	-1.5E+4	1	$2\ HL \rightleftharpoons Cr_2O_7$ $\log_{10}(\beta) = 1.52$ ΔH = -1.9E+4 $2\ H + 2\ L \rightleftharpoons 2\ HL$ $\log_{10}(\beta) = 13.02$ ΔH = 4E+3 $2\ H + 2\ L \rightleftharpoons Cr_2O_7$ $\log_{10}(\beta) = 14.54$ ΔH = -1.5E+4
$Na^+ + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{Na(CrO_4)^-}$	0.7		2	
$K^+ + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{K(CrO_4)^-}$	0.57		1	Original data for β at 18°C.
$2\ H^+ + K^+ + 2\ (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{KCr_2O_7^-}$	15.30	-4.2E+4	1	$K + Cr_2O_7 \rightleftharpoons KCr_2O_7$ $\log_{10}(\beta) = 0.76$ ΔH = -2.9E+4 $2\ H + 2\ L \rightleftharpoons Cr_2O_7$ $\log_{10}(\beta) = 14.54$ ΔH = -1.5E+4 $K + 2\ H + 2\ L \rightleftharpoons KCr_2O_7$ $\log_{10}(\beta) = 15.30$ ΔH = -4.2E+4
$Fe(III)^{3+} + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{Fe(III)(CrO_4)^+}$	7.8	2.0E+4	1	
$Ni^{2+} + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{Ni(CrO_4)}$ ***(aq)***	2.4		1	
$Cu(II)^{2+} + (CrO_4)^{2-} \rightleftharpoons$ $\mathbf{Cu(II)(CrO_4)}$ ***(aq)***	3.3		1	

2.2.16. Arsenite

The formula for the ligand arsenite is $H_2AsO_3^-$ so not the completely deprotonated form ; the molecular weight is 124.935.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (H_2AsO_3)^- \rightleftharpoons$ $\mathbf{H(H_2AsO_3)}$ ***(aq)***	9.32	-2.7E+4	1	
$H^+ + 2\ (H_2AsO_3)^- \rightleftharpoons$ $\mathbf{H(H_2AsO_3)_2^-}$	9.14161		1	$H_2L_2 \rightleftharpoons HL_2 + H$ $\log_{10}(\beta) = -8.31$ I = 0.5 M $2\ H + 2\ L \rightleftharpoons 2\ H_2L_2$ $\log_{10}(\beta) = 17.18322$ I = 0.5 M $H + 2\ L \rightleftharpoons HL_2$ $\log_{10}(\beta) = 8.87322$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 9.14161$
$2\ H^+ + 2\ (H_2AsO_3)^- \rightleftharpoons$ $\mathbf{H_2(H_2AsO_3)_2}$ ***(aq)***	17.72		1	$2\ HL \rightleftharpoons H_2L_2$ $\log_{10}(\beta) = -0.92$ $2\ H + 2\ L \rightleftharpoons 2\ HL$ $\log_{10}(\beta) = 18.64$ $2\ H + 2\ L \rightleftharpoons H_2L_2$ $\log_{10}(\beta) = 17.72$
$Ca^{2+} + (H_2AsO_3)^- \rightleftharpoons$ $\mathbf{Ca(H_2AsO_3)^+}$	1.36		1	

2.2.17. Arsenate

The formula for the ligand arsenate is AsO_4^{3-}; the molecular weight is 138.918.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (AsO_4)^{3-} \rightleftharpoons \mathbf{H(AsO_4)^{2-}}$	11.54	-1.7E+4	1	Original data for ΔH at I = 0.1 M.
$2\ H^+ + (AsO_4)^{3-} \rightleftharpoons \mathbf{H_2(AsO_4)^{-}}$	18.54	-2.0E+4	1	$H + HL \rightleftharpoons H_2L$ $log_{10}(\beta) = 7.00$ ΔH = -3E+3 (Original data for ΔH at I = 0.1 M) $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 11.54$ ΔH = -1.7E+4 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 18.54$ ΔH = -2E+4
$3\ H^+ + (AsO_4)^{3-} \rightleftharpoons \mathbf{H_3(AsO_4)}$ ***(aq)***	20.76	-1.29E+4	1	$H + H_2L \rightleftharpoons H_3L$ $log_{10}(\beta) = 2.22$ ΔH = 7.1E+3 (Original data for ΔH at I = 0.1 M) $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 18.54$ ΔH = -2E+4 $3\ H + L \rightleftharpoons H_3L$ $log_{10}(\beta) = 20.76$ ΔH = -1.29E+04
$Ca^{2+} + (AsO_4)^{3-} \rightleftharpoons \mathbf{Ca(AsO_4)^{-}}$	4.3		1	Original data for β at 40°C.
$H^+ + Ca^{2+} + (AsO_4)^{3-} \rightleftharpoons \mathbf{CaH(AsO_4)}$ ***(aq)***	14.29		1	$Ca + HL \rightleftharpoons CaHL$ $log_{10}(\beta) = 2.75$ $H + L = HL$ $log_{10}(\beta) = 11.54$ $Ca + H + L \rightleftharpoons CaHL$ $log_{10}(\beta) = 14.29$ Original data for β at 40°C.
$2\ H^+ + Ca^{2+} + (AsO_4)^{3-} \rightleftharpoons \mathbf{CaH_2(AsO_4)^{+}}$	19.93		1	$Ca + H_2L \rightleftharpoons CaH_2L$ $log_{10}(\beta) = 1.39$ $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 18.54$ $Ca + 2\ H + L \rightleftharpoons CaH_2L$ $log_{10}(\beta) = 19.93$ Original data for β at 40°C.

2.2.18. Selenite

The formula for the ligand selenite is SeO_3^{2-}; the molecular weight is 126.968.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (SeO_3)^{2-} \rightleftharpoons \mathbf{H(SeO_3)^{-}}$	8.40	-5.02E+3	1	Original data for ΔH at I = 1.0 M.
$2\ H^+ + (SeO_3)^{2-} \rightleftharpoons \mathbf{H_2(SeO_3)}$ ***(aq)***	11.03	1.18E+3	1	$HL + H \rightleftharpoons H_2L$ $log_{10}(\beta) = 2.63$ ΔH = 6.2E+3 (Original data for ΔH at I = 1.0 M) $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 8.40$ ΔH = -5.02E+3 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 11.03$ ΔH = 1.18E+3
$H^+ + Fe(III)^{3+} + (SeO_3)^{2-} \rightleftharpoons \mathbf{Fe(III)H(SeO_3)^{2+}}$	11.81948	-2.52E+3	1	$Fe(III) + HL \rightleftharpoons Fe(III)HL$ $log_{10}(\beta) = 2.81$ I = 1.0 M ΔH = 2.5E+3 (Original data for ΔH at I = 1.0 M) $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 7.99368$ I = 1.0 M ΔH = -5.02E+3 $Fe(III) + H + L \rightleftharpoons Fe(III)HL$ $log_{10}(\beta) = 10.80368$ I = 1.0 M ΔH = -2.52E+3 I = 0 M: $log_{10}(\beta) = 11.81948$
$Ag^+ + (SeO_3)^{2-} \rightleftharpoons \mathbf{Ag(SeO_3)^{-}}$	2.80632		1	Original data for β: $log_{10}(\beta) = 2.4$, at I = 1.0 M.

$Ag^{+} + 2\ (SeO_3)^{2-} \rightleftharpoons \mathbf{Ag(SeO_3)_2^{3-}}$	3.76		1	Original data for β: $\log_{10}(\beta)$ = 3.76, at I = 1.0 M.
$Cd^{2+} + 2\ (SeO_3)^{2-} \rightleftharpoons \mathbf{Cd(SeO_3)_2^{2-}}$	5.91264		1	Original data for β: $\log_{10}(\beta)$ = 5.1, at I = 1.0 M.
$Hg(II)^{2+} + 2\ (SeO_3)^{2-} \rightleftharpoons \mathbf{Hg(II)(SeO_3)_2^{2-}}$	13.31264		1	Original data for β: $\log_{10}(\beta)$ = 12.5, at I = 1.0 M.

2.2.19. Selenate

The formula for the ligand selenate is SeO_4^{2-}; the molecular weight is 142.967.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{H(SeO_4)^{-}}$	1.7	2.3E+4	1	
$Ca^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Ca(SeO_4)}$ ***(aq)***	2		1	
$Sc^{3+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Sc(SeO_4)^{+}}$	3.39033	-8E+3	1	Original data for β: $\log_{10}(\beta)$ = 1.78, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Sc^{3+} + 2\ (SeO_4)^{2-} \rightleftharpoons \mathbf{Sc(SeO_4)_2^{-}}$	4.78711		1	Original data for β: $\log_{10}(\beta)$ = 2.64, at I = 0.5 M.
$Mn(II)^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Mn(II)(SeO_4)}$ ***(aq)***	2.43	1.4E+4	1	
$Co(II)^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Co(II)(SeO_4)}$ ***(aq)***	2.7	1.2E+4	1	
$Ni^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Ni(SeO_4)}$ ***(aq)***	2.67	1.4E+4	1	
$Zn^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Zn(SeO_4)}$ ***(aq)***	2.19		1	
$Zn^{2+} + 2\ (SeO_4)^{2-} \rightleftharpoons \mathbf{Zn(SeO_4)_2^{2-}}$	2.19264		1	Original data for β: $\log_{10}(\beta)$ = 1.38, at I = 1.0 M.
$Cd^{2+} + (SeO_4)^{2-} \rightleftharpoons \mathbf{Cd(SeO_4)}$ ***(aq)***	2.27		1	

2.2.20. Bromide

The formula for the ligand bromide is Br^{-}; the molecular weight is 79.904.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Be^{2+} + Br^{-} \rightleftharpoons \mathbf{BeBr^{+}}$	-1.78352		1	Original data for β: $\log_{10}(\beta)$ = -0.7, at I = 4.0 M.
$Be^{2+} + 2\ Br^{-} \rightleftharpoons \mathbf{BeBr_2}$ ***(aq)***	-2.42528		1	Original data for β: $\log_{10}(\beta)$ = -0.8, at I = 4.0 M.
$Mg^{2+} + Br^{-} \rightleftharpoons \mathbf{MgBr^{+}}$	-1.94046		1	Original data for β: $\log_{10}(\beta)$ = -1.4, at I = 3.0 M.
$Sc^{3+} + Br^{-} \rightleftharpoons \mathbf{ScBr^{2+}}$	0.67824		1	Original data for β: $\log_{10}(\beta)$ = -0.07, at I = 0.7 M at 20°C.
$Sc^{3+} + 2\ Br^{-} \rightleftharpoons \mathbf{ScBr_2^{+}}$	0.94706		1	Original data for β: log10(β) = -0.3, at I = 0.7 M at 20°C.
$Cr(III)^{3+} + Br^{-} \rightleftharpoons \mathbf{Cr(III)Br^{2+}}$	2.52	3.7E+4	1	Original data for ΔH at I = 0.5 M.
$Cr(III)^{3+} + 2\ Br^{-} \rightleftharpoons \mathbf{Cr(III)Br_2^{+}}$	3.46		1	
$Cr(III)^{3+} + 3\ Br^{-} \rightleftharpoons \mathbf{Cr(III)Br_3}$ ***(aq)***	4.4		1	
$Mn(II)^{2+} + Br^{-} \rightleftharpoons \mathbf{Mn(II)Br^{+}}$	0.13678		1	Original data for β: $\log_{10}(\beta)$ = -0.4, at I = 0.5 M.
$Fe(III)^{3+} + Br^{-} \rightleftharpoons \mathbf{Fe(III)Br^{2+}}$	0.6	2.5E+4	1	
$Co(II)^{2+} + Br^{-} \rightleftharpoons \mathbf{Co(II)Br^{+}}$	-1.24046	9.2E+3	1	Original data for β: $\log_{10}(\beta)$ = -0.7, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Ni^{2+} + Br^{-} \rightleftharpoons \mathbf{NiBr^{+}}$	-1.34046	1.1E+4	1	Original data for β: $\log_{10}(\beta)$ = -0.8, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Cu(I)^{+} + Br^{-} \rightleftharpoons \mathbf{Cu(I)Br}$ ***(aq)***	3.53		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(I)^{+}$ + 2 Br^{-} ⇌ **$Cu(I)Br_2^{-}$**	5.86		1	
$Cu(I)^{+}$ + 3 Br^{-} ⇌ **$Cu(I)Br_3^{2-}$**	6.43		1	
$Cu(II)^{2+}$ + Br^{-} ⇌ **$Cu(II)Br^{+}$**	-0.04	1.2E+4	1	Original data for ΔH at I = 3.0 M.
Zn^{2+} + Br^{-} ⇌ **$ZnBr^{+}$**	-0.07	1E+3	1	Original data for ΔH at I = 3.0 M.
Ga^{3+} + Br^{-} ⇌ **$GaBr^{2+}$**	0.64824		1	Original data for β: $log_{10}(\beta)$ = -0.10, at I = 0.7 M at 20°C.
Y^{3+} + Br^{-} ⇌ **YBr^{2+}**	0.45948		1	Original data for β: $log_{10}(\beta)$ = -0.15, at I = 1.0 M.
Pd^{2+} + Br^{-} ⇌ **$PdBr^{+}$**	5.57632	-2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 5.17, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
Pd^{2+} + 2 Br^{-} ⇌ **$PdBr_2$ *(aq)***	10.02948		1	Original data for β: $log_{10}(\beta)$ = 9.42, at I = 1.0 M.
Pd^{2+} + 3 Br^{-} ⇌ **$PdBr_3^{-}$**	13.30948		1	Original data for β: $log_{10}(\beta)$ = 12.7, at I = 1.0 M.
Pd^{2+} + 4 Br^{-} ⇌ **$PdBr_4^{2-}$**	15.12715	-5.48E+4	1	Original data for β: $log_{10}(\beta)$ = 14.7, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ag^{+} + Br^{-} ⇌ **AgBr *(aq)***	4.6		1	
Ag^{+} + 2 Br^{-} ⇌ **$AgBr_2^{-}$**	7.5		1	
Ag^{+} + 3 Br^{-} ⇌ **$AgBr_3^{2-}$**	8.1	-5.48E+4	1	Original data for ΔH at I = 5.0 M.
Ag^{+} + 4 Br^{-} ⇌ **$AgBr_4^{3-}$**	8.7	-7.99E+4	1	Original data for ΔH at I = 5.0 M.
Cd^{2+} + Br^{-} ⇌ **$CdBr^{+}$**	2.15	-3E+3	1	
Cd^{2+} + 2 Br^{-} ⇌ **$CdBr_2$ *(aq)***	3	-3E+3	1	
Cd^{2+} + 3 Br^{-} ⇌ **$CdBr_3^{-}$**	3	0	1	Original data for ΔH at I = 1.0 M.
Cd^{2+} + 4 Br^{-} ⇌ **$CdBr_4^{2-}$**	2.9	-2E+3	1	Original data for ΔH at I = 3.0 M.
In^{3+} + Br^{-} ⇌ **$InBr^{2+}$**	1.94669	2E+3	1	Original data for β: $log_{10}(\beta)$ = 1.99, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
In^{3+} + 2 Br^{-} ⇌ **$InBr_2^{+}$**	2.52781	7.5E+3	1	Original data for β: $log_{10}(\beta)$ = 2.6, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Sn(II)^{2+}$ + Br^{-} ⇌ **$Sn(II)Br^{+}$**	1.16	4E+3	1	Original data for ΔH at I = 3.0 M.
$Sn(II)^{2+}$ + 2 Br^{-} ⇌ **$Sn(II)Br_2$ *(aq)***	1.7	1.2E+4	1	Original data for ΔH at I = 3.0 M.
$Sn(II)^{2+}$ + 3 Br^{-} ⇌ **$Sn(II)Br_3^{-}$**	0.38931	8E+3	1	Original data for β: $log_{10}(\beta)$ = 1.2, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Cs^{+} + Br^{-} ⇌ **CsBr *(aq)***	0.03		1	
Ce^{3+} + Br^{-} ⇌ **$CeBr^{2+}$**	0.40948		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M.
Pr^{3+} + Br^{-} ⇌ **$PrBr^{2+}$**	-1.01069		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 3.0 M.
Sm^{3+} + Br^{-} ⇌ **$SmBr^{2+}$**	-1.01069		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 3.0 M.
Eu^{3+} + Br^{-} ⇌ **$EuBr^{2+}$**	0.40948		1	Original data for β: $log_{10}(\beta)$ = -0.2, at I = 1.0 M.
Eu^{3+} + 2 Br^{-} ⇌ **$EuBr_2^{+}$**	0.61580		1	Original data for β: $log_{10}(\beta)$ = -0.4, at I = 1.0 M.
Gd^{3+} + Br^{-} ⇌ **$GdBr^{2+}$**	-1.21069		1	Original data for β: $log_{10}(\beta)$ = -0.4, at I = 3.0 M at 20°C.
Tb^{3+} + Br^{-} ⇌ **$TbBr^{2+}$**	-1.21069		1	Original data for β: $log_{10}(\beta)$ = -0.4, at I = 3.0 M at 20°C.
Ho^{3+} + Br^{-} ⇌ **$HoBr^{2+}$**	-1.41069		1	Original data for β: $log_{10}(\beta)$ = -0.6, at I = 3.0 M.
Er^{3+} + Br^{-} ⇌ **$ErBr^{2+}$**	-1.31069		1	Original data for β: $log_{10}(\beta)$ = -0.5, at I = 3.0 M.
$Pt(II)^{2+}$ + Br^{-} ⇌ **$Pt(II)Br^{+}$**	5.68632		1	Original data for β: $log_{10}(\beta)$ = 5.28, at I = 1.0 M.
$Pt(II)^{2+}$ + 2 Br^{-} ⇌ **$Pt(II)Br_2$ *(aq)***	10.30948		1	Original data for β: $log_{10}(\beta)$ = 9.7, at I = 1.0 M.
$Pt(II)^{2+}$ + 3 Br^{-} ⇌ **$Pt(II)Br_3^{-}$**	13.90948		1	Original data for β: $log_{10}(\beta)$ = 13.3, at I = 1.0 M.
$Pt(II)^{2+}$ + 4 Br^{-} ⇌ **$Pt(II)Br_4^{2-}$**	16.50632		1	Original data for β: $log_{10}(\beta)$ = 16.1, at I = 1.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Hg(II)^{2+} + Br^{-} \rightleftharpoons$ **$Hg(II)Br^{+}$**	9.60678	-4.22E+4	1	Original data for β: $log_{10}(\beta)$ = 9.07, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Hg(II)^{2+} + (OH)^{-} + Br^{-} \rightleftharpoons$ **$Hg(II)Br(OH)$ *(aq)***	20.23377		1	Hg(II)L ⇌ Hg(II)(OH)L + H $log_{10}(\beta)$ = -3.37 I = 0.5 M Hg(II) + L ⇌ Hg(II)L $log_{10}(\beta)$ = 9.07 I = 0.5 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.72861 I = 0.5 M Hg(II) + L + OH ⇌ Hg(II)(OH)L $log_{10}(\beta)$ = 19.42861 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 20.23377
$Hg(II)^{2+} + 2\ Br^{-} \rightleftharpoons$ **$Hg(II)Br_2$ *(aq)***	18.07516	-8.74E+4	1	Original data for β: $log_{10}(\beta)$ = 17.27, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Hg(II)^{2+} + 3\ Br^{-} \rightleftharpoons$ **$Hg(II)Br_3^{-}$**	20.50516	-9.91E+4	1	Original data for β: $log_{10}(\beta)$ = 19.7, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Hg(II)^{2+} + 4\ Br^{-} \rightleftharpoons$ **$Hg(II)Br_4^{2-}$**	21.73678	-1.14E+5	1	Original data for β: $log_{10}(\beta)$ = 21.2, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Pb(II)^{2+} + Br^{-} \rightleftharpoons$ **$Pb(II)Br^{+}$**	1.7	8E+3	1	
$Pb(II)^{2+} + 2\ Br^{-} \rightleftharpoons$ **$Pb(II)Br_2$ *(aq)***	2.6	-4E+3	1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+} + 3\ Br^{-} \rightleftharpoons$ **$Pb(II)Br_3^{-}$**	3.00516	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 2.2, at I = 0.5 M. Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+} + 4\ Br^{-} \rightleftharpoons$ **$Pb(II)Br_4^{2-}$**	2.37112	-1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 2.4, at I = 2.0 M. Original data for ΔH at I = 3.0 M.
$Bi^{3+} + Br^{-} \rightleftharpoons$ **$BiBr^{2+}$**	3.24	1.3E+4	1	
$Bi^{3+} + 2\ Br^{-} \rightleftharpoons$ **$BiBr_2^{+}$**	5.5		1	
$Bi^{3+} + 3\ Br^{-} \rightleftharpoons$ **$BiBr_3$ *(aq)***	7.7		1	
$Bi^{3+} + 4\ Br^{-} \rightleftharpoons$ **$BiBr_4^{-}$**	9		1	
$Bi^{3+} + 5\ Br^{-} \rightleftharpoons$ **$BiBr_5^{2-}$**	9.9		1	
$Bi^{3+} + 6\ Br^{-} \rightleftharpoons$ **$BiBr_6^{3-}$**	8.7		1	
$(U(VI)O_2)^{2+} + Br^{-} \rightleftharpoons$ **$(U(VI)O_2)Br^{+}$**	0.2		1	

2.2.21. Molybdate

The formula for the ligand molybdate is MoO_4^{2-}; the molecular weight is 159.946.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + (MoO_4)^{2-} \rightleftharpoons$ **$H(MoO_4)^{-}$**	4.20715	2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 3.78, at I = 0.1 M. Original data for ΔH at I = 1.0 M.
$2\ H^{+} + (MoO_4)^{2-} \rightleftharpoons$ **$H_2(MoO_4)$ *(aq)***	8.19073	-2.6E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 3.77 I = 0.1 M ΔH = -4.6E+4 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 3.78 I = 0.1 M ΔH = 2.0E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 7.55 I = 0.1 M ΔH = -2.6E+4 I = 0 M: $log_{10}(\beta)$ = 8.19073
$8\ H^{+} + 7\ (MoO_4)^{2-} \rightleftharpoons$ **$Mo_7O_{24}^{6-}$** $+ 4\ H_2O$	52.99	-2.28E+5	1	Original data for β: $log_{10}(\beta)$ = 52.99, at I = 0.1 M. Original data for ΔH at I = 1.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$9\ H^+ + 7\ (MoO_4)^{2-} \rightleftharpoons \mathbf{HMo_7O_{24}^{5-}} + 4\ H_2O$	59.37145	-2.18E+5	1	$Mo_7O_{24} + H \rightleftharpoons HMo_7O_{24}$ $log_{10}(\beta) = 5.10$ I = 0.1 M ΔH = 1E+4 (Original data for ΔH at I = 3.0 M) <u>$8\ H + 7\ L \rightleftharpoons Mo_7O_{24}$ $log_{10}(\beta) = 52.99$ I = 0.1 M ΔH = -2.28E+5</u> $9\ H + 7\ L \rightleftharpoons HMo_7O_{24}$ $log_{10}(\beta) = 58.09$ I = 0.1 M ΔH = -2.18E+5 I=0: 59.37145
$10\ H^+ + 7\ (MoO_4)^{2-} \rightleftharpoons \mathbf{H_2Mo_7O_{24}^{4-}} + 4\ H_2O$	64.14933	-2.15E+5	1	$HMo_7O_{24} + H \rightleftharpoons H_2Mo_7O_{24}$ $log_{10}(\beta) = 3.71$ I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 3.0 M) <u>$9\ H + 7\ L \rightleftharpoons HMo_7O_{24}$ $log_{10}(\beta) = 58.09$ I = 0.1 M ΔH = -2.18E+5</u> $10\ H + 7\ L \rightleftharpoons H_2Mo_7O_{24}$ $log_{10}(\beta) = 61.80$ I = 0.1 M ΔH = -2.15E+5 I = 0 M: $log_{10}(\beta) = 64.14933$
$11\ H^+ + 7\ (MoO_4)^{2-} \rightleftharpoons \mathbf{H_3Mo_7O_{24}^{3-}} + 4\ H_2O$	67.39197	-2.17E+5	1	$H_2Mo_7O_{24} + H \rightleftharpoons H_3Mo_7O_{24}$ $log_{10}(\beta) = 2.43$ I = 1.0 M ΔH = -2E+3 (Original data for ΔH at I = 3.0 M) <u>$10\ H + 7\ L \rightleftharpoons H_2Mo_7O_{24}$ $log_{10}(\beta) = 61.91457$ I = 1.0 M ΔH = -2.15E+5</u> $11\ H + 7\ L \rightleftharpoons H_3Mo_7O_{24}$ $log_{10}(\beta) = 64.34457$ I = 1.0 M ΔH = -2.17E+5 I = 0 M: $log_{10}(\beta) = 67.39197$
$34\ H^+ + 19\ (MoO_4)^{2-} \rightleftharpoons \mathbf{Mo_{19}O_{59}^{4-}} + 17\ H_2O$	183.59926		1	Original data for β: $log_{10}(\beta) = 196.3$, at I = 3.0 M.
$6\ H^+ + Al^{3+} + 6\ (MoO_4)^{2-} \rightleftharpoons \mathbf{AlMo_6O_{21}^{3-}} + 3\ H_2O$	54.97582		1	Original data for β: $log_{10}(\beta) = 50.95$, at I = 0.5 M.

2.2.22. Iodide

The formula for the ligand iodide is I^-; the molecular weight is 126.90.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$K^+ + I^- \rightleftharpoons$ **KI *(aq)***	-0.4	4E+3	1	
$Cu(I)^+ + I^- \rightleftharpoons$ **Cu(I)I *(aq)***	5.90316		1	Original data for β: $log_{10}(\beta) = 5.7$, at I = 1.0 M.
$Cu(I)^+ + 2\ I^- \rightleftharpoons \mathbf{Cu(I)I_2^-}$	8.9		1	
$Cu(I)^+ + 3\ I^- \rightleftharpoons \mathbf{Cu(I)I_3^{2-}}$	10.43		1	Original data for β: $log_{10}(\beta) = 10.43$, at I = 5.0 M.
$Cu(I)^+ + 4\ I^- \rightleftharpoons \mathbf{Cu(I)I_4^{3-}}$	11.04360		1	Original data for β: $log_{10}(\beta) = 9.4$, at I = 5.0 M.
$2\ Cu(I)^+ + 6\ I^- \rightleftharpoons \mathbf{Cu(I)_2I_6^{4-}}$	25.28720		1	Original data for β: $log_{10}(\beta) = 22.0$, at I = 5.0 M.
$Zn^{2+} + I^- \rightleftharpoons \mathbf{ZnI^+}$	-2.04046	-4E+3	1	Original data for β: $log_{10}(\beta) = -1.5$, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Ga^{3+} + I^- \rightleftharpoons \mathbf{GaI^{2+}}$	0.54824		1	Original data for β: $log_{10}(\beta) = -0.2$, at I = 0.7 M at 20°C.
$Rb^+ + I^- \rightleftharpoons$ **RbI *(aq)***	0.04		1	
$Pd^{2+} + I^- \rightleftharpoons \mathbf{PdI^+}$	6.48632		1	Original data for β: $log_{10}(\beta) = 6.08$, at I = 1.0 M.
$Pd^{2+} + 2\ I^- \rightleftharpoons \mathbf{PdI_2}$ ***(aq)***	22.60948		1	Original data for β: $log_{10}(\beta) = 22$, at I = 1.0 M.
$Pd^{2+} + 3\ I^- \rightleftharpoons \mathbf{PdI_3^-}$	26.40948		1	Original data for β: $log_{10}(\beta) = 25.8$, at I = 1.0 M.
$Pd^{2+} + 4\ I^- \rightleftharpoons \mathbf{PdI_4^{2-}}$	28.70632		1	Original data for β: $log_{10}(\beta) = 28.3$, at I = 1.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ Pd^{2+} + 6\ I^- \rightleftharpoons$ **$Pd_2I_6^{2-}$**	58.93580		1	$2\ PdL_4 \rightleftharpoons Pd_2L_6 + 2\ L$ $log_{10}(\beta) = 1.32$ I = 1.0 M $2\ Pd + 8\ L \rightleftharpoons 2\ PdL_4$ $log_{10}(\beta) = 56.6$ I = 1.0 M $2\ Pd + 6\ L \rightleftharpoons Pd_2L_6$ $log_{10}(\beta) = 57.92$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 58.93580$
$Ag^+ + I^- \rightleftharpoons$ **AgI *(aq)***	7.55824		1	Original data for β: $log_{10}(\beta) = 8.1$, at I = 4.0 M.
$Ag^+ + 2\ I^- \rightleftharpoons$ **AgI_2^-**	10.45824		1	Original data for β: $log_{10}(\beta) = 11.0$, at I = 4.0 M.
$Ag^+ + 3\ I^- \rightleftharpoons$ **AgI_3^{2-}**	12.6	-1.22E+5	1	
$Ag^+ + 4\ I^- \rightleftharpoons$ **AgI_4^{3-}**	14.22888		1	Original data for β: $log_{10}(\beta) = 14.2$, at I = 2.0 M.
$2\ Ag^+ + 6\ I^- \rightleftharpoons$ **$Ag_2I_6^{4-}$**	31.86704		1	Original data for β: $log_{10}(\beta) = 29.7$, at I = 4.0 M.
$3\ Ag^+ + 8\ I^- \rightleftharpoons$ **$Ag_3I_8^{5-}$**	50.19232		1	Original data for β: $log_{10}(\beta) = 46.4$, at I = 4.0 M.
$Cd^{2+} + I^- \rightleftharpoons$ **CdI^+**	2.28	-9.6E+3	1	
$Cd^{2+} + 2\ I^- \rightleftharpoons$ **CdI_2 *(aq)***	3.92	-1.2E+4	1	Original data for ΔH at I = 1.0 M.
$Cd^{2+} + 3\ I^- \rightleftharpoons$ **CdI_3^-**	5	-1.8E+4	1	Original data for ΔH at I = 1.0 M.
$Cd^{2+} + 4\ I^- \rightleftharpoons$ **CdI_4^{2-}**	6	-3.5E+4	1	Original data for ΔH at I = 1.0 M.
$In^{3+} + I^- \rightleftharpoons$ **InI^{2+}**	0.94669	-2E+3	1	Original data for β: $log_{10}(\beta) = 0.99$, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$In^{3+} + 2\ I^- \rightleftharpoons$ **InI_2^+**	2.18781	3E+3	1	Original data for β: $log_{10}(\beta) = 2.26$, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Sn(II)^{2+} + I^- \rightleftharpoons$ **$Sn(II)I^+$**	-0.38352		1	Original data for β: $log_{10}(\beta) = 0.70$, at I = 4.0 M.
$Sn(II)^{2+} + 2\ I^- \rightleftharpoons$ **$Sn(II)I_2$ *(aq)***	-0.49528		1	Original data for β: $log_{10}(\beta) = 1.13$, at I = 4.0 M.
$Sn(II)^{2+} + 3\ I^- \rightleftharpoons$ **$Sn(II)I_3^-$**	0.47472		1	Original data for β: $log_{10}(\beta) = 2.1$, at I = 4.0 M.
$Sn(II)^{2+} + 4\ I^- \rightleftharpoons$ **$Sn(II)I_4^{2-}$**	1.21648		1	Original data for β: $log_{10}(\beta) = 2.3$, at I = 4.0 M.
$Sn(II)^{2+} + 6\ I^- \rightleftharpoons$ **$Sn(II)I_6^{4-}$**	4.22528		1	Original data for β: $log_{10}(\beta) = 2.6$, at I = 4.0 M.
$Sn(II)^{2+} + 8\ I^- \rightleftharpoons$ **$Sn(II)I_8^{6-}$**	8.60112		1	Original data for β: $log_{10}(\beta) = 2.1$, at I = 4.0 M.
$Cs^+ + I^- \rightleftharpoons$ **CsI *(aq)***	-0.03		1	
$Eu^{3+} + I^- \rightleftharpoons$ **EuI^{2+}**	0.20948		1	Original data for β: $log_{10}(\beta) = -0.4$, at I = 1.0 M.
$Hf^{4+} + I^- \rightleftharpoons$ **HfI^{3+}**	-1.58091		1	Original data for β: $log_{10}(\beta) = -0.5$, at I = 3.0 M at 20°C.
$Pt(II)^{2+} + I^- \rightleftharpoons$ **$Pt(II)I^+$**	5.38632		1	Original data for β: $log_{10}(\beta) = 4.98$, at I = 1.0 M.
$Pt(II)^{2+} + 2\ I^- \rightleftharpoons$ **$Pt(II)I_2$ *(aq)***	25.60948		1	Original data for β: $log_{10}(\beta) = 25$, at I = 1.0 M.
$Pt(II)^{2+} + 3\ I^- \rightleftharpoons$ **$Pt(II)I_3^-$**	28.60948		1	Original data for β: $log_{10}(\beta) = 28$, at I = 1.0 M.
$Pt(II)^{2+} + 4\ I^- \rightleftharpoons$ **$Pt(II)I_4^{2-}$**	30.00632		1	Original data for β: $log_{10}(\beta) = 29.6$, at I = 1.0 M at 18°C.
$Hg(II)^{2+} + I^- \rightleftharpoons$ **$Hg(II)I^+$**	13.40678	-7.15E+4	1	Original data for β: $log_{10}(\beta) = 12.87$, at I = 0.5 M.
$Hg(II)^{2+} + (OH)^- + I^- \rightleftharpoons$ **Hg(II)I(OH) *(aq)***	23.40377		1	$Hg(II)L \rightleftharpoons Hg(II)OHL + H$ $log_{10}(\beta) = -4.0$ I = 0.5 M $Hg(II) + L \rightleftharpoons Hg(II)L$ $log_{10}(\beta) = 12.87$ I = 0.5 M $OH + H \rightleftharpoons H_2O$ $log_{10}(\beta) = 13.72861$ I = 0.5 M $Hg(II) + OH + L \rightleftharpoons Hg(II)OHL$ $log_{10}(\beta) = 22.59861$ I = 0.5 M I = 0 M: $log_{10}(\beta) = 23.40377$
$Hg(II)^{2+} + 2\ I^- \rightleftharpoons$ **$Hg(II)I_2$ *(aq)***	24.62516	-1.43E+5	1	Original data for β: $log_{10}(\beta) = 23.82$, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Hg(II)^{2+} + 3\ I^- \rightleftharpoons$ **$Hg(II)I_3^-$**	28.40516		1	Original data for β: $log_{10}(\beta) = 27.6$, at I = 0.5 M.
$Hg(II)^{2+} + 4\ I^- \rightleftharpoons$ **$Hg(II)I_4^{2-}$**	30.33678	-1.81E+5	1	Original data for β: $log_{10}(\beta) = 29.8$, at I = 0.5 M.
$Pb(II)^{2+} + I^- \rightleftharpoons$ **$Pb(II)I^+$**	2		1	
$Pb(II)^{2+} + 2\ I^- \rightleftharpoons$ **$Pb(II)I_2$ *(aq)***	3.2		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+}$ + 3 I^- ⇌ **$Pb(II)I_3^-$**	3.9		1	
$Pb(II)^{2+}$ + 4 I^- ⇌ **$Pb(II)I_4^{2-}$**	4.5		1	
Bi^{3+} + I^- ⇌ **BiI^{2+}**	4.43516		1	Original data for β: $log_{10}(\beta)$ = 3.63, at I = 0.5 M.
Bi^{3+} + 4 I^- ⇌ **BiI_4^-**	14.91337		1	Original data for β: $log_{10}(\beta)$ = 15.0, at I = 2.0 M at 20 °C.
Bi^{3+} + 5 I^- ⇌ **BiI_5^{2-}**	16.72781		1	Original data for β: $log_{10}(\beta)$ = 16.8, at I = 2.0 M.
Bi^{3+} + 6 I^- ⇌ **BiI_6^{3-}**	18.75669		1	Original data for β: $log_{10}(\beta)$ = 18.8, at I = 2.0 M.

2.2.23. Tungstate

The formula for the ligand tungstate is WO_4^{2-}; the molecular weight is 247.836.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(WO_4)^{2-}$ ⇌ **$H(WO_4)^-$**	3.6	4E+3	1	Original data for ΔH at I = 0.1 M.
2 H^+ + $(WO_4)^{2-}$ ⇌ **$H_2(WO_4)$ *(aq)***	5.8		1	

2.2.24. Cyanide

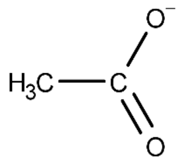
The formula for the ligand cyanide is CN^-; the molecular weight is 26.018.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(CN)^-$ ⇌ **H(CN) *(aq)***	9.21	-4.359E+4	1	
$Mn(II)^{2+}$ + $(CN)^-$ ⇌ **$Mn(II)(CN)^+$**	2.30632		1	Original data for β: $log_{10}(\beta)$ = 1.9, at I = 1.0 M.
$Mn(II)^{2+}$ + 2 $(CN)^-$ ⇌ **$Mn(II)(CN)_2$ *(aq)***	3.96948		1	Original data for β: $log_{10}(\beta)$ = 3.36, at I = 1.0 M.
$Fe(II)^{2+}$ + 6 $(CN)^-$ ⇌ **$Fe(II)(CN)_6^{4-}$**	35.4	-3.58E+5	1	
$Fe(III)^{3+}$ + 6 $(CN)^-$ ⇌ **$Fe(III)(CN)_6^{3-}$**	43.6	-2.93E+5	1	
$Co(II)^{2+}$ + 3 $(CN)^-$ ⇌ **$Co(II)(CN)_3^-$**	14.30948		1	Original data for β: $log_{10}(\beta)$ = 13.7, at I = 1.0 M.
$Co(II)^{2+}$ + 5 $(CN)^-$ ⇌ **$Co(II)(CN)_5^{3-}$**	23	-2.57E+5	1	Original data for β: $log_{10}(\beta)$ = 23.0, at I = 1.0 M.
Ni^{2+} + $(CN)^-$ ⇌ **$Ni(CN)^+$**	7.7		3	
Ni^{2+} + 4 $(CN)^-$ ⇌ **$Ni(CN)_4^{2-}$**	30.2	-1.80E+5	1	
H^+ + Ni^{2+} + 4 $(CN)^-$ ⇌ **$NiH(CN)_4^-$**	36.02715		1	NiL_4 + H ⇌ $NiHL_4$ $log_{10}(\beta)$ = 5.4 I = 0.1 M Ni + 4 L ⇌ NiL_4 $log_{10}(\beta)$ = 29.77285 I = 0.1 M Ni + H + 4 L ⇌ $NiHL_4$ $log_{10}(\beta)$ = 35.17285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 36.02715
2 H^+ + Ni^{2+} + 4 $(CN)^-$ ⇌ **$NiH_2(CN)_4$ *(aq)***	40.74073		1	$NiHL_4$ + H ⇌ NiH_2L_4 $log_{10}(\beta)$ = 4.5 I = 0.1 M Ni + H + 4 L ⇌ $NiHL_4$ $log_{10}(\beta)$ = 35.17285 I = 0.1 M Ni + 2 H + 4 L ⇌ NiH_2L_4 $log_{10}(\beta)$ = 39.67285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 40.74073

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ H^+ + Ni^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{NiH_3(CN)_4^+}$	43.34073		1	$NiH_2L_4 + H \rightleftharpoons NiH_3L_4$ $log_{10}(\beta) = 2.6$ I = 0.1 M $Ni + 2\ H + 4\ L \rightleftharpoons NiH_2L_4$ $log_{10}(\beta) = 39.67285$ I = 0.1 M $Ni + 3\ H + 4\ L \rightleftharpoons NiH_3L_4$ $log_{10}(\beta) = 42.27285$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 43.34073$
$Cu(I)^+ + 2\ (CN)^- \rightleftharpoons \mathbf{Cu(I)(CN)_2^-}$	23.9	-1.21E+5	1	
$Cu(I)^+ + 3\ (CN)^- \rightleftharpoons \mathbf{Cu(I)(CN)_3^{2-}}$	29.2	-1.674E+5	1	$Cu(I)L_2 + L \rightleftharpoons Cu(I)L_3$ $log_{10}(\beta) = 5.30$ ΔH = -4.64E+4 $Cu(I) + 2\ L \rightleftharpoons Cu(I)L_2$ $log_{10}(\beta) = 23.9$ ΔH = -1.21E+5 $Cu(I) + 3\ L \rightleftharpoons Cu(I)L_3$ $log_{10}(\beta) = 29.2$ ΔH = -1.674E+5
$Cu(I)^+ + 4\ (CN)^- \rightleftharpoons \mathbf{Cu(I)(CN)_4^{3-}}$	30.8	-2.142E+5	1	$Cu(I)L_3 + L \rightleftharpoons Cu(I)L_4$ $log_{10}(\beta) = 1.6$ ΔH = -4.68E+4 $Cu(I) + 3\ L \rightleftharpoons Cu(I)L_3$ $log_{10}(\beta) = 29.2$ ΔH = -1.674E+5 $Cu(I) + 4\ L \rightleftharpoons Cu(I)L_4$ $log_{10}(\beta) = 30.8$ ΔH = -2.142E+5
$Cu(II)^{2+} + 2\ (CN)^- \rightleftharpoons \mathbf{Cu(II)(CN)_2}$ ***(aq)***	16.3		3	
$Cu(II)^{2+} + 3\ (CN)^- \rightleftharpoons \mathbf{Cu(II)(CN)_3^-}$	21.6		3	
$Cu(II)^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{Cu(II)(CN)_4^{2-}}$	23.1		3	
$Zn^{2+} + (CN)^- \rightleftharpoons \mathbf{Zn(CN)^+}$	4.57954		1	Original data for β: $log_{10}(\beta) = 4.98$, at I = 3.0 M when NaCl is the background electrolyte; $log_{10}(\beta) = 5.26$ (also at I = 3.0 M) when $NaClO_4$ is the background electrolyte. The average log-value (5.12) was converted to I = 0 M.
$Zn^{2+} + 2\ (CN)^- \rightleftharpoons \mathbf{Zn(CN)_2}$ ***(aq)***	11.07	-4.60E+4	1	
$Zn^{2+} + 3\ (CN)^- \rightleftharpoons \mathbf{Zn(CN)_3^-}$	16.05	-8.45E+4	1	
$Zn^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{Zn(CN)_4^{2-}}$	19.62	-1.16E+5	1	
$Pd^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{Pd(CN)_4^{2-}}$	42.4	-3.86E+5	1	
$Pd^{2+} + 5\ (CN)^- \rightleftharpoons \mathbf{Pd(CN)_5^{3-}}$	45.3	-3.87E+5	1	
$Ag^+ + (OH)^- + (CN)^- \rightleftharpoons \mathbf{Ag(CN)(OH)^-}$	13.22		1	
$Ag^+ + 2\ (CN)^- \rightleftharpoons \mathbf{Ag(CN)_2^-}$	20.48	-1.37E+5	1	
$Ag^+ + 3\ (CN)^- \rightleftharpoons \mathbf{Ag(CN)_3^{2-}}$	21.7	-1.40E+5	1	
$Cd^{2+} + (CN)^- \rightleftharpoons \mathbf{Cd(CN)^+}$	6.01	-3.0E+4	1	
$Cd^{2+} + 2\ (CN)^- \rightleftharpoons \mathbf{Cd(CN)_2}$ ***(aq)***	11.12	-5.43E+4	1	
$Cd^{2+} + 3\ (CN)^- \rightleftharpoons \mathbf{Cd(CN)_3^-}$	15.65	-9.03E+4	1	
$Cd^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{Cd(CN)_4^{2-}}$	17.92	-1.12E+5	1	
$Pt(II)^{2+} + (CN)^- \rightleftharpoons \mathbf{Pt(II)(CN)^+}$	41.40632		1	Original data for β: $log_{10}(\beta) = 41.0$, at I = 1.0 M at 18°C.
$Hg(II)^{2+} + (CN)^- \rightleftharpoons \mathbf{Hg(II)(CN)^+}$	17.00	-9.70E+4	1	
$Hg(II)^{2+} + (OH)^- + (CN)^- \rightleftharpoons \mathbf{Hg(II)(CN)(OH)}$ ***(aq)***	28.85669	-1.94E+5	1	Original data for β: $log_{10}(\beta) = 28.9$, at I = 2.0 M at 30°C.
$Hg(II)^{2+} + 2\ (CN)^- \rightleftharpoons \mathbf{Hg(II)(CN)_2}$ ***(aq)***	32.75	-2.23E+5	1	
$Hg(II)^{2+} + 3\ (CN)^- \rightleftharpoons \mathbf{Hg(II)(CN)_3^-}$	36.31	-2.49E+5	1	
$Hg(II)^{2+} + 4\ (CN)^- \rightleftharpoons \mathbf{Hg(II)(CN)_4^{2-}}$	38.97		1	

2.2.25. Acetate

The ligand in its neutral form is acetic acid (ethanoic acid), $C_2H_4O_2$. The ligand L as it is present in the database is acetate, $C_2H_3O_2^-$. Its molecular weight is 59.044. Its structural formula is shown on the right.



Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(H_2BO_3)^-$ + (acetate)$^-$ ⇌ **B(OH)$_3$(acetate)$^-$**	8.806		1	H + H_2BO_3 ⇌ H_3BO_3 (=B(OH)$_3$) log$_{10}$(β) = 9.236 B(OH)$_3$ + L ⇌ B(OH)$_3$L log$_{10}$(β) = -0.43 H + H_2BO_3 + L ⇌ B(OH)$_3$L log$_{10}$(β) = 8.806
H^+ + (acetate)$^-$ ⇌ **H(acetate) *(aq)***	4.757	4.1E+2	1	
Li^+ + (acetate)$^-$ ⇌ **Li(acetate) *(aq)***	0.28		1	
Be^{2+} + (acetate)$^-$ ⇌ **Be(acetate)$^+$**	2.04715		1	Original data for β: log$_{10}$(β) = 1.62, at I = 0.1 M.
Be^{2+} + 2 (acetate)$^-$ ⇌ **Be(acetate)$_2$ *(aq)***	3.00073		1	Original data for β: log$_{10}$(β) = 2.36, at I = 0.1 M.
Na^+ + (acetate)$^-$ ⇌ **Na(acetate) *(aq)***	-0.12	8E+3	1	
Mg^{2+} + (acetate)$^-$ ⇌ **Mg(acetate)$^+$**	1.26		1	
Al^{3+} + (acetate)$^-$ ⇌ **Al(acetate)$^{2+}$**	2.75	1.6E+4	1	Original data for ΔH at I = 0.1 M.
Al^{3+} + $(OH)^-$ + (acetate)$^-$ ⇌ **Al(acetate)(OH)$^+$**	13.85016		1	AlL ⇌ AlOHL + H log$_{10}$(β) = -3.1 I = 1.0 Al + L ⇌ AlL log$_{10}$(β) = 2.14052 I = 1.0 OH + H ⇌ H_2O log$_{10}$(β) = 13.79384 I = 1.0 Al + L + OH ⇌ AlOHL log$_{10}$(β) = 12.83436 I = 1.0 I = 0 M: log$_{10}$(β) = 13.85016
Al^{3+} + 2 (acetate)$^-$ ⇌ **Al(acetate)$_2^+$**	4.6	4.1E+4	1	Original data for ΔH at I = 0.1 M.
2 Al^{3+} + 2 $(OH)^-$ + (acetate)$^-$ ⇌ **Al$_2$(acetate)(OH)$_2^{3+}$**	25.57755		1	2 Al + L ⇌ $Al_2(OH)_2$L + 2 H log$_{10}$(β) = -3.49 I = 0.5 2 OH + 2 H ⇌ 2 H_2O log$_{10}$(β) = 27.45722 I = 0.5 2 Al + L + 2 OH ⇌ $Al_2(OH)_2$L log$_{10}$(β) = 23.96722 I = 0.5 I = 0 M: log$_{10}$(β) = 25.57755
K^+ + (acetate)$^-$ ⇌ **K(acetate) *(aq)***	-0.27	4E+3	1	
Ca^{2+} + (acetate)$^-$ ⇌ **Ca(acetate)$^+$**	1.18	4E+3	1	
Sc^{3+} + (acetate)$^-$ ⇌ **Sc(acetate)$^{2+}$**	4.12073		1	Original data for β: log$_{10}$(β) = 3.48, at I = 0.1 M.
Cr(III)$^{3+}$ + (acetate)$^-$ ⇌ **Cr(III)(acetate)$^{2+}$**	5.43516	4E+3	1	Original data for β: log$_{10}$(β) = 4.63, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
Cr(III)$^{3+}$ + 2 (acetate)$^-$ ⇌ **Cr(III)(acetate)$_2^+$**	8.42194		1	Original data for β: log$_{10}$(β) = 7.08, at I = 0.5 M.
Cr(III)$^{3+}$ + 3 (acetate)$^-$ ⇌ **Cr(III)(acetate)$_3$ *(aq)***	11.21033		1	Original data for β: log$_{10}$(β) = 9.6, at I = 0.5 M.
Mn(II)$^{2+}$ + (acetate)$^-$ ⇌ **Mn(II)(acetate)$^+$**	1.4		1	
Fe(II)$^{2+}$ + (acetate)$^-$ ⇌ **Fe(II)(acetate)$^+$**	-0.00046		1	Original data for β: log$_{10}$(β) = 0.54, at I = 3.0 M.
Fe(III)$^{3+}$ + (acetate)$^-$ ⇌ **Fe(III)(acetate)$^{2+}$**	4.24073	2.5E+4	1	Original data for β: log$_{10}$(β) = 3.6, at I = 0.1 M. Original data for ΔH at I = 1.0 M.
Fe(III)$^{3+}$ + 2 (acetate)$^-$ ⇌ **Fe(III)(acetate)$_2^+$**	7.56788		1	Original data for β: log$_{10}$(β) = 6.5, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$3\ Fe(III)^{3+} + 3\ (OH)^{-} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Fe(III)_3(acetate)_2(OH)_3^{4+}}$	46.50986		1	$3\ Fe(III) + 2\ L \rightleftharpoons Fe(III)_3(OH)_3L_2 + 3\ H$ $\log_{10}(\beta) = 5.87$ I = 3.0 M $3\ OH + 3\ H \rightleftharpoons 3\ H_2O$ $\log_{10}(\beta) = 42.80169$ I = 3.0 M $3\ Fe(III) + 3\ OH + 2\ L \rightleftharpoons Fe(III)_3(OH)_3L_2$ $\log_{10}(\beta) = 48.67169$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 46.50986$
$3\ Fe(III)^{3+} + 2\ (OH)^{-} + 6\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Fe(III)_3(acetate)_6(OH)_2^{+}}$	51.0414	-4.15E+4	1	$3\ Fe(III) + 6\ L \rightleftharpoons Fe(III)_3(OH)_2L_6 + 2\ H$ $\log_{10}(\beta) = 20.0$ I = 1.0 M ΔH = 7.07E+4 (Original data for ΔH at I = 1.0 M) $2\ OH + 2\ H \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.58768$ I = 1.0 M ΔH = -1.122E+5 $3\ Fe(III) + 2\ OH + 6\ L \rightleftharpoons Fe(III)_3(OH)_2L_6$ $\log_{10}(\beta) = 47.58768$ I = 1.0 M ΔH = -4.15E+4 I = 0 M: $\log_{10}(\beta) = 51.04140$
$7\ Fe(III)^{3+} + 9\ (OH)^{-} + 6\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Fe(III)_7(acetate)_6(OH)_9^{6+}}$	139.99027		1	$7\ Fe(III) + 6\ L \rightleftharpoons Fe(III)_7(OH)_9L_6 + 9\ H$ $\log_{10}(\beta) = 17.26$ I = 3.0 M $9\ OH + 9\ H \rightleftharpoons 9\ H_2O$ $\log_{10}(\beta) = 128.40507$ I = 3.0 M $7\ Fe(III) + 9\ OH + 6\ L \rightleftharpoons Fe(III)_7(OH)_9L_6$ $\log_{10}(\beta) = 145.66507$ I = 3.0 M I = 0 M: $\log_{10}(\beta) = 139.99027$
$Co(II)^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Co(II)(acetate)^{+}}$	1.38		1	
$Co(II)^{2+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Co(II)(acetate)_2}$ ***(aq)***	0.75669		1	Original data for β: $\log_{10}(\beta) = 0.8$, at I = 2.0 M.
$Ni^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Ni(acetate)^{+}}$	1.44	8.7E+3	1	
$Ni^{2+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Ni(acetate)_2}$ ***(aq)***	2.4	1.0E+4	1	
$Cu(II)^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Cu(II)(acetate)^{+}}$	2.21	7.1E+3	1	
$Cu(II)^{2+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Cu(II)(acetate)_2}$ ***(aq)***	3.4	1.1E+4	1	
$Cu(II)^{2+} + 3\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Cu(II)(acetate)_3^{-}}$	3.94073	6.2E+3	1	Original data for β: $\log_{10}(\beta) = 3.3$, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Zn^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Zn(acetate)^{+}}$	1.57	8.3E+3	1	Original data for ΔH at I = 3.0 M.
$Zn^{2+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Zn(acetate)_2}$ ***(aq)***	1.90516	2.2E+4	1	Original data for β: $\log_{10}(\beta) = 1.1$, at I = 0.5 M. Original data for ΔH at I = 3.0 M.
$Zn^{2+} + 3\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Zn(acetate)_3^{-}}$	0.75931	2.6E+4	1	Original data for β: $\log_{10}(\beta) = 1.57$, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Rb^{+} + (acetate)^{-} \rightleftharpoons$ **Rb(acetate)** ***(aq)***	-0.15642		1	Original data for β: $\log_{10}(\beta) = -0.37$, at I = 0.1 M.
$Sr^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Sr(acetate)^{+}}$	1.12		1	
$Y^{3+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Y(acetate)^{2+}}$	2.32073	1.3E+4	1	Original data for β: $\log_{10}(\beta) = 1.68$, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
$Y^{3+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Y(acetate)_2^{+}}$	4.23788	2.2E+4	1	Original data for β: $\log_{10}(\beta) = 3.17$, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
$Y^{3+} + 3\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Y(acetate)_3}$ ***(aq)***	3.41337	2.1E+4	1	Original data for β: $\log_{10}(\beta) = 3.5$, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
$Pd^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Pd(acetate)^{+}}$	4.74632	-4E+3	1	Original data for β: $\log_{10}(\beta) = 4.34$, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$Ag^{+} + (acetate)^{-} \rightleftharpoons$ **Ag(acetate)** ***(aq)***	0.73	3E+3	1	
$Ag^{+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Ag(acetate)_2^{-}}$	0.64	3E+3	1	
$Cd^{2+} + (acetate)^{-} \rightleftharpoons$ $\mathbf{Cd(acetate)^{+}}$	1.92	9.6E+3	1	
$Cd^{2+} + 2\ (acetate)^{-} \rightleftharpoons$ $\mathbf{Cd(acetate)_2}$ ***(aq)***	2.71516	1.5E+4	1	Original data for β: $\log_{10}(\beta) = 1.91$, at I = 0.5 M.

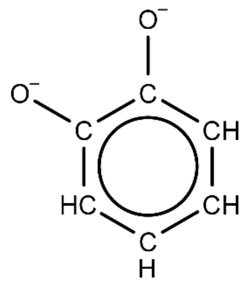
Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + 3 $(acetate)^-$ ⇌ **$Cd(acetate)_3^-$**	2.98516	1.5E+4	1	Original data for β: $log_{10}(β)$ = 2.18, at I = 0.5 M.
In^{3+} + $(acetate)^-$ ⇌ **$In(acetate)^{2+}$**	3.45669		1	Original data for β: $log_{10}(β)$ = 3.50, at I = 2.0 M at 20°C.
In^{3+} + 2 $(acetate)^-$ ⇌ **$In(acetate)_2^+$**	5.87781		1	Original data for β: $log_{10}(β)$ = 5.95, at I = 2.0 M at 20°C.
In^{3+} + 3 $(acetate)^-$ ⇌ **$In(acetate)_3$ *(aq)***	7.81337		1	Original data for β: $log_{10}(β)$ = 7.90, at I = 2.0 M at 20°C.
In^{3+} + 4 $(acetate)^-$ ⇌ **$In(acetate)_4^-$**	8.99337		1	Original data for β: $log_{10}(β)$ = 9.08, at I = 2.0 M at 20°C.
$Sn(II)^{2+}$ + $(acetate)^-$ ⇌ **$Sn(II)(acetate)^+$**	2.92954		1	Original data for β: $log_{10}(β)$ = 3.47, at I = 3.0 M.
$Sn(II)^{2+}$ + 2 $(acetate)^-$ ⇌ **$Sn(II)(acetate)_2$ *(aq)***	5.22931		1	Original data for β: $log_{10}(β)$ = 6.04, at I = 3.0 M.
$Sn(II)^{2+}$ + 3 $(acetate)^-$ ⇌ **$Sn(II)(acetate)_3^-$**	6.45931		1	Original data for β: $log_{10}(β)$ = 7.27, at I = 3.0 M.
Cs^+ + $(acetate)^-$ ⇌ **Cs(acetate) *(aq)***	-0.11642		1	Original data for β: $log_{10}(β)$ = -0.33, at I = 0.1 M.
Ba^{2+} + $(acetate)^-$ ⇌ **$Ba(acetate)^+$**	1.07		1	
La^{3+} + $(acetate)^-$ ⇌ **$La(acetate)^{2+}$**	2.55	9.2E+3	1	Original data for ΔH at I = 2.0 M.
La^{3+} + 2 $(acetate)^-$ ⇌ **$La(acetate)_2^+$**	4.12	1.5E+4	1	Original data for ΔH at I = 2.0 M.
La^{3+} + 3 $(acetate)^-$ ⇌ **$La(acetate)_3$ *(aq)***	4.81145	1.9E+4	1	Original data for β: $log_{10}(β)$ = 3.53, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Ce^{3+} + $(acetate)^-$ ⇌ **$Ce(acetate)^{2+}$**	2.55073	8.7E+3	1	Original data for β: $log_{10}(β)$ = 1.91, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Ce^{3+} + 2 $(acetate)^-$ ⇌ **$Ce(acetate)_2^+$**	4.15788	1.5E+4	1	Original data for β: $log_{10}(β)$ = 3.09, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Ce^{3+} + 3 $(acetate)^-$ ⇌ **$Ce(acetate)_3$ *(aq)***	4.96145	2.1E+4	1	Original data for β: $log_{10}(β)$ = 3.68, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Pr^{3+} + $(acetate)^-$ ⇌ **$Pr(acetate)^{2+}$**	2.65073	7.1E+3	1	Original data for β: $log_{10}(β)$ = 2.01, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Pr^{3+} + 2 $(acetate)^-$ ⇌ **$Pr(acetate)_2^+$**	4.47788	1.7E+4	1	Original data for β: $log_{10}(β)$ = 3.41, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Pr^{3+} + 3 $(acetate)^-$ ⇌ **$Pr(acetate)_3$ *(aq)***	3.24337	1.5E+4	1	Original data for β: $log_{10}(β)$ = 3.33, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
Nd^{3+} + $(acetate)^-$ ⇌ **$Nd(acetate)^{2+}$**	2.67	7.1E+3	1	Original data for ΔH at I = 2.0 M.
Nd^{3+} + 2 $(acetate)^-$ ⇌ **$Nd(acetate)_2^+$**	4.54	1.4E+4	1	Original data for ΔH at I = 2.0 M.
Nd^{3+} + 3 $(acetate)^-$ ⇌ **$Nd(acetate)_3$ *(aq)***	3.51337	1.8E+4	1	Original data for β: $log_{10}(β)$ = 3.60, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
Sm^{3+} + $(acetate)^-$ ⇌ **$Sm(acetate)^{2+}$**	2.84	6.2E+3	1	Original data for ΔH at I = 2.0 M.
Sm^{3+} + 2 $(acetate)^-$ ⇌ **$Sm(acetate)_2^+$**	4.8	1.2E+4	1	Original data for ΔH at I = 2.0 M.
Sm^{3+} + 3 $(acetate)^-$ ⇌ **$Sm(acetate)_3$ *(aq)***	3.81337	1.5E+4	1	Original data for β: $log_{10}(β)$ = 3.90, at I = 2.0 M. Original data for ΔH at I = 2.0 M.
Eu^{3+} + $(acetate)^-$ ⇌ **$Eu(acetate)^{2+}$**	2.77073	7.1E+3	1	Original data for β: $log_{10}(β)$ = 2.13, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Eu^{3+} + 2 $(acetate)^-$ ⇌ **$Eu(acetate)_2^+$**	4.70788		1	Original data for β: $log_{10}(β)$ = 3.64, at I = 0.1 M.
Eu^{3+} + 3 $(acetate)^-$ ⇌ **$Eu(acetate)_3$ *(aq)***	5.52145		1	Original data for β: $log_{10}(β)$ = 4.24, at I = 0.1 M.
Gd^{3+} + $(acetate)^-$ ⇌ **$Gd(acetate)^{2+}$**	2.66073	7.9E+3	1	Original data for β: $log_{10}(β)$ = 2.02, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Gd^{3+} + 2 $(acetate)^-$ ⇌ **$Gd(acetate)_2^+$**	4.53788	1.3E+4	1	Original data for β: $log_{10}(β)$ = 3.47, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Gd^{3+} + 3 $(acetate)^-$ ⇌ **$Gd(acetate)_3$ *(aq)***	5.54145	1.4E+4	1	Original data for β: $log_{10}(β)$ = 4.26, at I = 0.1 M. Original data for ΔH at I = 2.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Tb^{3+} + $(acetate)^{-}$ ⇌ **$Tb(acetate)^{2+}$**	2.55073		1	Original data for β: $log_{10}(\beta)$ = 1.91, at I = 0.1 M.
Tb^{3+} + 2 $(acetate)^{-}$ ⇌ **$Tb(acetate)_2^{+}$**	4.29788		1	Original data for β: $log_{10}(\beta)$ = 3.23, at I = 0.1 M.
Tb^{3+} + 3 $(acetate)^{-}$ ⇌ **$Tb(acetate)_3$ *(aq)***	5.67145		1	Original data for β: $log_{10}(\beta)$ = 4.39, at I = 0.1 M.
Dy^{3+} + $(acetate)^{-}$ ⇌ **$Dy(acetate)^{2+}$**	2.49073	1.2E+4	1	Original data for β: $log_{10}(\beta)$ = 1.85, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Dy^{3+} + 2 $(acetate)^{-}$ ⇌ **$Dy(acetate)_2^{+}$**	4.22788	1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 3.16, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Dy^{3+} + 3 $(acetate)^{-}$ ⇌ **$Dy(acetate)_3$ *(aq)***	5.58145	1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 4.30, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Dy^{3+} + 4 $(acetate)^{-}$ ⇌ **$Dy(acetate)_4^{-}$**	3.81337		1	Original data for β: $log_{10}(\beta)$ = 3.90, at I = 2.0 M at 20°C.
Ho^{3+} + $(acetate)^{-}$ ⇌ **$Ho(acetate)^{2+}$**	2.45073	1.3E+4	1	Original data for β: $log_{10}(\beta)$ = 1.81, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Ho^{3+} + 2 $(acetate)^{-}$ ⇌ **$Ho(acetate)_2^{+}$**	4.17788	2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 3.11, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Ho^{3+} + 3 $(acetate)^{-}$ ⇌ **$Ho(acetate)_3$ *(aq)***	5.55145	1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 4.27, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Er^{3+} + $(acetate)^{-}$ ⇌ **$Er(acetate)^{2+}$**	2.43073	1.3E+4	1	Original data for β: $log_{10}(\beta)$ = 1.79, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Er^{3+} + 2 $(acetate)^{-}$ ⇌ **$Er(acetate)_2^{+}$**	4.12788	2.3E+4	1	Original data for β: $log_{10}(\beta)$ = 3.06, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Er^{3+} + 3 $(acetate)^{-}$ ⇌ **$Er(acetate)_3$ *(aq)***	5.48145	2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 4.20, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Er^{3+} + 4 $(acetate)^{-}$ ⇌ **$Er(acetate)_4^{-}$**	3.61337		1	Original data for β: $log_{10}(\beta)$ = 3.7, at I = 2.0 M at 20°C.
Tm^{3+} + $(acetate)^{-}$ ⇌ **$Tm(acetate)^{2+}$**	2.47073		1	Original data for β: $log_{10}(\beta)$ = 1.83, at I = 0.1 M.
Tm^{3+} + 2 $(acetate)^{-}$ ⇌ **$Tm(acetate)_2^{+}$**	4.08788		1	Original data for β: $log_{10}(\beta)$ = 3.02, at I = 0.1 M.
Tm^{3+} + 3 $(acetate)^{-}$ ⇌ **$Tm(acetate)_3$ *(aq)***	5.45145		1	Original data for β: $log_{10}(\beta)$ = 4.17, at I = 0.1 M.
Yb^{3+} + $(acetate)^{-}$ ⇌ **$Yb(acetate)^{2+}$**	2.56	1.4E+4	1	Original data for ΔH at I = 2.0 M.
Yb^{3+} + 2 $(acetate)^{-}$ ⇌ **$Yb(acetate)_2^{+}$**	4.36	2.5E+4	1	Original data for ΔH at I = 2.0 M.
Yb^{3+} + 3 $(acetate)^{-}$ ⇌ **$Yb(acetate)_3$ *(aq)***	5.43145	2.7E+4	1	Original data for β: $log_{10}(\beta)$ = 4.15, at I = 0.1 M. Original data for ΔH at I = 2.0 M.
Lu^{3+} + $(acetate)^{-}$ ⇌ **$Lu(acetate)^{2+}$**	2.49073		1	Original data for β: $log_{10}(\beta)$ = 1.85, at I = 0.1 M.
Lu^{3+} + 2 $(acetate)^{-}$ ⇌ **$Lu(acetate)_2^{+}$**	4.22788		1	Original data for β: $log_{10}(\beta)$ = 3.16, at I = 0.1 M.
Lu^{3+} + 3 $(acetate)^{-}$ ⇌ **$Lu(acetate)_3$ *(aq)***	5.30145		1	Original data for β: $log_{10}(\beta)$ = 4.02, at I = 0.1 M.
$Hg(II)^{2+}$ + $(acetate)^{-}$ ⇌ **$Hg(II)(acetate)^{+}$**	4.3		1	
$Hg(II)^{2+}$ + 2 $(acetate)^{-}$ ⇌ **$Hg(II)(acetate)_2$ *(aq)***	7.63931		1	Original data for β: $log_{10}(\beta)$ = 8.45, at I = 3.0 M.
$Hg(II)^{2+}$ + 3 $(acetate)^{-}$ ⇌ **$Hg(II)(acetate)_3^{-}$**	14.1		3	
$Hg(II)^{2+}$ + 4 $(acetate)^{-}$ ⇌ **$Hg(II)(acetate)_4^{2-}$**	17.6		3	
$Pb(II)^{2+}$ + $(acetate)^{-}$ ⇌ **$Pb(II)(acetate)^{+}$**	2.58	-4E+2	1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + 2 $(acetate)^{-}$ ⇌ **$Pb(II)(acetate)_2$ *(aq)***	4.02	-8E+2	1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + 3 $(acetate)^{-}$ ⇌ **$Pb(II)(acetate)_3^{-}$**	3.37669	-4.6E+3	1	Original data for β: $log_{10}(\beta)$ = 3.42, at I = 2.0 M. Original data for ΔH at I = 3.0 M.
$(U(VI)O_2)^{2+}$ + $(acetate)^{-}$ ⇌ **$(U(VI)O_2)(acetate)^{+}$**	3.10715	2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 2.68, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$(U(VI)O_2)^{2+}$ + 2 $(acetate)^-$ ⇌ **$(U(VI)O_2)(acetate)_2$ *(aq)***	5.03948	1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 4.43, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$(U(VI)O_2)^{2+}$ + 3 $(acetate)^-$ ⇌ **$(U(VI)O_2)(acetate)_3^-$**	7.05948	1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 6.45, at I = 1.0 M. Original data for ΔH at I = 1.0 M.

2.2.26. Catechol

The ligand in its neutral form is 1,2-dihydroxybenzene (catechol), $C_6H_6O_2$. The ligand L as it is present in the database is the anion, $C_6H_4O_2^{2-}$. Its molecular weight is 108.096. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(catechol)^{2-}$ ⇌ **$H(catechol)^-$**	13.72715	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 13.3, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
2 H^+ + $(catechol)^{2-}$ ⇌ **$H_2(catechol)$ *(aq)***	23.17715	-4.5E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 9.45 ΔH = -2.5E+4 (Original data for ΔH at I = 0.1 M) <u>H + L ⇌ HL $log_{10}(\beta)$ = 13.72715 ΔH = -2.0E+4</u> 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 23.17715 ΔH = -4.5E+4
Be^{2+} + $(catechol)^{2-}$ ⇌ **Be(catechol) *(aq)***	13.84072		1	Be + H_2L ⇌ BeL + 2 H $log_{10}(\beta)$ = -9.55 I = 0.1 M (Original data for β at T = 20°C) <u>2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M</u> Be + L ⇌ BeL $log_{10}(\beta)$ = 12.98642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.84072
H^+ + Be^{2+} + $(catechol)^{2-}$ ⇌ **$BeH(catechol)^+$**	19.00072		1	BeL + H ⇌ BeHL $log_{10}(\beta)$ = 5.16 I = 0.1 M (Original data for β at T = 20°C) <u>Be + L ⇌ BeL $log_{10}(\beta)$ = 12.98642 I = 0.1 M</u> Be + H + L ⇌ BeHL $log_{10}(\beta)$ = 18.14642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.00072

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Be^{2+} + 2 $(catechol)^{2-}$ ⇌ **$Be(catechol)_2^{2-}$**	23.31714		1	BeL + H_2L ⇌ BeL_2 + 2 H $\log_{10}(\beta)$ = -13.06 I = 0.1 M (Original data for β at T = 20°C) Be + L ⇌ BeL $\log_{10}(\beta)$ = 12.98642 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Be + 2 L ⇌ BeL_2 $\log_{10}(\beta)$ = 22.46284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 23.31714
H^+ + Be^{2+} + 2 $(catechol)^{2-}$ ⇌ **$BeH(catechol)_2^-$**	30.43429		1	BeL_2 + H ⇌ $BeHL_2$ $\log_{10}(\beta)$ = 6.69 I = 0.1 M (Original data for β at T = 20°C) Be + 2 L ⇌ BeL_2 $\log_{10}(\beta)$ = 22.46284 I = 0.1 M Be + H + 2 L ⇌ $BeHL_2$ $\log_{10}(\beta)$ = 29.15284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 30.43429
Al^{3+} + $(catechol)^{2-}$ ⇌ **$Al(catechol)^+$**	17.73787		1	Al + H_2L ⇌ AlL + 2 H $\log_{10}(\beta)$ = -6.08 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 16.45642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 17.73787
Al^{3+} + 2 $(catechol)^{2-}$ ⇌ **$Al(catechol)_2^-$**	31.50144		1	AlL + H_2L ⇌ AlL_2 + 2 H $\log_{10}(\beta)$ = -9.20 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 16.45642 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Al + 2 L ⇌ AlL_2 $\log_{10}(\beta)$ = 29.79284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 31.50144
H^+ + Al^{3+} + 2 $(catechol)^{2-}$ ⇌ **$AlH(catechol)_2$ *(aq)***	37.76502		1	AlL_2 + H ⇌ $AlHL_2$ $\log_{10}(\beta)$ = 6.05 I = 0.1 M Al + 2 L ⇌ AlL_2 $\log_{10}(\beta)$ = 29.79284 I = 0.1 M Al + H + 2 L ⇌ $AlHL_2$ $\log_{10}(\beta)$ = 35.84284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 37.76502
Al^{3+} + 3 $(catechol)^{2-}$ ⇌ **$Al(catechol)_3^{3-}$**	40.05071		1	AlL_2 + H_2L ⇌ AlL_3 + 2 H $\log_{10}(\beta)$ = -13.56 I = 0.1 M Al + 2 L ⇌ AlL_2 $\log_{10}(\beta)$ = 29.79284 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Al + 3 L ⇌ AlL_3 $\log_{10}(\beta)$ = 38.76926 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 40.05071
H^+ + Al^{3+} + 3 $(catechol)^{2-}$ ⇌ **$AlH(catechol)_3^{2-}$**	48.74144		1	AlL_3 + H ⇌ $AlHL_3$ $\log_{10}(\beta)$ = 8.05 I = 0.1 M Al + 3 L ⇌ AlL_3 $\log_{10}(\beta)$ = 38.76926 I = 0.1 M Al + 3 L + H ⇌ $AlHL_3$ $\log_{10}(\beta)$ = 46.81926 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 48.74144
2 Al^{3+} + 2 $(OH)^-$ + 2 $(catechol)^{2-}$ ⇌ **$Al_2(catechol)_2(OH)_2$ *(aq)***	54.60689		1	2 Al + 2 L ⇌ $Al_2(OH)_2L_2$ + 2 H $\log_{10}(\beta)$ = 24.05 I = 0.1 M 2 OH + 2 H ⇌ 2 H_2O $\log_{10}(\beta)$ = 27.56684 I = 0.1 M 2 Al + 2 L + 2 OH ⇌ $Al_2(OH)_2L_2$ $\log_{10}(\beta)$ = 51.61684 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 54.60689
3 Al^{3+} + 3 $(OH)^-$ + 3 $(catechol)^{2-}$ ⇌ **$Al_3(catechol)_3(OH)_3$ *(aq)***	84.02795		1	3 Al + 3 H_2L ⇌ $Al_3(OH)_3L_3$ + 9 H $\log_{10}(\beta)$ = -29.91 I = 0.5 M 6 H + 3 L ⇌ 3 H_2L $\log_{10}(\beta)$ = 67.11597 I = 0.5 M 3 OH + 3 H ⇌ 3 H_2O $\log_{10}(\beta)$ = 41.18583 I = 0.5 M 3 Al + 3 OH + 3 L ⇌ $Al_3(OH)_3L_3$ $\log_{10}(\beta)$ = 78.39180 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 84.02795

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Sc^{3+} + $(catechol)^{2-}$ ⇌ **$Sc(catechol)^{+}$**	18.91787		1	Sc + H_2L ⇌ ScL + 2 H $\log_{10}(\beta)$ = -4.90 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Sc + L ⇌ ScL $\log_{10}(\beta)$ = 17.63642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.91787
$Mn(II)^{2+}$ + $(catechol)^{2-}$ ⇌ **Mn(II)(catechol) *(aq)***	8.69072		1	Mn(II) + H_2L ⇌ Mn(II)L + 2 H $\log_{10}(\beta)$ = -14.70 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Mn(II) + L ⇌ Mn(II)L $\log_{10}(\beta)$ = 7.83642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 8.69072
$Mn(II)^{2+}$ + 2 $(catechol)^{2-}$ ⇌ **$Mn(II)(catechol)_2^{2-}$**	14.12714		1	Mn(II)L + H_2L ⇌ Mn(II)L_2 + 2 H $\log_{10}(\beta)$ = -17.1 I = 0.1 M Mn(II) + L ⇌ Mn(II)L $\log_{10}(\beta)$ = 7.83642 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Mn(II) + 2 L ⇌ Mn(II)L_2 $\log_{10}(\beta)$ = 13.27284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 14.12714
$Fe(II)^{2+}$ + $(catechol)^{2-}$ ⇌ **Fe(II)(catechol) *(aq)***	9.09072		1	Fe(II) + H_2L ⇌ Fe(II)L + 2 H $\log_{10}(\beta)$ = -14.3 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Fe(II) + L ⇌ Fe(II)L $\log_{10}(\beta)$ = 8.23642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 9.09072
$Fe(II)^{2+}$ + 2 $(catechol)^{2-}$ ⇌ **$Fe(II)(catechol)_2^{2-}$**	14.95839		1	Fe(II)L + H_2L ⇌ Fe(II)L_2 + 2 H $\log_{10}(\beta)$ = -16.7 I = 1.0 M Fe(II) + L ⇌ Fe(II)L $\log_{10}(\beta)$ = 8.27808 I = 1.0 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.56767 I = 1.0 M Fe (II) + 2 L ⇌ Fe(II)L_2 $\log_{10}(\beta)$ = 14.14575 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 1495839
H^{+} + 2 $Fe(II)^{2+}$ + 2 $(catechol)^{2-}$ ⇌ **$Fe(II)_2H(catechol)_2^{+}$**	39.20860		1	2 Fe(II) + 2 HL ⇌ $Fe(II)_2HL_2$ + H $\log_{10}(\beta)$ = 10.9 I = 0.1 M 2 H + 2 L ⇌ 2 HL $\log_{10}(\beta)$ = 26.6 I = 0.1 M 2 Fe(II) + 2 H + 2 L ⇌ $Fe(II)_2HL_2$ $\log_{10}(\beta)$ = 37.5 I = 0.1 M I=0: 39.20860
$Fe(III)^{3+}$ + $(catechol)^{2-}$ ⇌ **$Fe(III)(catechol)^{+}$**	21.61787	-4.1E+4	1	Fe(III) + H_2L ⇌ Fe(III)L + 2 H $\log_{10}(\beta)$ = -2.2 I = 0.1 M ΔH = 4E+3 (Original data for ΔH at I = 1.0 M) 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M ΔH = -4.5E+4 Fe(III) + L ⇌ Fe(III)L $\log_{10}(\beta)$ = 20.33642 I = 0.1 M ΔH = -4.1E+4 I = 0 M: $\log_{10}(\beta)$ = 21.61787
$Fe(III)^{3+}$ + 2 $(catechol)^{2-}$ ⇌ **$Fe(III)(catechol)_2^{-}$**	37.05144		1	Fe(III)L + H_2L ⇌ Fe(III)L_2 + 2 H $\log_{10}(\beta)$ = -7.53 I = 0.1 M Fe(III) + L ⇌ Fe(III)L $\log_{10}(\beta)$ = 20.33642 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Fe(III) + 2 L ⇌ Fe(III)L_2 $\log_{10}(\beta)$ = 35.34284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 37.05144
$Fe(III)^{3+}$ + 3 $(catechol)^{2-}$ ⇌ **$Fe(III)(catechol)_3^{3-}$**	46.00071		1	Fe(III)L_2 + H_2L ⇌ Fe(III)L_3 + 2 H $\log_{10}(\beta)$ = -13.16 I = 0.1 M Fe(III) + 2 L ⇌ Fe(III)L_2 $\log_{10}(\beta)$ = 35.34284 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 22.53642 I = 0.1 M Fe(III) + 3 L ⇌ Fe(III)L_3 $\log_{10}(\beta)$ = 44.71926 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 46.00071

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+} + (catechol)^{2-} \rightleftharpoons$ **Co(II)(catechol) *(aq)***	9.67072		1	Co(II) + $H_2L \rightleftharpoons$ Co(II)L + 2 H $log_{10}(\beta)$ = -13.72 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Co(II) + L $\rightleftharpoons$ Co(II)L $log_{10}(\beta)$ = 8.81642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 9.67072
$Co(II)^{2+} + 2\ (catechol)^{2-} \rightleftharpoons$ **$Co(II)(catechol)_2^{2-}$**	16.10714		1	Co(II)L + $H_2L \rightleftharpoons Co(II)L_2$ + 2 H $log_{10}(\beta)$ = -16.1 I = 0.1 M Co(II) + L $\rightleftharpoons$ Co(II)L $log_{10}(\beta)$ = 8.81642 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Co(II) + 2 L $\rightleftharpoons Co(II)L_2$ $log_{10}(\beta)$ = 15.25284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.10714
$Ni^{2+} + (catechol)^{2-} \rightleftharpoons$ **Ni(catechol) *(aq)***	10.06072		1	Ni + $H_2L \rightleftharpoons$ NiL + 2 H $log_{10}(\beta)$ = -13.33 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Ni + L $\rightleftharpoons$ NiL $log_{10}(\beta)$ = 9.20642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.06072
$Ni^{2+} + 2\ (catechol)^{2-} \rightleftharpoons$ **$Ni(catechol)_2^{2-}$**	16.19714		1	NiL + $H_2L \rightleftharpoons NiL_2$ + 2 H $log_{10}(\beta)$ = -16.4 I = 0.1 M Ni + L $\rightleftharpoons$ NiL $log_{10}(\beta)$ = 9.20642 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Ni + 2 L $\rightleftharpoons NiL_2$ $log_{10}(\beta)$ = 15.34284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.19714
$Cu(II)^{2+} + (catechol)^{2-} \rightleftharpoons$ **Cu(II)(catechol) *(aq)***	15.07715	-3.2E+4	1	Cu(II) + $H_2L \rightleftharpoons$ Cu(II)L + 2 H $log_{10}(\beta)$ = -8.10 ΔH = 1.3E+4 (Original data for ΔH at I = 0.1 M) 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 23.17715 ΔH = -4.5E+4 Cu(II) + L $\rightleftharpoons$ Cu(II)L $log_{10}(\beta)$ = 15.07715 ΔH = -3.2E+4
$H^+ + Cu(II)^{2+} + (catechol)^{2-} \rightleftharpoons$ **$Cu(II)H(catechol)^+$**	15.92715	-5.2E+4	1	Cu(II)L + H $\rightleftharpoons$ Cu(II)HL $log_{10}(\beta)$ = 0.85 I = 0.1 M ΔH = -2.0E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + L $\rightleftharpoons$ Cu(II)L $log_{10}(\beta)$ = 14.22285 I = 0.1 M ΔH = -3.2E+4 Cu(II) + H + L $\rightleftharpoons$ Cu(II)HL $log_{10}(\beta)$ = 15.07285 I = 0.1 M ΔH = -5.2E+4 I = 0 M: $log_{10}(\beta)$ = 15.92715
$Cu(II)^{2+} + 2\ (catechol)^{2-} \rightleftharpoons$ **$Cu(II)(catechol)_2^{2-}$**	26.50430		1	Cu(II)L + $H_2L \rightleftharpoons Cu(II)L_2$ + 2 H $log_{10}(\beta)$ = -11.75 Cu(II) + L $\rightleftharpoons$ Cu(II)L $log_{10}(\beta)$ = 15.07715 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 23.17715 Cu(II) + 2 L $\rightleftharpoons Cu(II)L_2$ $log_{10}(\beta)$ = 26.50430
$Zn^{2+} + (catechol)^{2-} \rightleftharpoons$ **Zn(catechol) *(aq)***	10.89072		1	Zn + $H_2L \rightleftharpoons$ ZnL + 2 H $log_{10}(\beta)$ = -12.5 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Zn + L $\rightleftharpoons$ ZnL $log_{10}(\beta)$ = 10.03642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.89072
$Zn^{2+} + 2\ (catechol)^{2-} \rightleftharpoons$ **$Zn(catechol)_2^{2-}$**	18.92714		1	ZnL + $H_2L \rightleftharpoons ZnL_2$ + 2 H $log_{10}(\beta)$ = -14.5 I = 0.1 M Zn + L $\rightleftharpoons$ ZnL $log_{10}(\beta)$ = 10.03642 I = 0.1 M 2 H + L $\rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M Zn + 2 L $\rightleftharpoons ZnL_2$ $log_{10}(\beta)$ = 18.07284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.92714

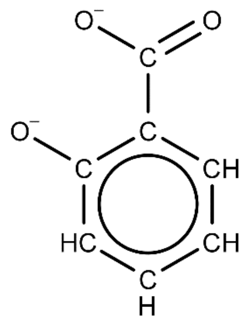
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ga^{3+} + $(catechol)^{2-}$ ⇌ **$Ga(catechol)^{+}$**	20.81787		1	Ga + H_2L ⇌ GaL + 2 H $log_{10}(\beta)$ = -3.0 I = 0.1 M (Original data for β at T = 20°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Ga + L ⇌ GaL $log_{10}(\beta)$ = 19.53642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.81787
Pd^{2+} + $(catechol)^{2-}$ ⇌ **Pd(catechol) *(aq)***	21.17072		1	Pd + H_2L ⇌ PdL + 2 H $log_{10}(\beta)$ = -2.22 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Pd + L ⇌ PdL $log_{10}(\beta)$ = 20.31642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.17072
Cd^{2+} + $(catechol)^{2-}$ ⇌ **Cd(catechol) *(aq)***	9.69072		1	Cd + H_2L ⇌ CdL + 2 H $log_{10}(\beta)$ = -13.7 I = 0.1 M (Original data for β at T = 30°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Cd + L ⇌ CdL $log_{10}(\beta)$ = 8.83642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 9.69072
La^{3+} + $(catechol)^{2-}$ ⇌ **$La(catechol)^{+}$**	11.33787		1	La + H_2L ⇌ LaL + 2 H $log_{10}(\beta)$ = -12.48 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M La + L ⇌ LaL $log_{10}(\beta)$ = 10.05642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 11.33787
Pr^{3+} + $(catechol)^{2-}$ ⇌ **$Pr(catechol)^{+}$**	12.18787		1	Pr + H_2L ⇌ PrL + 2 H $log_{10}(\beta)$ = -11.63 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Pr + L ⇌ PrL $log_{10}(\beta)$ = 10.90642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.18787
Nd^{3+} + $(catechol)^{2-}$ ⇌ **$Nd(catechol)^{+}$**	12.37787		1	Nd + H_2L ⇌ NdL + 2 H $log_{10}(\beta)$ = -11.44 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Nd + L ⇌ NdL $log_{10}(\beta)$ = 11.09642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.37787
Sm^{3+} + $(catechol)^{2-}$ ⇌ **$Sm(catechol)^{+}$**	13.37787		1	Sm + H_2L ⇌ SmL + 2 H $log_{10}(\beta)$ = -10.44 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Sm + L ⇌ SmL $log_{10}(\beta)$ = 12.09642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.37787
Eu^{3+} + $(catechol)^{2-}$ ⇌ **$Eu(catechol)^{+}$**	12.93787		1	Eu + H_2L ⇌ EuL + 2 H $log_{10}(\beta)$ = -10.88 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Eu + L ⇌ EuL $log_{10}(\beta)$ = 11.65642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.93787
Gd^{3+} + $(catechol)^{2-}$ ⇌ **$Gd(catechol)^{+}$**	13.07787		1	Gd + H_2L ⇌ GdL + 2 H $log_{10}(\beta)$ = -10.74 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Gd + L ⇌ GdL $log_{10}(\beta)$ = 11.79642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.07787
Dy^{3+} + $(catechol)^{2-}$ ⇌ **$Dy(catechol)^{+}$**	13.21787		1	Dy + H_2L ⇌ DyL + 2 H $log_{10}(\beta)$ = -10.60 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Dy + L ⇌ DyL $log_{10}(\beta)$ = 11.93642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.21787

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ho^{3+} + $(catechol)^{2-}$ ⇌ **$Ho(catechol)^{+}$**	13.29787		1	Ho + H_2L ⇌ HoL + 2 H $log_{10}(\beta)$ = -10.52 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Ho + L ⇌ HoL $log_{10}(\beta)$ = 12.01642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.29787
Er^{3+} + $(catechol)^{2-}$ ⇌ **$Er(catechol)^{+}$**	13.30787		1	Er + H_2L ⇌ ErL + 2 H $log_{10}(\beta)$ = -10.51 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Er + L ⇌ ErL $log_{10}(\beta)$ = 12.02642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.30787
Tm^{3+} + $(catechol)^{2-}$ ⇌ **$Tm(catechol)^{+}$**	13.43787		1	Tm + H_2L ⇌ TmL + 2 H $log_{10}(\beta)$ = -10.38 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Tm + L ⇌ TmL $log_{10}(\beta)$ = 12.15642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.43787
Yb^{3+} + $(catechol)^{2-}$ ⇌ **$Yb(catechol)^{+}$**	13.54787		1	Yb + H_2L ⇌ YbL + 2 H $log_{10}(\beta)$ = -10.27 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Yb + L ⇌ YbL $log_{10}(\beta)$ = 12.26642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.54787
Lu^{3+} + $(catechol)^{2-}$ ⇌ **$Lu(catechol)^{+}$**	13.18787		1	Lu + H_2L ⇌ LuL + 2 H $log_{10}(\beta)$ = -10.63 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M Lu + L ⇌ LuL $log_{10}(\beta)$ = 11.90642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.18787
$(U(VI)O_2)^{2+}$ + $(catechol)^{2-}$ ⇌ **$(U(VI)O_2)(catechol)$ *(aq)***	16.25072		1	$(U(VI)O_2)$ + H_2L ⇌ $(U(VI)O_2)L$ + 2 H $log_{10}(\beta)$ = -7.14 I = 0.1 M (Original data for β at T = 20°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M $(U(VI)O_2)$ + L ⇌ $(U(VI)O_2)L$ $log_{10}(\beta)$ = 15.39642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.25072
H^{+} + $(U(VI)O_2)^{2+}$ + $(catechol)^{2-}$ ⇌ **$(U(VI)O_2)H(catechol)^{+}$**	20.18072		1	$(U(VI)O_2)L$ + H ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 3.93 I = 0.1 M (Original data for β at T = 20°C) $(U(VI)O_2)$ + L ⇌ $(U(VI)O_2)L$ $log_{10}(\beta)$ = 15.39642 I = 0.1 M $(U(VI)O_2)$ + H + L ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 19.32642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.18072
H^{+} + $(U(VI)O_2)^{2+}$ + 2 $(catechol)^{2-}$ ⇌ **$(U(VI)O_2)H(catechol)_2^{-}$**	34.83429		1	$(UO_2)L$ + H_2L ⇌ $(UO_2)HL_2$ + H $log_{10}(\beta)$ = -4.38 I = 0.1 M (Original data for β at T = 20°C) (UO_2) + L ⇌ $(UO_2)L$ $log_{10}(\beta)$ = 15.39642 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 22.53642 I = 0.1 M (UO_2) + 2 L + H ⇌ $(UO_2)HL_2$ $log_{10}(\beta)$ = 33.55284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 34.83429

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + (U(VI)O_2)^{2+} + 3\ (catechol)^{2-} \rightleftharpoons$ **$(U(VI)O_2)H_2(catechol)_3^{2-}$**	51.98429		1	$(UO_2)HL_2 + H_2L \rightleftharpoons (UO_2)H_2L_3 + H$ $log_{10}(\beta)$ = -5.60 I = 0.1 M (Original data for β at T = 20°C) $(UO_2) + 2\ L + H \rightleftharpoons (UO_2)HL_2$ $log_{10}(\beta)$ = 33.55284 I = 0.1 M $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 22.53642 I = 0.1 M $(UO_2) + 3\ L + 2\ H \rightleftharpoons (UO_2)H_2L_3$ $log_{10}(\beta)$ = 50.48926 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 51.98429

2.2.27. Salicylate

The ligand in its neutral form is 2-hydroxybenzoic acid (salicylic acid), $C_7H_6O_3$. The ligand L as it is present in the database is salicylate, $C_7H_4O_3^{2-}$. Its molecular weight is 136.106. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (salicylate)^{2-} \rightleftharpoons$ **$H(salicylate)^-$**	13.7	-3.57E+4	1	
$2\ H^+ + (salicylate)^{2-} \rightleftharpoons$ **$H_2(salicylate)$ *(aq)***	16.672	-3.87E+4	1	$HL + H \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 2.972 ΔH = -3.57E+4 $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 13.7 ΔH = -3E+3 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 16.672 ΔH = -3.87E+4
$Be^{2+} + (salicylate)^{2-} \rightleftharpoons$ **Be(salicylate) *(aq)***	13.49715		1	$Be + HL \rightleftharpoons BeL + H$ $log_{10}(\beta)$ = -0.63 I = 0.1 M ΔH = 4E+3 $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 $Be + L \rightleftharpoons BeL$ $log_{10}(\beta)$ = 12.64285 I = 0.1 M ΔH = -3.17E+4 I = 0 M: $log_{10}(\beta)$ = 13.49715
$H^+ + Be^{2+} + (salicylate)^{2-} \rightleftharpoons$ **$BeH(salicylate)^+$**	15.70632		1	$Be + HL \rightleftharpoons BeHL$ $log_{10}(\beta)$ = 1.6 I = 1.0 M $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 13.29368 I = 1.0 M $Be + H + L \rightleftharpoons BeHL$ $log_{10}(\beta)$ = 14.89368 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 15.70632

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Be^{2+} + $(OH)^{-}$ + $(salicylate)^{2-}$ ⇌ **Be(salicylate)(OH)$^{-}$**	20.19099		1	BeL ⇌ BeOHL + H $\log_{10}(\beta)$ = -7.1 I = 1.0 M Be + L ⇌ BeL $\log_{10}(\beta)$ = 12.68451 I = 1.0 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.79384 I = 1.0 M Be + L + OH ⇌ BeOHL $\log_{10}(\beta)$ = 19.37835 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 20.19099
Be^{2+} + 2 $(salicylate)^{2-}$ ⇌ **Be(salicylate)$_2^{2-}$**	23.37		1	BeL + HL ⇌ BeL_2 + H $\log_{10}(\beta)$ = -3.4 I = 0.1 M Be + L ⇌ BeL $\log_{10}(\beta)$ = 12.64285 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M Be + 2 L ⇌ BeL_2 $\log_{10}(\beta)$ = 22.51570 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 23.37000
H^{+} + Be^{2+} + 2 $(salicylate)^{2-}$ ⇌ **BeH(salicylate)$_2^{-}$**	28.70632		1	BeH_2L_2 ⇌ $BeHL_2$ + H $\log_{10}(\beta)$ = -2.9 I = 1.0 M Be + 2 H + 2 L ⇌ BeH_2L_2 $\log_{10}(\beta)$ = 30.38736 I = 1.0 M Be + H + 2 L ⇌ $BeHL_2$ $\log_{10}(\beta)$ = 27.48736 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 28.70632
2 H^{+} + Be^{2+} + 2 $(salicylate)^{2-}$ ⇌ **BeH$_2$(salicylate)$_2$ *(aq)***	31.80948		1	Be + 2 HL ⇌ BeH_2L_2 $\log_{10}(\beta)$ = 3.8 I = 1.0 M 2 H + 2 L ⇌ 2 HL $\log_{10}(\beta)$ = 26.58736 I = 1.0 M Be + 2 H + 2 L ⇌ BeH_2L_2 $\log_{10}(\beta)$ = 30.38736 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 31.80948
3 Be^{2+} + 3 $(OH)^{-}$ + 3 $(salicylate)^{2-}$ ⇌ **Be$_3$(salicylate)$_3$(OH)$_3^{3-}$**	66.891		1	3 Be + 3 HL ⇌ $Be_3L_3(OH)_3$ + 6 H $\log_{10}(\beta)$ = -16.2 I = 1.0 M 3 H + 3 L ⇌ 3 HL $\log_{10}(\beta)$ = 39.88104 I = 1.0 M 3 OH + 3 H ⇌ 3 H_2O $\log_{10}(\beta)$ = 41.38152 I = 1.0 M 3 Be + 3 L + 3 OH ⇌ $Be_3L_3(OH)_3$ $\log_{10}(\beta)$ = 65.06256 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 66.89100
H^{+} + Na^{+} + $(salicylate)^{2-}$ ⇌ **NaH(salicylate) *(aq)***	13.41358		1	Na + HL ⇌ NaHL $\log_{10}(\beta)$ = -0.5 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M Na + H + L ⇌ NaHL $\log_{10}(\beta)$ = 12.77285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 13.41358
Mg^{2+} + $(salicylate)^{2-}$ ⇌ **Mg(salicylate) *(aq)***	5.75677		1	Mg + HL ⇌ MgL + H $\log_{10}(\beta)$ = -8.48 I = 0.5 M H + L ⇌ HL $\log_{10}(\beta)$ = 13.16322 I = 0.5 M Mg + L ⇌ MgL $\log_{10}(\beta)$ = 4.68322 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 5.75677
H^{+} + Mg^{2+} + $(salicylate)^{2-}$ ⇌ **MgH(salicylate)$^{+}$**	14.1	-2.65E+4	1	Mg + HL ⇌ MgHL $\log_{10}(\beta)$ = 0.4 ΔH = 9.2E+3 H + L ⇌ HL $\log_{10}(\beta)$ = 13.7 ΔH = -3.57E+4 Mg + H + L ⇌ MgHL $\log_{10}(\beta)$ = 14.1 ΔH = -2.65E+4
Al^{3+} + $(salicylate)^{2-}$ ⇌ **Al(salicylate)$^{+}$**	14.37430		1	Al + HL ⇌ AlL + H $\log_{10}(\beta)$ = -0.18 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 13.09285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 14.37430
Al^{3+} + 2 $(salicylate)^{2-}$ ⇌ **Al(salicylate)$_2^{-}$**	25.18430		1	AlL + HL ⇌ AlL_2 + H $\log_{10}(\beta)$ = -2.89 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 13.09285 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M Al + 2 L ⇌ AlL_2 $\log_{10}(\beta)$ = 23.47570 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 25.18430

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Al^{3+} + (OH)$^{-}$ + 2 (salicylate)$^{2-}$ ⇌ **Al(salicylate)$_2$(OH)$^{2-}$**	31.62415		1	AlL$_2$ ⇌ Al(OH)L$_2$ + H log$_{10}$(β) = -7.13 I = 0.1 M Al + 2 L ⇌ AlL$_2$ log$_{10}$(β) = 23.47570 I = 0.1 M OH + H ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Al + 2 L + OH ⇌ Al(OH)L$_2$ log$_{10}$(β) = 30.12912 I = 0.1 M I = 0 M: log$_{10}$(β) = 31.62415
Al^{3+} + 2 (OH)$^{-}$ + 2 (salicylate)$^{2-}$ ⇌ **Al(salicylate)$_2$(OH)$_2$$^{3-}$**	35.51598		1	Al(OH)L$_2$ ⇌ Al(OH)$_2$L$_2$ + H log$_{10}$(β) = -9.3 I = 0.5 M Al + 2 L + OH ⇌ Al(OH)L$_2$ log$_{10}$(β) = 29.74543 I = 0.5 M OH + H ⇌ H$_2$O log$_{10}$(β) = 13.72861 I = 0.5 M Al + 2 L + 2 OH ⇌ Al(OH)$_2$L$_2$ log$_{10}$(β) = 34.17404 I = 0.5 M I = 0 M: log$_{10}$(β) = 35.51598
Al^{3+} + 3 (salicylate)$^{2-}$ ⇌ **Al(salicylate)$_3$$^{3-}$**	32.8		3	
2 Al^{3+} + 2 (OH)$^{-}$ + 2 (salicylate)$^{2-}$ ⇌ **Al$_2$(salicylate)$_2$(OH)$_2$ *(aq)***	48.45689		1	2 Al + 2 L ⇌ Al$_2$(OH)$_2$L$_2$ + 2 H log$_{10}$(β) = 17.9 I = 0.1 M 2 OH + 2 H ⇌ 2 H$_2$O log$_{10}$(β) = 27.56684 I = 0.1 M 2 Al + 2 L + 2 OH ⇌ Al$_2$(OH)$_2$L$_2$ log$_{10}$(β) = 45.46684 I = 0.1 M I = 0 M: log$_{10}$(β) = 48.45689
H^{+} + K^{+} + (salicylate)$^{2-}$ ⇌ **KH(salicylate) *(aq)***	13.41358		1	K + HL ⇌ KHL log$_{10}$(β) = -0.5 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M K + H + L ⇌ KHL log$_{10}$(β) = 12.77285 I = 0.1 M I = 0 M: log$_{10}$(β) = 13.41358
Ca^{2+} + (salicylate)$^{2-}$ ⇌ **Ca(salicylate) *(aq)***	4.04677		1	Ca + HL ⇌ CaL + H log$_{10}$(β) = -10.19 I = 0.5 M H + L ⇌ HL log$_{10}$(β) = 13.16322 I = 0.5 M Ca + L ⇌ CaL log$_{10}$(β) = 3.97322 I = 0.5 M I = 0 M: log$_{10}$(β) = 4.04677
H^{+} + Ca^{2+} + (salicylate)$^{2-}$ ⇌ **CaH(salicylate)$^{+}$**	14.2	-2.95E+4	1	Ca + HL ⇌ CaHL log$_{10}$(β) = 0.5 ΔH = 6.2E+3 H + L ⇌ HL log$_{10}$(β) = 13.7 ΔH = -3.57E+4 Ca + H + L ⇌ CaHL log$_{10}$(β) = 14.2 ΔH = -2.95E+4
Mn(II)$^{2+}$ + (salicylate)$^{2-}$ ⇌ **Mn(II)(salicylate) *(aq)***	6.62715		1	Mn(II) + HL ⇌ Mn(II)L + H log$_{10}$(β) = -7.5 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Mn(II) + L ⇌ Mn(II)L log$_{10}$(β) = 5.77285 I = 0.1 M I = 0 M: log$_{10}$(β) = 6.62715
Mn(II)$^{2+}$ + 2 (salicylate)$^{2-}$ ⇌ **Mn(II)(salicylate)$_2$$^{2-}$**	10.2		1	Mn(II)L + HL ⇌ Mn(II)L$_2$ + H log$_{10}$(β) = -9.7 I = 0.1 M (Original data for β at T = 20°C) Mn(II) + L ⇌ Mn(II)L log$_{10}$(β) = 5.77285 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Mn(II) + 2 L ⇌ Mn(II)L$_2$ log$_{10}$(β) = 9.34570 I = 0.1 M I = 0 M: log$_{10}$(β) = 10.20000

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Fe(II)$^{2+}$ + (salicylate)$^{2-}$ ⇌ **Fe(II)(salicylate) *(aq)***	7.32715		1	Fe(II) + HL ⇌ Fe(II)+ H log$_{10}$(β) = -6.8 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Fe(II)+ L ⇌ Fe(II)L log$_{10}$(β) = 6.47285 I = 0.1 M I = 0 M: log$_{10}$(β) = 7.32715
Fe(II)$^{2+}$ + 2 (salicylate)$^{2-}$ ⇌ **Fe(II)(salicylate)$_2^{2-}$**	11.7		1	Fe(II)L + HL ⇌ Fe(II)L$_2$ + H log$_{10}$(β) = -8.9 I = 0.1 M (Original data for β at T = 20°C) Fe(II) + L ⇌ Fe(II)L log$_{10}$(β) = 6.47285 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Fe(II) + 2 L ⇌ Fe(II)L$_2$ log$_{10}$(β) = 10.84570 I = 0.1 M I = 0 M: log$_{10}$(β) = 11.70000
Fe(III)$^{3+}$ + (salicylate)$^{2-}$ ⇌ **Fe(III)(salicylate)$^+$**	17.55	-2.37E+4	1	Fe(III) + HL ⇌ Fe(III)L + H log$_{10}$(β) = 3.85 ΔH = 1.2E+4 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL log$_{10}$(β) = 13.7 ΔH = -3.57E+4 Fe(III) + L ⇌ Fe(III)L log$_{10}$(β) = 17.55 ΔH = -2.37E+4
H$^+$ + Fe(III)$^{3+}$ + (salicylate)$^{2-}$ ⇌ **Fe(III)H(salicylate)$^{2+}$**	18.74073		1	Fe(III) + HL ⇌ Fe(III)HL log$_{10}$(β) = 4.4 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Fe(III) + H + L ⇌ Fe(III)HL log$_{10}$(β) = 17.67285 I = 0.1 M I = 0 M: log$_{10}$(β) = 18.74073
Fe(III)$^{3+}$ + 2 (salicylate)$^{2-}$ ⇌ **Fe(III)(salicylate)$_2^-$**	29.55		1	Fe(III)L + HL ⇌ Fe(III)L$_2$ + H log$_{10}$(β) = -1.7 I = 0.1 M Fe(III) + L ⇌ Fe(III)L log$_{10}$(β) = 16.26855 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Fe(III) + 2 L ⇌ Fe(III)L$_2$ log$_{10}$(β) = 27.84140 I = 0.1 M I = 0 M: log$_{10}$(β) = 29.55000
Fe(III)$^{3+}$ + 3 (salicylate)$^{2-}$ ⇌ **Fe(III)(salicylate)$_3^{3-}$**	37.2		3	
Co(II)$^{2+}$ + (salicylate)$^{2-}$ ⇌ **Co(II)(salicylate) *(aq)***	7.92715		1	Co(II) + HL ⇌ Co(II)L + H log$_{10}$(β) = -6.2 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Co(II) + L ⇌ Co(II)L log$_{10}$(β) = 7.07285 I = 0.1 M I = 0 M: log$_{10}$(β) = 7.92715
Co(II)$^{2+}$ + 2 (salicylate)$^{2-}$ ⇌ **Co(II)(salicylate)$_2^{2-}$**	12.3		1	Co(II)L + HL ⇌ Co(II)L$_2$ + H log$_{10}$(β) = -8.9 I = 0.1 M (Original data for β at T = 20°C) Co(II) + L ⇌ Co(II)L log$_{10}$(β) = 7.07285 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Co(II) + 2 L ⇌ Co(II)L$_2$ log$_{10}$(β) = 11.44570 I = 0.1 M I = 0 M: log$_{10}$(β) = 12.30000
Ni^{2+} + (salicylate)$^{2-}$ ⇌ **Ni(salicylate) *(aq)***	8.12715		1	Ni + HL ⇌ NiL + H log$_{10}$(β) = -6.0 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M Ni + L ⇌ NiL log$_{10}$(β) = 7.27285 I = 0.1 M I = 0 M: log$_{10}$(β) = 8.12715

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ni^{2+} + 2 $(salicylate)^{2-}$ ⇌ **$Ni(salicylate)_2^{2-}$**	12.6		1	NiL + HL ⇌ NiL_2 + H $log_{10}(\beta)$ = -8.8 I = 0.1 M (Original data for β at T = 20°C) Ni + L ⇌ NiL $log_{10}(\beta)$ = 7.27285 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Ni + 2 L ⇌ NiL_2 $log_{10}(\beta)$ = 11.74570 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.60000
$Cu(II)^{2+}$ + $(salicylate)^{2-}$ ⇌ **Cu(II)(salicylate) *(aq)***	11.34715	-1.87E+4	1	Cu(II) + HL ⇌ Cu(II)L + H $log_{10}(\beta)$ = -2.78 I = 0.1 M ΔH = 1.7E+4 (Original data for ΔH at I = 0.5 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH =-3.57E+4 Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 10.49285 I = 0.1 M ΔH =-1.87E+4 I = 0 M: $log_{10}(\beta)$ = 11.34715
$Cu(II)^{2+}$ + 2 $(salicylate)^{2-}$ ⇌ **$Cu(II)(salicylate)_2^{2-}$**	19.62		1	Cu(II)L + HL ⇌ $Cu(II)L_2$ + H $log_{10}(\beta)$ = -5.0 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 10.49285 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Cu(II) + 2 L ⇌ $Cu(II)L_2$ $log_{10}(\beta)$ = 18.76570 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.62000
Zn^{2+} + $(salicylate)^{2-}$ ⇌ **Zn(salicylate) *(aq)***	7.62715		1	Zn + HL ⇌ ZnL + H $log_{10}(\beta)$ = -6.5 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Zn + L ⇌ ZnL $log_{10}(\beta)$ = 6.77285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 7.62715
Ga^{3+} + $(salicylate)^{2-}$ ⇌ **$Ga(salicylate)^{+}$**	15.28430		1	Ga + HL ⇌ GaL + H $log_{10}(\beta)$ = 0.73 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Ga + L ⇌ GaL $log_{10}(\beta)$ = 14.00285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.28430
H^{+} + Ga^{3+} + $(salicylate)^{2-}$ ⇌ **$GaH(salicylate)^{2+}$**	16.24073		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 1.9 I = 0.1 H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 15.17285 I = 0.1 I = 0 M: $log_{10}(\beta)$ = 16.24073
Cd^{2+} + $(salicylate)^{2-}$ ⇌ **Cd(salicylate) *(aq)***	6.32715		1	Cd + HL ⇌ CdL + H $log_{10}(\beta)$ = -7.8 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Cd + L ⇌ CdL $log_{10}(\beta)$ = 5.47285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 6.32715
Ba^{2+} + $(salicylate)^{2-}$ ⇌ **Ba(salicylate) *(aq)***	0.2		3	
H^{+} + Ba^{2+} + $(salicylate)^{2-}$ ⇌ **$BaH(salicylate)^{+}$**	14.0		1	Ba + HL ⇌ BaHL $log_{10}(\beta)$ = 0.3 H + L ⇌ HL $log_{10}(\beta)$ = 13.7 Ba + H + L ⇌ BaHL $log_{10}(\beta)$ = 14.0

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + La^{3+} + (salicylate)^{2-} \rightleftharpoons$ **LaH(salicylate)$^{2+}$**	15.78	-3.37E+4	1	La + HL ⇌ LaHL log$_{10}$(β) = 2.08 ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 13.7 ΔH = -3.57E+4 La + H + L ⇌ LaHL log$_{10}$(β) = 15.78 ΔH = -3.37E+4
$2\ H^+ + La^{3+} + 2\ (salicylate)^{2-} \rightleftharpoons$ **LaH$_2$(salicylate)$_2^+$**	32.06788	-6.64E+4	1	La + 2 HL ⇌ LaH_2L_2 log$_{10}$(β) = 3.6 I = 0.1 M ΔH = 5.0E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL log$_{10}$(β) = 26.54570 I = 0.1 M ΔH = -7.14E+4 La + 2 H + 2 L ⇌ LaH_2L_2 log$_{10}$(β) = 30.14570 I = 0.1 M ΔH = -6.64E+4 I = 0 M: log$_{10}$(β) = 32.06788
$H^+ + Pr^{3+} + (salicylate)^{2-} \rightleftharpoons$ **PrH(salicylate)$^{2+}$**	16.24073	-3.37E+4	1	Pr + HL ⇌ PrHL log$_{10}$(β) = 1.9 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M ΔH = -3.57E+4 Pr + H + L ⇌ PrHL log$_{10}$(β) = 15.17285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: log$_{10}$(β) = 16.24073
$2\ H^+ + Pr^{3+} + 2\ (salicylate)^{2-} \rightleftharpoons$ **PrH$_2$(salicylate)$_2^+$**	32.16788	-6.73E+4	1	Pr + 2 HL ⇌ PrH_2L_2 log$_{10}$(β) = 3.7 I = 0.1 M ΔH = 4.1E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL log$_{10}$(β) = 26.54570 I = 0.1 M ΔH = -7.14E+4 Pr + 2 H + 2 L ⇌ PrH_2L_2 log$_{10}$(β) = 30.24570 I = 0.1 M ΔH = -6.73E+4 I = 0 M: log$_{10}$(β) = 32.16788
$H^+ + Nd^{3+} + (salicylate)^{2-} \rightleftharpoons$ **NdH(salicylate)$^{2+}$**	16.24073	-3.47E+4	1	Nd + HL ⇌ NdHL log$_{10}$(β) = 1.9 I = 0.1 M ΔH = 1E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M ΔH = -3.57E+4 Nd + H + L ⇌ NdHL log$_{10}$(β) = 15.17285 I = 0.1 M ΔH = -3.47E+4 I = 0 M: log$_{10}$(β) = 16.24073
$2\ H^+ + Nd^{3+} + 2\ (salicylate)^{2-} \rightleftharpoons$ **NdH$_2$(salicylate)$_2^+$**	32.06788	-6.56E+4	1	Nd + 2 HL ⇌ NdH_2L_2 log$_{10}$(β) = 3.6 I = 0.1 M ΔH = 5.8E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL log$_{10}$(β) = 26.54570 I = 0.1 M ΔH = -7.14E+4 Nd + 2 H + 2 L ⇌ NdH_2L_2 log$_{10}$(β) = 30.14570 I = 0.1 M ΔH = -6.56E+4 I = 0 M: log$_{10}$(β) = 32.06788
$H^+ + Sm^{3+} + (salicylate)^{2-} \rightleftharpoons$ **SmH(salicylate)$^{2+}$**	16.44073	-3.49E+4	1	Sm + HL ⇌ SmHL log$_{10}$(β) = 2.1 I = 0.1 M ΔH = 8E+2 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 13.27285 I = 0.1 M ΔH = -3.57E+4 Sm + H + L ⇌ SmHL log$_{10}$(β) = 15.37285 I = 0.1 M ΔH = -3.49E+4 I = 0 M: log$_{10}$(β) = 16.44073

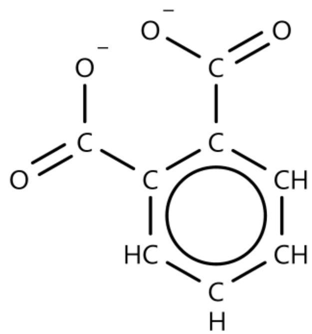
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + Sm^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$SmH_2(salicylate)_2^+$**	32.26788	-6.84E+4	1	Sm + 2 HL ⇌ SmH_2L_2 $log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Sm + 2 H + 2 L ⇌ SmH_2L_2 $log_{10}(\beta)$ = 30.34570 I = 0.1 M ΔH = -6.84E+4 I = 0 M: $log_{10}(\beta)$ = 32.26788
H^+ + Eu^{3+} + $(salicylate)^{2-}$ ⇌ **$EuH(salicylate)^{2+}$**	16.34073	-3.477E+4	1	Eu + HL ⇌ EuHL $log_{10}(\beta)$ = 2.0 I = 0.1 M ΔH = 1E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Eu + H + L ⇌ EuHL $log_{10}(\beta)$ = 15.27285 I = 0.1 M ΔH = -3.47E+4 I = 0 M: $log_{10}(\beta)$ = 16.34073
2 H^+ + Eu^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$EuH_2(salicylate)_2^+$**	32.26788	-6.56E+4	1	Eu + 2 HL ⇌ EuH_2L_2 $log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 5.8E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Eu + 2 H + 2 L ⇌ EuH_2L_2 $log_{10}(\beta)$ = 30.34570 I = 0.1 M ΔH = -6.56E+4 I = 0 M: $log_{10}(\beta)$ = 32.26788
H^+ + Gd^{3+} + $(salicylate)^{2-}$ ⇌ **$GdH(salicylate)^{2+}$**	16.24073	-3.37E+4	1	Gd + HL ⇌ GdHL $log_{10}(\beta)$ = 1.9 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Gd + H + L ⇌ GdHL $log_{10}(\beta)$ = 15.17285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: $log_{10}(\beta)$ = 16.24073
2 H^+ + Gd^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$GdH_2(salicylate)_2^+$**	32.26788	-6.56E+4	1	Gd + 2 HL ⇌ GdH_2L_2 $log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 5.8E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Gd + 2 H + 2 L ⇌ GdH_2L_2 $log_{10}(\beta)$ = 30.344570 I = 0.1 M ΔH = -6.56E+4 I = 0 M: $log_{10}(\beta)$ = 32.26788
H^+ + Tb^{3+} + $(salicylate)^{2-}$ ⇌ **$TbH(salicylate)^{2+}$**	16.24073	-3.37E+4	1	Tb + HL ⇌ TbHL $log_{10}(\beta)$ = 1.9 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Tb + H + L ⇌ TbHL $log_{10}(\beta)$ = 15.17285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: $log_{10}(\beta)$ = 16.24073
2 H^+ + Tb^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$TbH_2(salicylate)_2^+$**	32.36788	-6.68E+4	1	Tb + 2 HL ⇌ TbH_2L_2 $log_{10}(\beta)$ = 3.9 I = 0.1 M ΔH = 4.6E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Tb + 2 H + 2 L ⇌ Tb H_2L_2 $log_{10}(\beta)$ = 30.44570 I = 0.1 M ΔH = -6.68E+4 I = 0 M: $log_{10}(\beta)$ = 32.36788

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Dy^{3+}$ + (salicylate)$^{2-}$ ⇌ **DyH(salicylate)$^{2+}$**	16.04073	-3.27E+4	1	Dy + HL ⇌ DyHL $\log_{10}(\beta)$ = 1.7 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Dy + H + L ⇌ DyHL $\log_{10}(\beta)$ = 14.97285 I = 0.1 M ΔH = -3.27E+4 I = 0 M: $\log_{10}(\beta)$ = 16.04073
2 $H^+ + Dy^{3+}$ + 2 (salicylate)$^{2-}$ ⇌ **DyH_2(salicylate)$_2^+$**	32.26788	-6.22E+4	1	Dy + 2 HL ⇌ Dy H_2L_2 $\log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 9.2E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $\log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Dy + 2 H + 2 L ⇌ Dy H_2L_2 $\log_{10}(\beta)$ = 30.34570 I = 0.1 M ΔH = -6.22E+4 I = 0 M: $\log_{10}(\beta)$ = 32.26788
$H^+ + Ho^{3+}$ + (salicylate)$^{2-}$ ⇌ **HoH(salicylate)$^{2+}$**	16.14073	-3.37E+4	1	Ho + HL ⇌ HoHL $\log_{10}(\beta)$ = 1.8 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Ho + H + L ⇌ HoHL $\log_{10}(\beta)$ = 15.07285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: $\log_{10}(\beta)$ = 16.14073
2 $H^+ + Ho^{3+}$ + 2 (salicylate)$^{2-}$ ⇌ **HoH_2(salicylate)$_2^+$**	32.26788	-6.43E+4	1	Ho + 2 HL ⇌ HoH_2L_2 $\log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 7.1E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $\log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Ho + 2 H + 2 L ⇌ Ho H_2L_2 $\log_{10}(\beta)$ = 30.34570 I = 0.1 M ΔH = -6.43E+4 I = 0 M: $\log_{10}(\beta)$ = 32.26788
$H^+ + Er^{3+}$ + (salicylate)$^{2-}$ ⇌ **ErH(salicylate)$^{2+}$**	16.14073	-3.27E+4	1	Er + HL ⇌ ErHL $\log_{10}(\beta)$ = 1.8 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Er + H + L ⇌ ErHL $\log_{10}(\beta)$ = 15.07285 I = 0.1 M ΔH = -3.27E+4 I = 0 M: $\log_{10}(\beta)$ = 16.14073
2 $H^+ + Er^{3+}$ + 2 (salicylate)$^{2-}$ ⇌ **ErH_2(salicylate)$_2^+$**	32.06788	-6.56E+4	1	Er + 2 HL ⇌ ErH_2L_2 $\log_{10}(\beta)$ = 3.6. I = 0.1 M ΔH = 5.8E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $\log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Er + 2 H + 2 L ⇌ Er H_2L_2 $\log_{10}(\beta)$ = 30.14570 I = 0.1 M ΔH = -6.56E+4 I = 0 M: $\log_{10}(\beta)$ = 32.06788
$H^+ + Tm^{3+}$ + (salicylate)$^{2-}$ ⇌ **TmH(salicylate)$^{2+}$**	16.14073	-3.27E+4	1	Tm + HL ⇌ TmHL $\log_{10}(\beta)$ = 1.8 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Tm + H + L ⇌ TmHL $\log_{10}(\beta)$ = 15.07285 I = 0.1 M ΔH = -3.27E+4 I = 0 M: $\log_{10}(\beta)$ = 16.14073

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + Tm^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$TmH_2(salicylate)_2^+$**	32.16788	-6.39E+4	1	Tm + 2 HL ⇌ Tm H_2L_2 $log_{10}(\beta)$ = 3.7 I = 0.1 M ΔH = 7.5E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Tm + 2 H + 2 L ⇌ Tm H_2L_2 $log_{10}(\beta)$ = 30.24570 I = 0.1 M ΔH = -6.39E+4 I = 0 M: $log_{10}(\beta)$ = 32.16788
H^+ + Yb^{3+} + $(salicylate)^{2-}$ ⇌ **$YbH(salicylate)^{2+}$**	16.14073	-3.37E+4	1	Yb + HL ⇌ YbHL $log_{10}(\beta)$ = 1.8 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Yb + H + L ⇌ YbHL $log_{10}(\beta)$ = 15.07285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: $log_{10}(\beta)$ = 16.14073
2 H^+ + Yb^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$YbH_2(salicylate)_2^+$**	31.96788	-5.34E+4	1	Yb + 2 HL ⇌ YbH_2L_2 $log_{10}(\beta)$ = 3.5 I = 0.1 M ΔH = 1.8E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Yb + 2 H + 2 L ⇌ Yb H_2L_2 $log_{10}(\beta)$ = 30.04570 I = 0.1 M ΔH = -5.34E+4 I = 0 M: $log_{10}(\beta)$ = 32. ??788
H^+ + Lu^{3+} + $(salicylate)^{2-}$ ⇌ **$LuH(salicylate)^{2+}$**	16.04073	-3.27E+4	1	Lu + HL ⇌ LuHL $log_{10}(\beta)$ = 1.7 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M ΔH = -3.57E+4 Lu + H + L ⇌ LuHL $log_{10}(\beta)$ = 14.97285 I = 0.1 M ΔH = -3.37E+4 I = 0 M: $log_{10}(\beta)$ = 16.04073
2 H^+ + Lu^{3+} + 2 $(salicylate)^{2-}$ ⇌ **$LuH_2(salicylate)_2^+$**	32.16788	-6.22E+4	1	Lu + 2 HL ⇌ Lu H_2L_2 $log_{10}(\beta)$ = 3.7 I = 0.1 M ΔH = 9.2E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.54570 I = 0.1 M ΔH = -7.14E+4 Lu + 2 H + 2 L ⇌ Lu H_2L_2 $log_{10}(\beta)$ = 30.24570 I = 0.1 M ΔH = -6.22E+4 I = 0 M: $log_{10}(\beta)$ = 32.16788
$(U(VI)O_2)^{2+}$ + $(salicylate)^{2-}$ ⇌ **$(U(VI)O_2)(salicylate)$ *(aq)***	13.23		1	$(U(VI)O_2)$ + HL ⇌ $(U(VI)O_2)L$ + H $log_{10}(\beta)$ = -0.57 H + L ⇌ HL $log_{10}(\beta)$ = 13.7 $(U(VI)O_2)$ + L ⇌ $(U(VI)O_2)L$ $log_{10}(\beta)$ = 13.23
H^+ + $(U(VI)O_2)^{2+}$ + $(salicylate)^{2-}$ ⇌ **$(U(VI)O_2)H(salicylate)^+$**	15.73715		1	$(U(VI)O_2)$ + HL ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 1.61 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M $(U(VI)O_2)$ + H + L ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 14.88285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.73715
$(U(VI)O_2)^{2+}$ + 2 $(salicylate)^{2-}$ ⇌ **$(U(VI)O_2)(salicylate)_2^{2-}$**	23.40285		1	$(U(VI)O_2)L$ + HL ⇌ $(U(VI)O_2)L_2$ + H $log_{10}(\beta)$ = -3.0 I = 0.1 M $(U(VI)O_2)$ + L ⇌ $(U(VI)O_2)L$ $log_{10}(\beta)$ = 12.27570 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 13.27285 I = 0.1 M Co(II) + 2 L ⇌ $Co(II)L_2$ $log_{10}(\beta)$ = 22.54855 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 23.40285

2.2.28. Phthalate

The ligand in its neutral form is benzene-1,2-dicarboxylic acid (phthalic acid), $C_8H_6O_4$. The ligand L as it is present in the database is phthalate, $C_8H_4O_4^{2-}$. Its molecular weight is 164.116. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (H_2BO_3)^- + (phthalate)^{2-} \rightleftharpoons$ **$H(H_2BO_3)(phthalate)^{2-}$**	9.166		1	$B(OH)_3 + L \rightleftharpoons B(OH)_3L$ $log_{10}(\beta) = -0.07$ $H + H_2BO_3 \rightleftharpoons H_3BO_3$ $log_{10}(\beta) = 9.236$ $H + H_2BO_3 + L \rightleftharpoons B(OH)_3L$ $log_{10}(\beta) = 9.166$
$2\ H^+ + (H_2BO_3)^- + (phthalate)^{2-} \rightleftharpoons$ **$H_2(H_2BO_3)(phthalate)^-$**	13.647		1	$B(OH)_3 + HL \rightleftharpoons B(OH)_3HL$ $log_{10}(\beta) = -1$ $H + H_2BO_3 \rightleftharpoons H_3BO_3$ $log_{10}(\beta) = 9.236$ $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 5.411$ $2\ H + H_2BO_3 + L \rightleftharpoons B(OH)_3HL$ $log_{10}(\beta) = 13.647$
$H^+ + (NH_3)$ *(aq)* $+ (phthalate)^{2-} \rightleftharpoons$ **$H(phthalate)(NH_3)^-$**	10.544		1	$NH_4 + L \rightleftharpoons NH_4L$ $log_{10}(\beta) = 1.3$ $NH_3 + H \rightleftharpoons NH_4$ $log_{10}(\beta) = 9.244$ $H + NH_3 + L \rightleftharpoons NH_4L$ $log_{10}(\beta) = 10.544$
$H^+ + (phthalate)^{2-} \rightleftharpoons$ **$H(phthalate)^-$**	5.411	2.1E+3	1	
$2\ H^+ + (phthalate)^{2-} \rightleftharpoons$ **$H_2(phthalate)$ *(aq)***	8.361	4.7E+3	1	$HL + H \rightleftharpoons H_2L$ $log_{10}(\beta) = 2.950$ ΔH = 2.1E+3 $H + L \rightleftharpoons HL$ $log_{10}(\beta) = 5.411$ ΔH = 2.6E+3 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 8.361$ ΔH = 4.7E+3
$Li^+ + (phthalate)^{2-} \rightleftharpoons$ **$Li(phthalate)^-$**	0.9		1	
$Be^{2+} + (phthalate)^{2-} \rightleftharpoons$ **$Be(phthalate)$ *(aq)***	4.24355		1	Original data for β: $log_{10}(\beta) = 3.17$, at I = 0.5 M.
$Be^{2+} + 2\ (phthalate)^{2-} \rightleftharpoons$ **$Be(phthalate)_2^{2-}$**	6.39355		1	Original data for β: $log_{10}(\beta) = 5.32$, at I = 0.5 M.
$3\ Be^{2+} + 3\ (OH)^- + (phthalate)^{2-} \rightleftharpoons$ **$Be_3(phthalate)(OH)_3^+$**	37.15033		1	$Be_3(OH)_3 + L \rightleftharpoons Be_3(OH)_3L$ $log_{10}(\beta) = 2.44$ I = 0.5 M $3\ Be + 3\ OH \rightleftharpoons Be_3OH_3$ $log_{10}(\beta) = 32.29484$ I = 0.5 M $3\ Be + 3\ OH + L \rightleftharpoons Be_3(OH)_3L$ $log_{10}(\beta) = 34.73484$ I = 0.5 M I = 0 M: $log_{10}(\beta) = 37.15033$
$Na^+ + (phthalate)^{2-} \rightleftharpoons$ **$Na(phthalate)^-$**	0.8	4E+3	1	
$Mg^{2+} + (phthalate)^{2-} \rightleftharpoons$ **$Mg(phthalate)$ *(aq)***	2.52		1	
$Al^{3+} + (phthalate)^{2-} \rightleftharpoons$ **$Al(phthalate)^+$**	4.55033		1	Original data for β: $log_{10}(\beta) = 2.94$, at I = 0.5 M.
$Al^{3+} + 2\ (phthalate)^{2-} \rightleftharpoons$ **$Al(phthalate)_2^-$**	7.14711		1	Original data for β: $log_{10}(\beta) = 5.0$, at I = 0.5 M.

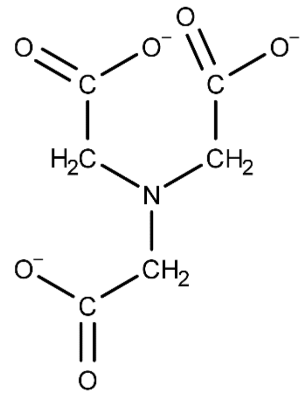
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 Al^{3+} + 2 $(OH)^-$ + $(phthalate)^{2-}$ ⇌ **$Al_2(phthalate)(OH)_2^{2+}$**	27.64110		1	2 Al + L ⇌ $Al_2(OH)_2L$ + 2 H $log_{10}(\beta)$ = -2.50 I = 0.5 M 2 OH + 2 H ⇌ 2 H_2O $log_{10}(\beta)$ = 27.45722 I = 0.5 M 2 Al + L + 2 OH ⇌ $Al_2(OH)_2L$ $log_{10}(\beta)$ = 24.95722 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 27.64110
2 Al^{3+} + 2 $(OH)^-$ + 2 $(phthalate)^{2-}$ ⇌ **$Al_2(phthalate)_2(OH)_2$ *(aq)***	31.14465		1	2 Al + 2 L ⇌ $Al_2(OH)_2L_2$ + 2 H $log_{10}(\beta)$ = -0.07 I = 0.5 M 2 OH + 2 H ⇌ 2 H_2O $log_{10}(\beta)$ = 27.45722 I = 0.5 M 2 Al + 2 L + 2 OH ⇌ $Al_2(OH)_2L_2$ $log_{10}(\beta)$ = 27.37722 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 31.14465
3 Al^{3+} + 4 $(OH)^-$ + $(phthalate)^{2-}$ ⇌ **$Al_3(phthalate)(OH)_4^{3+}$**	49.93349		1	3 Al + L ⇌ $Al_3(OH)_4L$ + 4 H $log_{10}(\beta)$ = -8.47 I = 0.5 M 4 OH + 4 H ⇌ 4 H_2O $log_{10}(\beta)$ = 54.91444 I = 0.5 M 3 Al + L + 4 OH ⇌ $Al_3(OH)_4L$ $log_{10}(\beta)$ = 46.44444 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 49.93349
K^+ + $(phthalate)^{2-}$ ⇌ **$K(phthalate)^-$**	0.7	4E+3	1	
Ca^{2+} + $(phthalate)^{2-}$ ⇌ **Ca(phthalate) *(aq)***	2.45		1	
H^+ + Ca^{2+} + $(phthalate)^{2-}$ ⇌ **$CaH(phthalate)^+$**	6.431		1	Ca + HL ⇌ CaHL $log_{10}(\beta)$ = 1.02 H + L ⇌ HL $log_{10}(\beta)$ = 5.411 Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 6.431
$Mn(II)^{2+}$ + $(phthalate)^{2-}$ ⇌ **Mn(II)(phthalate) *(aq)***	2.74	1.0E+4	1	
$Fe(III)^{3+}$ + $(phthalate)^{2-}$ ⇌ **$Fe(III)(phthalate)^+$**	7.35145		1	Original data for β: $log_{10}(\beta)$ = 6.07, at I = 0.1 M at 30°C.
$Fe(III)^{3+}$ + 2 $(phthalate)^{2-}$ ⇌ **$Fe(III)(phthalate)_2^-$**	12.2686		1	Original data for β: $log_{10}(\beta)$ = 10.56, at I = 0.1 M at 30°C.
$Fe(III)^{3+}$ + 3 $(phthalate)^{2-}$ ⇌ **$Fe(III)(phthalate)_3^{3-}$**	14.54145		1	Original data for β: $log_{10}(\beta)$ = 13.26, at I = 0.1 M at 30°C.
$Co(II)^{2+}$ + $(phthalate)^{2-}$ ⇌ **Co(II)(phthalate) *(aq)***	2.83	7.9E+3	1	
H^+ + $Co(II)^{2+}$ + $(phthalate)^{2-}$ ⇌ **$Co(II)H(phthalate)^+$**	7.22777		1	Co(II) + HL ⇌ Co(II)HL $log_{10}(\beta)$ = 1.28 I = 0.5 H + L ⇌ HL $log_{10}(\beta)$ = 4.87422 I = 0.5 Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 6.15422 I = 0.5 I = 0 M: $log_{10}(\beta)$ = 7.22777
Ni^{2+} + $(phthalate)^{2-}$ ⇌ **Ni(phthalate) *(aq)***	2.95	7.9E+3	1	
H^+ + Ni^{2+} + $(phthalate)^{2-}$ ⇌ **$NiH(phthalate)^+$**	6.64777		1	Ni + HL ⇌ NiHL $log_{10}(\beta)$ = 0.7 I = 0.5 H + L ⇌ HL $log_{10}(\beta)$ = 4.87422 I = 0.5 Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 5.57422 I = 0.5 I = 0 M: $log_{10}(\beta)$ = 6.64777
$Cu(II)^{2+}$ + $(phthalate)^{2-}$ ⇌ **Cu(II)(phthalate) *(aq)***	4.02	8.3E+3	1	
H^+ + $Cu(II)^{2+}$ + $(phthalate)^{2-}$ ⇌ **$Cu(II)H(phthalate)^+$**	7.13815	3.1E+3	1	Cu(II) + HL ⇌ Cu(II)HL $log_{10}(\beta)$ = 1.3 I = 0.1 M ΔH = 1E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 4.98385 I = 0.1 M ΔH = 2.1E+3 Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 6.28385 I = 0.1 M ΔH = 3.1E+3 I = 0 M: $log_{10}(\beta)$ = 7.13815

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cu(II)$^{2+}$ + 2 (phthalate)$^{2-}$ ⇌ **Cu(II)(phthalate)$_2^{2-}$**	5.3	1.5E+4	1	Original data for ΔH at I = 0.1 M.
Zn^{2+} + (phthalate)$^{2-}$ ⇌ **Zn(phthalate) *(aq)***	2.91	1.3E+4	1	
Zn^{2+} + 2 (phthalate)$^{2-}$ ⇌ **Zn(phthalate)$_2^{2-}$**	4.2		1	
Ga^{3+} + (phthalate)$^{2-}$ ⇌ **Ga(phthalate)$^+$**	6.43145		1	Original data for β: $log_{10}(\beta)$ = 5.15, at I = 0.1 M.
Sr^{2+} + (phthalate)$^{2-}$ ⇌ **Sr(phthalate) *(aq)***	2.38		1	
Y^{3+} + (phthalate)$^{2-}$ ⇌ **Y(phthalate)$^+$**	4.74145		1	Original data for β: $log_{10}(\beta)$ = 3.46, at I = 0.1 M.
Cd^{2+} + (phthalate)$^{2-}$ ⇌ **Cd(phthalate) *(aq)***	3.35430		1	Original data for β: $log_{10}(\beta)$ = 2.5, at I = 0.1 M.
H^+ + Cd^{2+} + (phthalate)$^{2-}$ ⇌ **CdH(phthalate)$^+$**	6.29732		1	Cd + HL ⇌ CdHL $log_{10}(\beta)$ = 0.48 I = 1.0 M H + L ⇌ HL $log_{10}(\beta)$ = 5.00468 I = 1.0 M Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 5.48468 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 6.29732
Cd^{2+} + 2 (phthalate)$^{2-}$ ⇌ **Cd(phthalate)$_2^{2-}$**	3.69264		1	Original data for β: $log_{10}(\beta)$ = 2.88, at I = 1.0 M.
H^+ + Cd^{2+} + 2 (phthalate)$^{2-}$ ⇌ **CdH(phthalate)$_2^-$**	7.76145		1	CdL_2 + H ⇌ $CdHL_2$ $log_{10}(\beta)$ = 3.60 I = 1.0 M Cd + 2 L ⇌ CdL_2 $log_{10}(\beta)$ = 2.88 I = 1.0 M Cd + 2 L + H ⇌ $CdHL_2$ $log_{10}(\beta)$ = 6.48 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 7.76145
Ba^{2+} + (phthalate)$^{2-}$ ⇌ **Ba(phthalate) *(aq)***	2.3		1	
La^{3+} + (phthalate)$^{2-}$ ⇌ **La(phthalate)$^+$**	4.74		1	
Pr^{3+} + (phthalate)$^{2-}$ ⇌ **Pr(phthalate)$^+$**	4.84145		1	Original data for β: $log_{10}(\beta)$ = 3.56, at I = 0.1 M.
Nd^{3+} + (phthalate)$^{2-}$ ⇌ **Nd(phthalate)$^+$**	5.16145		1	Original data for β: $log_{10}(\beta)$ = 3.88, at I = 0.1 M.
Sm^{3+} + (phthalate)$^{2-}$ ⇌ **Sm(phthalate)$^+$**	4.98145		1	Original data for β: $log_{10}(\beta)$ = 3.70, at I = 0.1 M.
Eu^{3+} + (phthalate)$^{2-}$ ⇌ **Eu(phthalate)$^+$**	4.98145		1	Original data for β: $log_{10}(\beta)$ = 3.70, at I = 0.1 M.
Gd^{3+} + (phthalate)$^{2-}$ ⇌ **Gd(phthalate)$^+$**	4.91145		1	Original data for β: $log_{10}(\beta)$ = 3.63, at I = 0.1 M.
Tb^{3+} + (phthalate)$^{2-}$ ⇌ **Tb(phthalate)$^+$**	4.74145		1	Original data for β: $log_{10}(\beta)$ = 3.46, at I = 0.1 M.
Dy^{3+} + (phthalate)$^{2-}$ ⇌ **Dy(phthalate)$^+$**	4.76145		1	Original data for β: $log_{10}(\beta)$ = 3.48, at I = 0.1 M.
Ho^{3+} + (phthalate)$^{2-}$ ⇌ **Ho(phthalate)$^+$**	4.83145		1	Original data for β: $log_{10}(\beta)$ = 3.55, at I = 0.1 M.
Er^{3+} + (phthalate)$^{2-}$ ⇌ **Er(phthalate)$^+$**	5.04145		1	Original data for β: $log_{10}(\beta)$ = 3.76, at I = 0.1 M.
Tm^{3+} + (phthalate)$^{2-}$ ⇌ **Tm(phthalate)$^+$**	4.81145		1	Original data for β: $log_{10}(\beta)$ = 3.53, at I = 0.1 M.
Yb^{3+} + (phthalate)$^{2-}$ ⇌ **Yb(phthalate)$^+$**	4.76145		1	Original data for β: $log_{10}(\beta)$ = 3.48, at I = 0.1 M.
Lu^{3+} + (phthalate)$^{2-}$ ⇌ **Lu(phthalate)$^+$**	4.93145		1	Original data for β: $log_{10}(\beta)$ = 3.65, at I = 0.1 M.
Pb(II)$^{2+}$ + (phthalate)$^{2-}$ ⇌ **Pb(II)(phthalate) *(aq)***	3.59264		1	Original data for β: $log_{10}(\beta)$ = 2.78, at I = 1.0 M.
H^+ + Pb(II)$^{2+}$ + (phthalate)$^{2-}$ ⇌ **Pb(II)H(phthalate)$^+$**	6.97732		1	Pb(II) + HL ⇌ Pb(II)HL $log_{10}(\beta)$ = 1.16 I = 1.0 M H + L ⇌ HL $log_{10}(\beta)$ = 5.00468 I = 1.0 M Pb(II) + H + L ⇌ Pb(II)HL $log_{10}(\beta)$ = 6.16468 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 6.97732
Pb(II)$^{2+}$ + 2 (phthalate)$^{2-}$ ⇌ **Pb(II)(phthalate)$_2^{2-}$**	4.82264		1	Original data for β: $log_{10}(\beta)$ = 4.01, at I = 1.0 M.
H^+ + Pb(II)$^{2+}$ + 2 (phthalate)$^{2-}$ ⇌ **Pb(II)H(phthalate)$_2^-$**	8.99896		1	Pb(II)L_2 + H ⇌ Pb(II)HL_2 $log_{10}(\beta)$ = 3.77 I = 1.0 M Pb(II) + 2 L ⇌ Pb(II)L_2 $log_{10}(\beta)$ = 4.01 I = 1.0 M Pb(II) + 2 L ⇌ H ⇌ Pb(II)HL_2 $log_{10}(\beta)$ = 7.78 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 8.99896

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$(U(VI)O_2)^{2+}$ + $(phthalate)^{2-}$ ⇌ **$(U(VI)O_2)(phthalate)$ *(aq)***	5.6643		1	Original data for β: $log_{10}(\beta)$ = 4.81, at I = 0.1 M.
$(U(VI)O_2)^{2+}$ + 2 $(phthalate)^{2-}$ ⇌ **$(U(VI)O_2)(phthalate)_2^{2-}$**	8.5843		1	Original data for β: $log_{10}(\beta)$ = 7.73, at I = 0.1 M.
2 $(U(VI)O_2)^{2+}$ + 2 $(OH)^-$ + 2 $(phthalate)^{2-}$ ⇌ **$(U(VI)O_2)_2(phthalate)_2(OH)_2^{2-}$**	31.43187		1	2 $(U(VI)O_2)$ + 2 L ⇌ $(U(VI)O_2)_2(OH)_2L_2$ + 2 H $log_{10}(\beta)$ = 2.37 I = 0.1 M 2 H + 2 OH ⇌ 2 H_2O $log_{10}(\beta)$ = 27.56684 I = 0.1 M 2 $(U(VI)O_2)$ + 2 L + 2 OH ⇌ $(U(VI)O_2)_2L_2(OH)_2$ $log_{10}(\beta)$ = 29.93684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 31.43187

2.2.29. NTA

The ligand in its neutral form is NTA (nitrilotriacetic acid; $C_6H_9NO_6$). The ligand L as it is present in the database is the anion $C_6H_6NO_6^{3-}$. Its molecular weight is 188.115. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(NTA)^{3-}$ ⇌ **$H(NTA)^{2-}$**	10.29406	-1.9E+4	1	Original data for β: $log_{10}(\beta)$ = 9.46 or 9.66 or 9.84, depending on the background electrolytes (Na/K/N(alkyl)$_4$), all at 0.1 M. The average log-value (9.65333) was converted to I = 0 M.
2 H^+ + $(NTA)^{3-}$ ⇌ **$H_2(NTA)^-$**	13.24121	-1.8E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.52 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 9.65333 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 12.17333 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.24121

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 H^+ + $(NTA)^{3-}$ ⇌ **$H_3(NTA)$ *(aq)***	15.24121	-1.6E+4	1	$H_2L + H \rightleftharpoons H_3L$ $\log_{10}(\beta) = 2.0$ $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta) = 13.24121$ $3\ H + L \rightleftharpoons H_3L$ $\log_{10}(\beta) = 15.24121$
4 H^+ + $(NTA)^{3-}$ ⇌ **$H_4(NTA)^+$**	16.24121	-7.7E+3	1	$H_3L + H \rightleftharpoons H_4L$ $\log_{10}(\beta) = 1.0$ I = 0.1 M $3\ H + L \rightleftharpoons H_3L$ $\log_{10}(\beta) = 13.95976$ I = 0.1 M $4\ H + L \rightleftharpoons H_4L$ $\log_{10}(\beta) = 14.95976$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 16.24121$
Li^+ + $(NTA)^{3-}$ ⇌ **$Li(NTA)^{2-}$**	3.09073	8E+3	1	Original data for β: $\log_{10}(\beta) = 2.45$, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Be^{2+} + $(NTA)^{3-}$ ⇌ **$Be(NTA)^-$**	9.07145	2.5E+4	1	Original data for β: $\log_{10}(\beta) = 7.79$, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Na^+ + $(NTA)^{3-}$ ⇌ **$Na(NTA)^{2-}$**	1.84073	8E+3	1	Original data for β: $\log_{10}(\beta) = 1.2$, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Na^+ + $(NTA)^{3-}$ ⇌ **$NaH(NTA)^-$**	10.808		4	
Mg^{2+} + $(NTA)^{3-}$ ⇌ **$Mg(NTA)^-$**	6.78145	1.7E+4	1	Original data for β: $\log_{10}(\beta) = 5.50$, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
Al^{3+} + $(NTA)^{3-}$ ⇌ **$Al(NTA)$ *(aq)***	13.32218		1	Original data for β: $\log_{10}(\beta) = 11.4$, at I = 0.1 M.
H^+ + Al^{3+} + $(NTA)^{3-}$ ⇌ **$AlH(NTA)^+$**	15.22218		1	$AlL + H \rightleftharpoons AlHL$ $\log_{10}(\beta) = 1.90$ I = 0.1 M $Al + L \rightleftharpoons AlL$ $\log_{10}(\beta) = 11.4$ I = 0.1 M $Al + H + L \rightleftharpoons AlHL$ $\log_{10}(\beta) = 13.3$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 15.22218$
Al^{3+} + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Al(NTA)(OH)^-$**	22.01560		1	$AlL \rightleftharpoons Al(OH)L + H$ $\log_{10}(\beta) = -5.09$ I = 0.1 M $Al + L \rightleftharpoons AlL$ $\log_{10}(\beta) = 11.4$ I = 0.1 M $OH + H \rightleftharpoons H_2O$ $\log_{10}(\beta) = 13.78342$ I = 0.1 M $Al + L + OH \rightleftharpoons Al(OH)L$ $\log_{10}(\beta) = 20.09342$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 22.01560$
Al^{3+} + 2 $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Al(NTA)(OH)_2^{2-}$**	27.30544		1	$Al(OH)L \rightleftharpoons Al(OH)_2L + H$ $\log_{10}(\beta) = -8.28$ I = 0.1 M $Al + L + OH \rightleftharpoons Al(OH)L$ $\log_{10}(\beta) = 20.09342$ I = 0.1 M $OH + H \rightleftharpoons H_2O$ $\log_{10}(\beta) = 13.78342$ I = 0.1 M $Al + L + 2\ OH \rightleftharpoons Al(OH)_2L$ $\log_{10}(\beta) = 25.59684$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 27.30544$
2 Al^{3+} + 2 $(OH)^-$ + 2 $(NTA)^{3-}$ ⇌ **$Al_2(NTA)_2(OH)_2^{2-}$**	45.58282		1	$2\ Al(OH)L \rightleftharpoons Al_2(OH)_2L_2$ $\log_{10}(\beta) = 1.82$ I = 0.5 M $2\ Al + 2\ OH + 2\ L \rightleftharpoons 2\ Al(OH)L$ $\log_{10}(\beta) = 39.20022$ I = 0.5 M $2\ Al + 2\ OH + 2\ L \rightleftharpoons Al_2(OH)_2L_2$ $\log_{10}(\beta) = 41.02022$ I = 0.5 M I = 0 M: $\log_{10}(\beta) = 45.58282$
K^+ + $(NTA)^{3-}$ ⇌ **$K(NTA)^{2-}$**	1.24073	1.6E+4	1	Original data for β: $\log_{10}(\beta) = 0.6$, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + K^+ + $(NTA)^{3-}$ ⇌ **$KH(NTA)^-$**	10.788		4	
Ca^{2+} + $(NTA)^{3-}$ ⇌ **$Ca(NTA)^-$**	7.74145	-5.69E+3	1	Original data for β: $\log_{10}(\beta) = 6.3$ or 6.44 or 6.64, depending on the background electrolytes ($Na/K/N(alkyl)_4$), all at 0.1 M. The average log-value (6.46) was converted to I = 0 M. Original data for ΔH at I = 0.1 M and 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ca^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Ca(NTA)_2^{4-}$**	9.68073	-3.2E+4	1	Original data for β: $log_{10}(\beta)$ = 8.81 or 9.27, depending on the background electrolytes (K/N(alkyl)$_4$), both at 0.1 M. The average log-value (9.04) was converted to I = 0 M. Original data for ΔH at I = 0.1 M and 20°C.
Sc^{3+} + $(NTA)^{3-}$ ⇌ **Sc(NTA) *(aq)***	14.62218		1	Original data for β: $log_{10}(\beta)$ = 12.7, at I = 0.1 M.
Sc^{3+} + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Sc(NTA)(OH)^-$**	22.06218		1	ScL + OH ⇌ Sc(OH)L $log_{10}(\beta)$ = 7.44 I = 0.1 M (Original data for β at T = 20°C) Sc + L ⇌ ScL $log_{10}(\beta)$ = 12.7 I = 0.1 M Sc + L + OH ⇌ Sc(OH)L $log_{10}(\beta)$ = 20.14 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.06218
Sc^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Sc(NTA)_2^{3-}$**	26.02218		1	Original data for β: $log_{10}(\beta)$ = 24.1, at I = 0.1 M and 20°C.
$Mn(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Mn(II)(NTA)^-$**	8.64645	5.4E+3	1	Original data for β: $log_{10}(\beta)$ = 7.46 or 7.27, depending on the background electrolytes (K/Na), both at 0.1 M. The average log-value (7.365) was converted to I = 0 M. Original data for ΔH at I = 0.1 M and 20°C.
$Mn(II)^{2+}$ + 2 $(NTA)^{3-}$ ⇌ **$Mn(II)(NTA)_2^{4-}$**	11.33073	-1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 10.44 or 10.94, depending on the background electrolytes (K/Na), both at 0.1 M. The average log-value (10.69) was converted to I = 0 M. Original data for ΔH at I = 0.1 M and 20°C.
$Fe(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Fe(II)(NTA)^-$**	10.18145		1	Original data for β: $log_{10}(\beta)$ = 8.90, at I = 0.1 M.
$Fe(II)^{2+}$ + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Fe(II)(NTA)(OH)^{2-}$**	12.93130		1	Fe(II)L ⇌ Fe(II)(OH)L + H $log_{10}(\beta)$ = -10.82 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(II) + L ⇌ Fe(II)L $log_{10}(\beta)$ = 8.90 I = 0.1 M Fe(II) + L + OH ⇌ Fe(II)(OH)L $log_{10}(\beta)$ = 11.86342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.93130
$Fe(II)^{2+}$ + 2 $(NTA)^{3-}$ ⇌ **$Fe(II)(NTA)_2^{4-}$**	12.62073		1	Original data for β: $log_{10}(\beta)$ = 11.98, at I = 0.1 M.
$Fe(III)^{3+}$ + $(NTA)^{3-}$ ⇌ **Fe(III)(NTA) *(aq)***	17.92218	1.3E+4	1	Original data for β: $log_{10}(\beta)$ = 16.00, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
H^+ + $Fe(III)^{3+}$ + $(NTA)^{3-}$ ⇌ **$Fe(III)H(NTA)^+$**	18.92218		1	Fe(III)L + H ⇌ Fe(III)HL $log_{10}(\beta)$ = 1.0 I = 0.5 M Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 15.50669 I = 0.5 M Fe(III) + L + H ⇌ Fe(III)HL $log_{10}(\beta)$ = 16.50669 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 18.92218
$Fe(III)^{3+}$ + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Fe(III)(NTA)(OH)^-$**	27.34560		1	Fe(III)L ⇌ Fe(III)(OH)L + H $log_{10}(\beta)$ = -4.36 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 16.00 I = 0.1 M Fe(III) + L + OH ⇌ Fe(III)(OH)L $log_{10}(\beta)$ = 25.42342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 27.34560
$Fe(III)^{3+}$ + 2 $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Fe(III)(NTA)(OH)_2^{2-}$**	33.33544		1	Fe(III)(OH)L ⇌ Fe(III)$(OH)_2$L + H $log_{10}(\beta)$ = -7.58 I = 0.1 M Fe(III) + L + OH ⇌ Fe(III)(OH)L $log_{10}(\beta)$ = 25.42342 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + 2 OH + L ⇌ Fe(III)$(OH)_2$L $log_{10}(\beta)$ = 31.62684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 33.33544

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Fe(III)^{3+}$ + 3 $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Fe(III)(NTA)(OH)_3^{3-}$**	35.97171		1	$Fe(III)(OH)_2L$ ⇌ $Fe(III)(OH)_3L$ + H $log_{10}(\beta)$ = -10.72 I = 0.1 M Fe(III) + 2 OH + L ⇌ $Fe(III)(OH)_2L$ $log_{10}(\beta)$ = 31.62684 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + 3 OH + L ⇌ $Fe(III)(OH)_3L$ $log_{10}(\beta)$ = 34.69026 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 35.97171
$Fe(III)^{3+}$ + 2 $(NTA)^{3-}$ ⇌ **$Fe(III)(NTA)_2^{3-}$**	25.92218		1	Original data for β: $log_{10}(\beta)$ = 24.0, at I = 0.1 M.
2 $Fe(III)^{3+}$ + 2 $(NTA)^{3-}$ ⇌ **$Fe(III)_2(NTA)_2$ *(aq)***	35.73099		1	Original data for β: $log_{10}(\beta)$ = 30.9, at I = 0.5 M.
2 $Fe(III)^{3+}$ + 2 $(OH)^-$ + 2 $(NTA)^{3-}$ ⇌ **$Fe(III)_2(NTA)_2(OH)_2^{2-}$**	63.56282		1	2 Fe(III)(OH)L ⇌ $Fe(III)_2(OH)_2L_2$ $log_{10}(\beta)$ = 9.14 I = 0.5 M 2 Fe(III) + 2 L + 2 OH ⇌ 2 Fe(III)(OH)L $log_{10}(\beta)$ = 49.86022 I = 0.5 M 2 Fe(III) + 2 L + 2 OH ⇌ $Fe(III)_2(OH)_2L_2$ $log_{10}(\beta)$ = 59.00022 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 63.56282
$Co(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Co(II)(NTA)^-$**	11.66145	-2E+3	1	Original data for β: $log_{10}(\beta)$ = 10.38, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
$Co(II)^{2+}$ + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Co(II)(NTA)(OH)^{2-}$**	14.43130		1	Co(II)L ⇌ Co(II)(OH)L + H $log_{10}(\beta)$ = -10.80 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Co(II) + L ⇌ Co(II)L $log_{10}(\beta)$ = 10.38 I = 0.1 M Co(II) + L + OH ⇌ Co(II)(OH)L $log_{10}(\beta)$ = 13.36342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 14.43130
$Co(II)^{2+}$ + 2 $(NTA)^{3-}$ ⇌ **$Co(II)(NTA)_2^{4-}$**	14.97073	-1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 14.33, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Ni^{2+} + $(NTA)^{3-}$ ⇌ **$Ni(NTA)^-$**	12.79145	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 11.51, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Ni(NTA)(OH)^{2-}$**	15.49130	-4.081E+4	1	NiL ⇌ Ni(OH)L + H $log_{10}(\beta)$ = -10.86 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 0.1 M) OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Ni + L ⇌ NiL $log_{10}(\beta)$ = 11.50 I = 0.1 M ΔH = -1E+4 Ni + L + OH ⇌ Ni(OH)L $log_{10}(\beta)$ = 14.42342 I = 0.1 M ΔH = -4.081E+4 I = 0 M: $log_{10}(\beta)$ = 15.49130
Ni^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Ni(NTA)_2^{4-}$**	16.96073	-3.2E+4	1	Original data for β: $log_{10}(\beta)$ = 16.32, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Cu(II)(NTA)^-$**	14.28145	-7.9E+3	1	Three values (12.7, 13.0, 13.3) for resp. Na as background electrolyte; "corrected for background electrolyte" and K as background electrolyte. The average log-value (13.0) was converted to I = 0 M. Original data for ΔH at I = 0.1 M and 20°C.
H^+ + $Cu(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **Cu(II)H(NTA) *(aq)***	16.09503		1	Cu(II)L + H ⇌ Cu(II)HL $log_{10}(\beta)$ = 1.6 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 13.0 I = 0.1 M Cu(II) + L + H ⇌ Cu(II)HL $log_{10}(\beta)$ = 14.6 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.09503

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(II)^{2+}$ + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Cu(II)(NTA)(OH)^{2-}$**	18.6513	-3.071E+4	1	Cu(II)L ⇌ Cu(II)(OH)L + H $log_{10}(\beta)$ = -9.2 I = 0.1 M ΔH = 3.3E+4 (Original data for ΔH at I = 0.1 M) OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 13.0 I = 0.1 M ΔH = -7.9E+3 Cu(II) + L + OH ⇌ Cu(II)(OH)L $log_{10}(\beta)$ = 13.36342 I = 0.1 M ΔH = -3.071E+4 I = 0 M: $log_{10}(\beta)$ = 14.43130
$Cu(II)^{2+}$ + 2 $(NTA)^{3-}$ ⇌ **$Cu(II)(NTA)_2^{4-}$**	18.04073	-3.5E+4	1	Original data for β: $log_{10}(\beta)$ = 17.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + $(NTA)^{3-}$ ⇌ **$Zn(NTA)^{-}$**	11.83645	-5.0E+3	1	Original data for β: $log_{10}(\beta)$ = 10.45 or 10.66, depending on the background electrolytes (KCl/KNO_3), both at 0.1 M. The average log-value (10.555) was converted to I = 0 M. Original data for ΔH at I = 0.5 M.
Zn^{2+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Zn(NTA)(OH)^{2-}$**	15.4313	-1.081E+4	1	Original data for β: $log_{10}(\beta)$ = -10.1 or -10.06, depending on the background electrolytes ($NaNO_3$/KNO_3), both at 0.1 M. The average log-value (-10.08) was used. ZnL ⇌ Zn(OH)L + H $log_{10}(\beta)$ = -10.08 I = 0.1 M ΔH = 5.0E+4 (Original data for ΔH at I = 0.1 M) OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Zn + L ⇌ ZnL $log_{10}(\beta)$ = 10.66 I = 0.1 M ΔH = -5.0E+3 Zn + L + OH ⇌ Zn(OH)L $log_{10}(\beta)$ = 14.36342 I = 0.1 M ΔH = -1.081E+4 I = 0 M: $log_{10}(\beta)$ = 15.43130
Zn^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Zn(NTA)_2^{4-}$**	14.88073	-1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 14.24, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Ga^{3+} + $(NTA)^{3-}$ ⇌ **Ga(NTA) *(aq)***	15.67218		1	Original data for β: $log_{10}(\beta)$ = 13.6 or 13.9, depending on the background electrolytes (Na/K), both at 0.1 M and 20°C. The average log-value (13.75) was converted to I = 0 M.
Ga^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Ga(NTA)(OH)^{-}$**	25.1856		1	GaL ⇌ GaOHL + H $log_{10}(\beta)$ = -4.27 I = 0.1 M Ga + L ⇌ GaL $log_{10}(\beta)$ = 13.75 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Ga + L + OH ⇌ GaOHL $log_{10}(\beta)$ = 23.26342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 25.18560
Ga^{3+} + 2 $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Ga(NTA)(OH)_2^{2-}$**	31.11544		1	GaOHL ⇌ $Ga(OH)_2L$ + H $log_{10}(\beta)$ = -7.64 I = 0.1 M Ga + L + OH ⇌ GaOHL $log_{10}(\beta)$ = 23.26342 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Ga + 2 OH + L ⇌ $Ga(OH)_2L$ $log_{10}(\beta)$ = 29.40684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 31.11544
Rb^{+} + $(NTA)^{3-}$ ⇌ **$Rb(NTA)^{2-}$**	1.04073		1	Original data for β: $log_{10}(\beta)$ = 0.4, at I = 0.1 M.
Sr^{2+} + $(NTA)^{3-}$ ⇌ **$Sr(NTA)^{-}$**	6.27145	-2.2E+3	1	Original data for β: $log_{10}(\beta)$ = 4.99, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
Y^{3+} + $(NTA)^{3-}$ ⇌ **Y(NTA) *(aq)***	13.34218	-2E+3	1	Original data for β: $log_{10}(\beta)$ = 11.42, at I = 0.1 M. Original data for ΔH at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Y^{3+} + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Y(NTA)(OH)^-$**	19.73218		1	YL + OH ⇌ Y(OH)L $log_{10}(\beta)$ = 6.39 I = 0.1 M Y + L ⇌ YL $log_{10}(\beta)$ = 11.42 I = 0.1 M Y + OH + L ⇌ Y(OH)L $log_{10}(\beta)$ = 17.81 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.73218
Y^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Y(NTA)_2^{3-}$**	22.33218	-1.3E+4	1	Original data for β: $log_{10}(\beta)$ = 20.41, at I = 0.1 M.
Zr^{4+} + $(NTA)^{3-}$ ⇌ **$Zr(NTA)^+$**	24.1	2.5E+4	1	
Pd^{2+} + $(NTA)^{3-}$ ⇌ **$Pd(NTA)^-$**	18.21896		1	Original data for β: $log_{10}(\beta)$ = 17.0, at I = 1.0 M at 20°C.
H^+ + Pd^{2+} + $(NTA)^{3-}$ ⇌ **PdH(NTA) *(aq)***	26.24212		1	PdL + H ⇌ PdHL $log_{10}(\beta)$ = 7.82 I = 1.0 M (Original data for β at T = 20°C) Pd + L ⇌ PdL $log_{10}(\beta)$ = 17.0 I = 1.0 M Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 24.82 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 26.24212
2 H^+ + Pd^{2+} + $(NTA)^{3-}$ ⇌ **$PdH_2(NTA)^+$**	26.74212		1	PdHL + H ⇌ PdH_2L $log_{10}(\beta)$ = 0.5 I = 1.0 M (Original data for β at T = 20°C) Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 24.82 I = 1.0 M Pd + 2 H + L ⇌ PdH_2L $log_{10}(\beta)$ = 25.32 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 26.74212
Pd^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Pd(NTA)_2^{4-}$**	24.30948		1	Original data for β: $log_{10}(\beta)$ = 23.7, at I = 1.0 M at 20°C.
2 Pd^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Pd_2(NTA)_2^{2-}$**	38.23476		1	2 PdL ⇌ Pd_2L_2 $log_{10}(\beta)$ = 2 I = 1.0 M (Original data for β at T = 20°C) 2 Pd + 2 L ⇌ 2 PdL $log_{10}(\beta)$ = 34.0 I = 1.0 M 2 Pd + 2 L ⇌ Pd_2L_2 $log_{10}(\beta)$ = 36.0 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 38.23476
Ag^+ + $(NTA)^{3-}$ ⇌ **$Ag(NTA)^{2-}$**	5.60573	-2.6E+4	1	Original data for β: $log_{10}(\beta)$ = 4.85 or 5.08, depending on the background electrolytes (Na/K), both at 0.1 M. The average log-value (4.965) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
H^+ + Ag^+ + $(NTA)^{3-}$ ⇌ **$AgH(NTA)^-$**	13.01205		1	AgL + H ⇌ AgHL $log_{10}(\beta)$ = 7.0 I = 1.0 M Ag + L ⇌ AgL $log_{10}(\beta)$ = 4.99625 I = 1.0 M Ag + H + L ⇌ AgHL $log_{10}(\beta)$ = 11.99625 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 13.01205
Cd^{2+} + $(NTA)^{3-}$ ⇌ **$Cd(NTA)^-$**	11.04145	-1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 9.76, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
Cd^{2+} + $(OH)^-$ + $(NTA)^{3-}$ ⇌ **$Cd(NTA)(OH)^{2-}$**	13.36130	2.581E+4	1	CdL ⇌ Cd(OH)L + H $log_{10}(\beta)$ = -11.25 I = 0.1 M ΔH = 4.6E+4 (Original data for ΔH at I = 0.1 M) Cd + L ⇌ CdL $log_{10}(\beta)$ = 9.76 I = 0.1 M ΔH = -1.6E+4 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cd + L + OH ⇌ Cd(OH)L $log_{10}(\beta)$ = 12.29342 I = 0.1 M ΔH = 2.581E+4 I = 0 M: $log_{10}(\beta)$ = 13.36130
Cd^{2+} + 2 $(NTA)^{3-}$ ⇌ **$Cd(NTA)_2^{4-}$**	15.11073	-3.7E+4	1	Original data for β: $log_{10}(\beta)$ = 14.47, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$In^{3+} + (NTA)^{3-} \rightleftharpoons$ **In(NTA) *(aq)***	15.73218		1	Original data for β: $\log_{10}(\beta)$ = 13.81, at I = 0.1 M.
$In^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$In(NTA)_2^{3-}$**	25.62218		1	Original data for β: $\log_{10}(\beta)$ = 23.70, at I = 0.1 M.
$H^{+} + In^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$InH(NTA)_2^{2-}$**	29.13290		1	$InL_2 + H \rightleftharpoons InHL_2$ $\log_{10}(\beta)$ = 2.87 I = 0.1 M $In + 2\ L \rightleftharpoons InL_2$ $\log_{10}(\beta)$ = 23.70 I = 0.1 M In + H + 2 L $\rightleftharpoons$ InHL2 $\log_{10}(\beta)$ = 26.57 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 29.13290
$Cs^{+} + (NTA)^{3-} \rightleftharpoons$ **$Cs(NTA)^{2-}$**	0.84073		1	Original data for β: $\log_{10}(\beta)$ = 0.2, at I = 0.1 M.
$Ba^{2+} + (NTA)^{3-} \rightleftharpoons$ **$Ba(NTA)^{-}$**	6.09145	-6.02E+3	1	Original data for β: $\log_{10}(\beta)$ = 4.81, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
$La^{3+} + (NTA)^{3-} \rightleftharpoons$ **La(NTA) *(aq)***	12.39218	-3E+3	1	Original data for β: $\log_{10}(\beta)$ = 10.47, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
$La^{3+} + (OH)^{-} + (NTA)^{3-} \rightleftharpoons$ **$La(NTA)(OH)^{-}$**	18.29218		1	LaL + OH $\rightleftharpoons$ La(OH)L $\log_{10}(\beta)$ = 5.9 I = 0.1 M La + L $\rightleftharpoons$ LaL $\log_{10}(\beta)$ = 10.47 I = 0.1 M La + OH + L $\rightleftharpoons$ La(OH)L $\log_{10}(\beta)$ = 16.37 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.29218
$La^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$La(NTA)_2^{3-}$**	19.76218	-8.7E+3	1	Original data for β: $\log_{10}(\beta)$ = 17.84, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Ce^{3+} + (NTA)^{3-} \rightleftharpoons$ **Ce(NTA) *(aq)***	12.62218	-4.6E+3	1	Original data for β: $\log_{10}(\beta)$ = 10.70, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
$Ce^{3+} + (OH)^{-} + (NTA)^{3-} \rightleftharpoons$ **$Ce(NTA)(OH)^{-}$**	18.40218		1	CeL + OH $\rightleftharpoons$ Ce(OH)L $\log_{10}(\beta)$ = 5.78 I = 0.1 M (Original data for β at T = 20°C) Ce + L $\rightleftharpoons$ CeL $\log_{10}(\beta)$ = 10.70 I = 0.1 M Ce + OH + L $\rightleftharpoons$ Ce(OH)L $\log_{10}(\beta)$ = 16.48 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.40218
$Ce^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$Ce(NTA)_2^{3-}$**	20.58218	-1.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 18.66, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Pr^{3+} + (NTA)^{3-} \rightleftharpoons$ **Pr(NTA) *(aq)***	12.79218	-5.8E+3	1	Original data for β: $\log_{10}(\beta)$ = 10.87, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
$Pr^{3+} + (OH)^{-} + (NTA)^{3-} \rightleftharpoons$ **$Pr(NTA)(OH)^{-}$**	18.51218		1	PrL + OH $\rightleftharpoons$ Pr(OH)L $\log_{10}(\beta)$ = 5.72 I = 0.1 M Pr + L $\rightleftharpoons$ PrL $\log_{10}(\beta)$ = 10.87 I = 0.1 M Pr + OH + L $\rightleftharpoons$ Pr(OH)L $\log_{10}(\beta)$ = 16.59 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.51218
$Pr^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$Pr(NTA)_2^{3-}$**	20.94218	-1.7E+4	1	Original data for β: $\log_{10}(\beta)$ = 19.02, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Nd^{3+} + (NTA)^{3-} \rightleftharpoons$ **Nd(NTA) *(aq)***	13.02218	-6.2E+3	1	Original data for β: $\log_{10}(\beta)$ = 11.10, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
$Nd^{3+} + (OH)^{-} + (NTA)^{3-} \rightleftharpoons$ **$Nd(NTA)(OH)^{-}$**	18.88218		1	NdL + OH $\rightleftharpoons$ Nd(OH)L $\log_{10}(\beta)$ = 5.86 I = 0.1 M Nd + L $\rightleftharpoons$ NdL $\log_{10}(\beta)$ = 11.10 I = 0.1 M Nd + OH + L $\rightleftharpoons$ Nd(OH)L $\log_{10}(\beta)$ = 16.96 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.88218
$Nd^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$Nd(NTA)_2^{3-}$**	21.43218	-1.9E+4	1	Original data for β: $\log_{10}(\beta)$ = 19.51, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Pm^{3+} + 2\ (NTA)^{3-} \rightleftharpoons$ **$Pm(NTA)_2^{3-}$**	21.62218		1	Original data for β: $\log_{10}(\beta)$ = 19.7, at I = 0.1 M at 20°C.

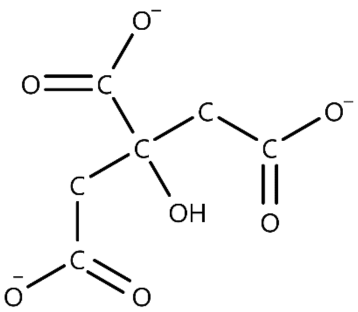
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Sm^{3+} + $(NTA)^{3-}$ ⇌ **Sm(NTA)** ***(aq)***	13.24218	-7.1E+3	1	Original data for β: $\log_{10}(\beta)$ = 11.32, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Sm^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Sm(NTA)(OH)^{-}$**	19.83218		1	SmL + OH ⇌ Sm(OH)L $\log_{10}(\beta)$ = 6.59 I = 0.1 M Sm + L ⇌ SmL $\log_{10}(\beta)$ = 11.32 I = 0.1 M Sm + OH + L ⇌ Sm(OH)L $\log_{10}(\beta)$ = 17.91 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.83218
Sm^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Sm(NTA)_2^{3-}$**	22.35218	-2.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.43, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Eu^{3+} + $(NTA)^{3-}$ ⇌ **Eu(NTA)** ***(aq)***	13.24218	-6.2E+3	1	Original data for β: $\log_{10}(\beta)$ = 11.32, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Eu^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Eu(NTA)(OH)^{-}$**	20.08218		1	EuL + OH ⇌ Eu(OH)L $\log_{10}(\beta)$ = 6.84 I = 0.1 M Eu + L ⇌ EuL $\log_{10}(\beta)$ = 11.32 I = 0.1 M Eu + OH + L ⇌ Eu(OH)L $\log_{10}(\beta)$ = 18.16 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.08218
Eu^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Eu(NTA)_2^{3-}$**	22.56218	-2.5E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.64, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Gd^{3+} + $(NTA)^{3-}$ ⇌ **Gd(NTA)** ***(aq)***	13.27218	-3E+3	1	Original data for β: $\log_{10}(\beta)$ = 11.35, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Gd^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Gd(NTA)(OH)^{-}$**	19.81218		1	GdL + OH ⇌ Gd(OH)L $\log_{10}(\beta)$ = 6.54 I = 0.1 M Gd + L ⇌ GdL $\log_{10}(\beta)$ = 11.35 I = 0.1 M Gd + OH + L ⇌ Gd(OH)L $\log_{10}(\beta)$ = 17.89 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.81218
Gd^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Gd(NTA)_2^{3-}$**	22.58218	-2.6E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.66, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Tb^{3+} + $(NTA)^{3-}$ ⇌ **Tb(NTA)** ***(aq)***	13.42218	-1E+3	1	Original data for β: $\log_{10}(\beta)$ = 11.50, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Tb^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Tb(NTA)(OH)^{-}$**	20.09218		1	TbL + OH ⇌ Tb(OH)L $\log_{10}(\beta)$ = 6.67 I = 0.1 M Tb + L ⇌ TbL $\log_{10}(\beta)$ = 11.50 I = 0.1 M Tb + OH + L ⇌ Tb(OH)L $\log_{10}(\beta)$ = 18.17 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.09218
Tb^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Tb(NTA)_2^{3-}$**	22.87218	-2.4E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.95, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Dy^{3+} + $(NTA)^{3-}$ ⇌ **Dy(NTA)** ***(aq)***	13.55218	0	1	Original data for β: $\log_{10}(\beta)$ = 11.63, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Dy^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Dy(NTA)(OH)^{-}$**	20.39218		1	DyL + OH ⇌ Dy(OH)L $\log_{10}(\beta)$ = 6.84 I = 0.1 M Dy + L ⇌ DyL $\log_{10}(\beta)$ = 11.63 I = 0.1 M Dy + OH + L ⇌ Dy(OH)L $\log_{10}(\beta)$ = 18.47 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.39218
Dy^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Dy(NTA)_2^{3-}$**	22.90218	-2.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.98, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ho^{3+} + $(NTA)^{3-}$ ⇌ **Ho(NTA)** ***(aq)***	13.68218	8E+2	1	Original data for β: $\log_{10}(\beta)$ = 11.76, at I = 0.1 M. Original data for ΔH at I = 0.5 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ho^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Ho(NTA)(OH)^{-}$**	20.34218		1	HoL + OH ⇌ Ho(OH)L $\log_{10}(\beta)$ = 6.66 I = 0.1 M Ho + L ⇌ HoL $\log_{10}(\beta)$ = 11.76 I = 0.1 M Ho + OH + L ⇌ Ho(OH)L $\log_{10}(\beta)$ = 18.42 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.34218
Ho^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Ho(NTA)_2^{3-}$**	22.98218	-1.9E+4	1	Original data for β: $\log_{10}(\beta)$ = 21.06, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Er^{3+} + $(NTA)^{3-}$ ⇌ **Er(NTA) *(aq)***	13.82218	0	1	Original data for β: $\log_{10}(\beta)$ = 11.90, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Er^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Er(NTA)(OH)^{-}$**	20.38218		1	ErL + OH ⇌ Er(OH)L $\log_{10}(\beta)$ = 6.56 I = 0.1 M Er + L ⇌ ErL $\log_{10}(\beta)$ = 11.90 I = 0.1 M Er + OH + L ⇌ Er(OH)L $\log_{10}(\beta)$ = 18.46 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.38218
Er^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Er(NTA)_2^{3-}$**	23.01218	-1.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 21.09, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Tm^{3+} + $(NTA)^{3-}$ ⇌ **Tm(NTA) *(aq)***	13.99218	-4E+2	1	Original data for β: $\log_{10}(\beta)$ = 12.07, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Tm^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Tm(NTA)(OH)^{-}$**	20.23218		1	TmL + OH ⇌ Tm(OH)L $\log_{10}(\beta)$ = 6.24 I = 0.1 M Tm + L ⇌ TmL $\log_{10}(\beta)$ = 12.07 I = 0.1 M Tm + OH + L ⇌ Tm(OH)L $\log_{10}(\beta)$ = 18.31 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.23218
Tm^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Tm(NTA)_2^{3-}$**	23.14218	-7.5E+3	1	Original data for β: $\log_{10}(\beta)$ = 21.22, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Yb^{3+} + $(NTA)^{3-}$ ⇌ **Yb(NTA) *(aq)***	14.13218	-1E+3	1	Original data for β: $\log_{10}(\beta)$ = 12.21, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Yb^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Yb(NTA)(OH)^{-}$**	20.42218		1	YbL + OH ⇌ Yb(OH)L $\log_{10}(\beta)$ = 6.29 I = 0.1 M Yb + L ⇌ YbL $\log_{10}(\beta)$ = 12.21 I = 0.1 M Yb + OH + L ⇌ Yb(OH)L $\log_{10}(\beta)$ = 18.50 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.42218
Yb^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Yb(NTA)_2^{3-}$**	23.33218	-6.2E+3	1	Original data for β: $\log_{10}(\beta)$ = 21.41, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Lu^{3+} + $(NTA)^{3-}$ ⇌ **Lu(NTA) *(aq)***	14.24218	-1E+3	1	Original data for β: $\log_{10}(\beta)$ = 12.32, at I = 0.1 M. Original data for ΔH at I = 0.5 M.
Lu^{3+} + $(OH)^{-}$ + $(NTA)^{3-}$ ⇌ **$Lu(NTA)(OH)^{-}$**	20.54218		1	LuL + OH ⇌ Lu(OH)L $\log_{10}(\beta)$ = 6.30 I = 0.1 M Lu + L ⇌ LuL $\log_{10}(\beta)$ = 12.32 I = 0.1 M Lu + OH + L ⇌ Lu(OH)L $\log_{10}(\beta)$ = 18.62 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.54218
Lu^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Lu(NTA)_2^{3-}$**	23.57218	-3E+3	1	Original data for β: $\log_{10}(\beta)$ = 21.65, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Hf^{4+} + $(NTA)^{3-}$ ⇌ **$Hf(NTA)^{+}$**	23.6	2.0E+4	1	
$Hg(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Hg(II)(NTA)^{-}$**	15.58145		1	Original data for β: $\log_{10}(\beta)$ = 14.3, at I = 0.1 M.
$Pb(II)^{2+}$ + $(NTA)^{3-}$ ⇌ **$Pb(II)(NTA)^{-}$**	12.76145	-1.5E+4	1	Original data for β: $\log_{10}(\beta)$ = 11.48, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.

Equilibrium reaction	$\text{Log}_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Pb(II)^{2+} + (NTA)^{3-}$ ⇌ **Pb(II)H(NTA) *(aq)***	15.32984		1	Pb(II)L + OH ⇌ Pb(II)(OH)L $\log_{10}(\beta)$ = 2.3 I = 0.5 M Pb(II) + L ⇌ Pb(II)L $\log_{10}(\beta)$ = 11.15112 I = 0.5 M Pb(II) + OH + L ⇌ Pb(II)(OH)L $\log_{10}(\beta)$ = 13.45112 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 15.32984
$Pb(II)^{2+}$ + 2 $(NTA)^{3-}$ ⇌ **$Pb(II)(NTA)_2^{4-}$**	13.44073		1	Original data for β: $\log_{10}(\beta)$ = 12.8, at I = 0.1 M at 20°C.
$Bi^{3+} + (NTA)^{3-}$ ⇌ **Bi(NTA) *(aq)***	20.12218		1	Original data for β: $\log_{10}(\beta)$ = 18.2, at I = 0.1 M.
Bi^{3+} + 2 $(NTA)^{3-}$ ⇌ **$Bi(NTA)_2^{3-}$**	28.42844		1	Original data for β: $\log_{10}(\beta)$ = 26.6, at I = 1.0 M at 20°C.
$(U(VI)O_2)^{2+} + (NTA)^{3-}$ ⇌ **$(U(VI)O_2)(NTA)^-$**	10.78145		1	Original data for β: $\log_{10}(\beta)$ = 9.50, at I = 0.1 M.

2.2.30. Citrate

The ligand in its neutral form is 2-hydroxypropane-1,2,3-tricarboxylic acid (citric acid; $C_6H_8O_7$). The ligand L as it is present in the database is the anion $C_6H_5O_7^{3-}$. Its molecular weight is 189.099. Its structural formula is shown on the right.



Equilibrium reaction	$\text{Log}_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (citrate)^{3-}$ ⇌ **$H(citrate)^{2-}$**	6.396	3.3E+3	1	
2 $H^+ + (citrate)^{3-}$ ⇌ **$H_2(citrate)^-$**	11.157	1.3E+3	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 4.761 ΔH = -2.0E+3 H + L ⇌ HL $\log_{10}(\beta)$ = 6.396 ΔH = 3.3E+3 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 11.157 ΔH = 1.3E+3
3 $H^+ + (citrate)^{3-}$ ⇌ **$H_3(citrate)$ *(aq)***	14.285	-2.7E+3	1	H_2L + H ⇌ H_3L $\log_{10}(\beta)$ = 3.128 ΔH = -4.0E+3 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 11.157 ΔH = 1.3E+3 3 H + L ⇌ H_3L $\log_{10}(\beta)$ = 14.285 ΔH = -2.7E+3
$Li^+ + (citrate)^{3-}$ ⇌ **$Li(citrate)^{2-}$**	1.47073		1	Original data for β: $\log_{10}(\beta)$ = 0.83, at I = 0.1 M.
$Be^{2+} + (citrate)^{3-}$ ⇌ **$Be(citrate)^-$**	6.01033		1	Original data for β: $\log_{10}(\beta)$ = 4.40, at I = 0.5 M.
$H^+ + Be^{2+} + (citrate)^{3-}$ ⇌ **BeH(citrate) *(aq)***	9.56955		1	Be + HL ⇌ BeHL $\log_{10}(\beta)$ = 2.1 I = 0.5 M H + L ⇌ HL $\log_{10}(\beta)$ = 5.59084 I = 0.5 M Be + H + L ⇌ BeHL $\log_{10}(\beta)$ = 7.69084 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 9.56956

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + Be^{2+} + $(citrate)^{3-}$ ⇌ **$BeH_2(citrate)^+$**	12.98415		1	Be + H_2L ⇌ Be H_2L $\log_{10}(\beta)$ = 1.4 I = 0.1 M (Original data for β at T = 35°C) 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 10.08912 I = 0.1 M Be + 2 H + L ⇌ BeH_2L $\log_{10}(\beta)$ = 11.48912 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 12.98415
Be^{2+} + 2 $(citrate)^{3-}$ ⇌ **$Be(citrate)_2^{4-}$**	8.90516		1	Original data for β: $\log_{10}(\beta)$ = 8.1, at I = 0.5 M.
2 Be^{2+} + 2 $(citrate)^{3-}$ ⇌ **$Be_2(citrate)_2^{2-}$**	15.72227		1	Original data for β: $\log_{10}(\beta)$ = 12.77, at I = 0.5 M.
2 Be^{2+} + $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Be_2(citrate)_2(OH)^{3-}$**	24.23979		1	Be_2L_2 ⇌ $Be_2L_2(OH)$ + H $\log_{10}(\beta)$ = -4.87 I = 1.0 M 2 Be + 2 L ⇌ Be_2L_2 $\log_{10}(\beta)$ = 13.48751 I = 1.0 M H + OH ⇌ 2 H_2O $\log_{10}(\beta)$ = 13.79384 I = 1.0 M 2 Be + 2 L + OH = $Be_2L_2(OH)$ $\log_{10}(\beta)$ = 22.41135 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 24.23979
2 Be^{2+} + 2 $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Be_2(citrate)_2(OH)_2^{4-}$**	32.03755		1	Be $_2L_2$ ⇌ $Be_2L_2(OH)_2$ + 2 H $\log_{10}(\beta)$ = -9.8 I = 0.5 M 2 Be + 2 L ⇌ Be_2L_2 $\log_{10}(\beta)$ = 12.77 I = 0.5 M 2 H + 2 OH ⇌ 2 H_2O $\log_{10}(\beta)$ = 27.45722 I = 0.5 M 2 Be + 2 L + 2 OH ⇌ $Be_2L_2(OH)_2$ $\log_{10}(\beta)$ = 30.42722 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 32.03755
4 Be^{2+} + 2 $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Be_4(citrate)_2(OH)_2$ *(aq)***	42.10547		1	2 Be + $Be_2L_2(OH)_2$ ⇌ Be $_4L_2(OH)_2$ $\log_{10}(\beta)$ = 7.63 I = 1.0 M 2 Be + 2 L + 2 OH ⇌ $Be_2L_2(OH)_2$ $\log_{10}(\beta)$ = 30.81859 I = 1.0 M 4 Be + 2 L + 2 OH ⇌ $Be_4L_2(OH)_2$ $\log_{10}(\beta)$ = 38.44859 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 42.10547
4 Be^{2+} + 3 $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Be_4(citrate)_2(OH)_3^-$**	52.19931		1	Be $_4L_2(OH)_2$ ⇌ $Be_4L_2(OH)_3$ + H $\log_{10}(\beta)$ = -3.70 I = 1.0 M 4 Be + 2 L + 2 OH ⇌ $Be_4L_2(OH)_2$ $\log_{10}(\beta)$ = 38.44859 I = 1.0 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.79384 I = 1.0 M 4 Be + 2 L + 3 OH ⇌ $Be_4L_2(OH)_3$ $\log_{10}(\beta)$ = 48.54243 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 52.19931
4 Be^{2+} + 4 $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Be_4(citrate)_2(OH)_4^{2-}$**	60.67999		1	Be $_4L_2(OH)_3$ ⇌ $Be_4L_2(OH)_4$ + H $\log_{10}(\beta)$ = -5.11 I = 1.0 M 4 Be + 2 L + 3 OH ⇌ $Be_4L_2(OH)_3$ $\log_{10}(\beta)$ = 48.54243 I = 1.0 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.79384 I = 1.0 M 4 Be + 2 L + 4 OH ⇌ $Be_4L_2(OH)_4$ $\log_{10}(\beta)$ = 57.22627 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 60.67999
Na^+ + $(citrate)^{3-}$ ⇌ **$Na(citrate)^{2-}$**	1.39073	1E+3	1	Original data for β: $\log_{10}(\beta)$ = 0.75, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Mg^{2+} + $(citrate)^{3-}$ ⇌ **$Mg(citrate)^-$**	4.86	8E+3	1	Original data for ΔH at I = 0.1 M.
Mg^{2+} + H^+ + $(citrate)^{3-}$ ⇌ **MgH(citrate) *(aq)***	8.986		1	Mg + HL ⇌ MgHL $\log_{10}(\beta)$ = 2.59 H + L ⇌ HL $\log_{10}(\beta)$ = 6.396 Mg + H + L ⇌ MgHL $\log_{10}(\beta)$ = 8.986
Mg^{2+} + 2 H^+ + $(citrate)^{3-}$ ⇌ **$MgH_2(citrate)^+$**	12.157		1	Mg + H_2L ⇌ MgH_2L $\log_{10}(\beta)$ = 1.0 H + L ⇌ HL $\log_{10}(\beta)$ = 11.157 Mg + H + L ⇌ MgHL $\log_{10}(\beta)$ = 12.157

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Al^{3+} + $(citrate)^{3-}$ ⇌ **Al(citrate) *(aq)***	10.10718		1	Original data for β: $log_{10}(\beta)$ = 8.04, at I = 0.1 M when a K^+-salt is the background electrolyte; $log_{10}(\beta)$ = 8.35 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (8.185) was converted to I = 0 M.
Al^{3+} + 2 $(citrate)^{3-}$ ⇌ **$Al(citrate)_2^{3-}$**	15.07218		1	Original data for β: $log_{10}(\beta)$ = 12.9, at I = 0.1 M when KCl is the background electrolyte; $log_{10}(\beta)$ = 13.4 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (13.15) was converted to I = 0 M.
H^+ + Al^{3+} + $(citrate)^{3-}$ ⇌ **$AlH(citrate)^+$**	12.91245		1	Original data for β: $log_{10}(\beta)$ = 5.16, at I = 0.1 M when a K^+-salt is the background electrolyte; $log_{10}(\beta)$ = 5.31 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (5.235) was used in the conversion given below. Al + HL ⇌ AlHL $log_{10}(\beta)$ = 5.235 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M Al + H + L = AlHL $log_{10}(\beta)$ = 10.99027 I = 0.1 M I = 0 M: $log_{10}(\beta)$ ⇌ 12.91245
3 Al^{3+} + 4 $(OH)^-$ + 3 $(citrate)^{3-}$ ⇌ **$Al_3(citrate)_3(OH)_4^{4-}$**	75.11817		1	3 Al + 3 L ⇌ $Al_3L_3(OH)_4$ + 4 H $log_{10}(\beta)$ = 14.83 I = 0.2 M 4 H + 4 OH ⇌ 4 H_2O $log_{10}(\beta)$ = 54.97619 I = 0.2 M 3 Al + 3 L + 4 OH ⇌ $Al_3L_3(OH)_4$ $log_{10}(\beta)$ = 69.80619 I = 0.2 M I = 0 M: $log_{10}(\beta)$ = 75.11817
K^+ + $(citrate)^{3-}$ ⇌ **$K(citrate)^{2-}$**	1.17	5.4E+3	1	
Ca^{2+} + $(citrate)^{3-}$ ⇌ **$Ca(citrate)^-$**	4.85	-5.8E+2	1	
H^+ + Ca^{2+} + $(citrate)^{3-}$ ⇌ **CaH(citrate) *(aq)***	9.256		1	Ca + HL ⇌ CaHL $log_{10}(\beta)$ = 2.86 H + L ⇌ HL $log_{10}(\beta)$ = 6.396 Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 9.256
2 H^+ + Ca^{2+} + $(citrate)^{3-}$ ⇌ **$CaH_2(citrate)^+$**	12.557		1	Ca + H_2L ⇌ CaH_2L $log_{10}(\beta)$ = 1.4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.157 Ca + 2 H + L ⇌ CaH_2L $log_{10}(\beta)$ = 12.557
$Mn(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Mn(II)(citrate)^-$**	5.18812		1	Original data for β: $log_{10}(\beta)$ = 3.76, at I = 0.1 M when a Na^+-salt is the background electrolyte; $log_{10}(\beta)$ = 3.81 (also at I = 0.1 M) when a K^+-salt is the background electrolyte; $log_{10}(\beta)$ = 4.15 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (3.90667) was converted to I = 0 M.
H^+ + $Mn(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **Mn(II)H(citrate) *(aq)***	9.55030		1	Mn(II) + HL ⇌ Mn(II)HL $log_{10}(\beta)$ = 2.3 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M Mn(II) + H + L ⇌ Mn(II)HL $log_{10}(\beta)$ = 8.05527 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 9.55030
2 H^+ + $Mn(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Mn(II)H_2(citrate)^+$**	13.13275		1	Mn(II) + H_2L ⇌ $Mn(II)H_2L$ $log_{10}(\beta)$ = 1.53 I = 0.15 M (Original data for β at T = 37°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 9.96763 I = 0.15 M Mn(II) + 2 H + L ⇌ $Mn(II)H_2L$ $log_{10}(\beta)$ = 11.46763 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 13.13275
$Fe(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Fe(II)(citrate)^-$**	6.08145		1	Original data for β: $log_{10}(\beta)$ = 4.8, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $Fe(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **Fe(II)H(citrate)** ***(aq)***	10.15030		1	Fe(II) + HL ⇌ Fe(II)HL $log_{10}(\beta)$ = 2.9 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M Fe(II) + H + L ⇌ Fe(II)HL $log_{10}(\beta)$ = 8.65527 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.15030
2 H^+ + $Fe(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Fe(II)H_2(citrate)^+$**	12.73275		1	Fe(II) + H_2L ⇌ $Fe(II)H_2L$ $log_{10}(\beta)$ = 1.1 I = 0.15 M (Original data for β at T = 37°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 9.96763 I = 0.15 M Fe(II) + 2 H + L ⇌ $Fe(II)H_2L$ $log_{10}(\beta)$ = 11.06763 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 12.73275
H^+ + $Fe(II)^{2+}$ + 2 $(citrate)^{3-}$ ⇌ **$Fe(II)H(citrate)_2^{3-}$**	13.34030		1	Fe(II)HL + L ⇌ $Fe(II)HL_2$ $log_{10}(\beta)$ = 3.19 I = 0.15 M (Original data for β at T = 37°C) Fe(II) + H + L ⇌ Fe(II)HL $log_{10}(\beta)$ = 8.48518 I = 0.15 M Fe(II) + H + 2 L ⇌ $Fe(II)HL_2$ $log_{10}(\beta)$ = 11.67518 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 13.34030
$Fe(III)^{3+}$ + $(citrate)^{3-}$ ⇌ **Fe(III)(citrate)** ***(aq)***	13.15218	-2.8E+4	1	Original data for β: $log_{10}(\beta)$ = 11.19, at I = 0.1 M when a Na^+-salt is the background electrolyte; $log_{10}(\beta)$ = 11.27 (also at I = 0.1 M) when a K^+-salt is the background electrolyte. The average log-value (11.23) was converted to I = 0 M.
H^+ + $Fe(III)^{3+}$ + $(citrate)^{3-}$ ⇌ **$Fe(III)H(citrate)^+$**	14.37745		1	Fe(III) + HL ⇌ Fe(III)HL $log_{10}(\beta)$ = 6.7 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M Fe(III) + H + L ⇌ Fe(III)HL $log_{10}(\beta)$ = 12.45527 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 14.37745
$Fe(III)^{3+}$ + $(OH)^-$ + $(citrate)^{3-}$ ⇌ **$Fe(III)(OH)(citrate)^-$**	18.76087		1	Fe(III)L ⇌ Fe(III)OHL + H $log_{10}(\beta)$ = -2.7 I = 0.1 M Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 5.75527 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + L + OH ⇌ Fe(III)OHL $log_{10}(\beta)$ = 16.83869 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.76087
2 $Fe(III)^{3+}$ + 2 $(OH)^-$ + 2 $(citrate)^{3-}$ ⇌ **$Fe(III)_2(OH)_2(citrate)_2^{2-}$**	52.39762		1	2 Fe(III) + 2 L ⇌ $Fe(III)_2(OH)_2L_2$ + 2 H $log_{10}(\beta)$ = 21.2 I = 0.1 M (Original data for β at T = 20°C) 2 OH + 2 H ⇌ 2 H_2O $log_{10}(\beta)$ = 27.56684 I = 0.1 M 2 Fe(III) + 2 OH + 2 L ⇌ $Fe(III)_2(OH)_2L_2$ $log_{10}(\beta)$ = 48.76684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 52.39762
$Co(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Co(II)(citrate)^-$**	6.18145		1	Original data for β: $log_{10}(\beta)$ = 4.9, at I = 0.1 M.
H^+ + $Co(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **Co(II)H(citrate)** ***(aq)***	10.44030		1	Co(II) + HL ⇌ Co(II)HL $log_{10}(\beta)$ = 3.19 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 8.94527 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.4403
2 H^+ + $Co(II)^{2+}$ + $(citrate)^{3-}$ ⇌ **$Co(II)H_2(citrate)^+$**	12.76332		1	Co(II) + H_2L ⇌ $Co(II)H_2L$ $log_{10}(\beta)$ = 1.2 I = 1.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 10.14120 I = 1.0 M Co(II) + 2 H + L ⇌ $Co(II)H_2L$ $log_{10}(\beta)$ = 11.34120 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 12.76332

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ni^{2+} + $(citrate)^{3-}$ $\rightleftharpoons$ **$Ni(citrate)^{-}$**	6.63478	1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 5.18, at I = 0.1 M when a Na^{+}-salt is the background electrolyte; $log_{10}(\beta)$ = 5.32 (also at I = 0.1 M) when a K^{+}-salt is the background electrolyte, 5.56 (also at 0.1 M) when a tetralkyl ammonium salt is the background electrolyte. The average log-value (5.35333) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 $(citrate)^{3-}$ $\rightleftharpoons$ **$Ni(citrate)_2^{4-}$**	8.99573	1.2E+4	1	Original data for β: $log_{10}(\beta)$ = 8.13, at I = 0.1 M when a K^{+}-salt is the background electrolyte; $log_{10}(\beta)$ = 8.58 (also at I = 0.1 M) when a tetralkyl ammonium salt is the background electrolyte. The average log-value (8.355) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
H^{+} + Ni^{2+} + $(citrate)^{3-}$ $\rightleftharpoons$ **NiH(citrate) *(aq)***	10.63530	1.53E+4	1	Ni + HL $\rightleftharpoons$ NiHL $log_{10}(\beta)$ = 3.385 I = 0.1 M ΔH = 1.2E+4 (Original data for ΔH at I = 0.1 M) H + L $\rightleftharpoons$ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M ΔH = 3.3E+3 Ni + H + L $\rightleftharpoons$ NiHL $log_{10}(\beta)$ = 9.14027 I = 0.1 M ΔH = 1.53E+4 I = 0 M: $log_{10}(\beta)$ = 10.6353
2 H^{+} + Ni^{2+} + $(citrate)^{3-}$ $\rightleftharpoons$ **$NiH_2(citrate)^{+}$**	13.33623		1	Ni + H_2L $\rightleftharpoons$ Ni H_2L $log_{10}(\beta)$ = 1.7 I = 0.1 M 2 H + L $\rightleftharpoons$ H_2L $log_{10}(\beta)$ = 10.14120 I = 0.1 M Ni + 2 H + L $\rightleftharpoons$ NiH_2L $log_{10}(\beta)$ = 11.84120 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.33623
H^{+} + Ni^{2+} + 2 $(citrate)^{3-}$ $\rightleftharpoons$ **$NiH(citrate)_2^{3-}$**	15.22003	2.8E+4	1	Original data for β: $log_{10}(\beta)$ = 5.3, at I = 0.1 M when a K^{+}-salt is the background electrolyte; $log_{10}(\beta)$ = 5.44 (also at I = 0.1 M) when a tetralkyl ammonium salt is the background electrolyte. The average log-value (5.37) was used here. NiL_2 + H $\rightleftharpoons$ $NiHL_2$ $log_{10}(\beta)$ = 5.37 I = 0.1 M ΔH = 1.6E+4 (Original data for ΔH at I = 0.1 M) Ni + 2 L $\rightleftharpoons$ NiL_2 $log_{10}(\beta)$ = 8.355 I = 0.1 M ΔH = 1.2E+4 Ni + H + 2 $\rightleftharpoons$ = Ni HL_2 $log_{10}(\beta)$ = 13.725 I = 0.1 M ΔH = 2.8E+4 I = 0 M: $log_{10}(\beta)$ = 15.22003
H^{+} + $Cu(II)^{2+}$ + $(citrate)^{3-}$ $\rightleftharpoons$ **Cu(II)H(citrate) *(aq)***	11.05030	1.13E+4	1	Original data for β: $log_{10}(\beta)$ = 3.7, at I = 0.1 M when a K^{+}-salt is the background electrolyte; $log_{10}(\beta)$ = 3.9 (also at I = 0.1 M) when a tetralkyl ammonium salt is the background electrolyte. The average log-value (3.8) was used here. Cu(II) + HL $\rightleftharpoons$ Cu(II)HL $log_{10}(\beta)$ = 3.8 I = 0.1 M ΔH = 8E+3 (Original data for ΔH at I = 0.1 M) H + L $\rightleftharpoons$ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M ΔH = 3.3E+3 Cu(II) + H + L $\rightleftharpoons$ Cu(II)HL $log_{10}(\beta)$ = 9.55527 I = 0.1 M ΔH = 1.13E+4 I = 0 M: $log_{10}(\beta)$ = 11.0503

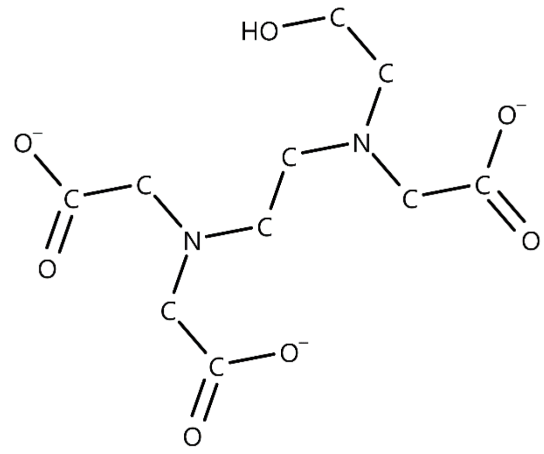
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ Cu(II)^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$Cu(II)_2(citrate)_2^{2-}$**	16.94933	4.1E+4	1	Original data for β: $log_{10}(\beta)$ = 14.4, at I = 0.1 M when a K^+-salt is the background electrolyte; $log_{10}(\beta)$ = 14.8 (also at I = 0.1 M) when a tetralkyl ammonium salt is the background electrolyte. The average log-value (14.6) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
$Zn^{2+} + (citrate)^{3-} \rightleftharpoons$ **$Zn(citrate)^-$**	6.24645	8E+3	1	Original data for β: $log_{10}(\beta)$ = 4.93, at I = 0.1 M when a Na^+-salt is the background electrolyte; $log_{10}(\beta)$ = 5.00 (also at I = 0.1 M) when a K^+-salt is the background electrolyte. The average log-value (4.965) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
$Zn^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$Zn(citrate)_2^{4-}$**	7.44073	2.5E+4	1	Original data for β: $log_{10}(\beta)$ = 6.8, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Zn^{2+} + (citrate)^{3-} \rightleftharpoons$ **$ZnH(citrate)$ *(aq)***	10.25030	3.3E+3	1	Zn + HL ⇌ ZnHL $log_{10}(\beta)$ = 3.00 I = 0.1 M ΔH = 0 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 5.75527 I = 0.1 M ΔH = 3.3E+3 Zn + H + L ⇌ ZnHL $log_{10}(\beta)$ = 8.75527 I = 0.1 M ΔH = 3.3E+3 I = 0 M: $log_{10}(\beta)$ = 10.25030
$2\ H^+ + Zn^{2+} + (citrate)^{3-} \rightleftharpoons$ **$ZnH_2(citrate)^+$**	12.83623		1	Zn + H_2L ⇌ ZnH_2L $log_{10}(\beta)$ = 1.2 I = 0.1 M (Original data for β at T = 20°C) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 10.14120 I = 0.1 M Zn + 2 H + L ⇌ ZnH_2L $log_{10}(\beta)$ = 11.34120 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.83623
$Ga^{3+} + (citrate)^{3-} \rightleftharpoons$ **$Ga(citrate)$ *(aq)***	11.94218		1	Original data for β: $log_{10}(\beta)$ = 10.02, at I = 0.1 M.
$Ga^{3+} + (OH)^- + (citrate)^{3-} \rightleftharpoons$ **$Ga(OH)(citrate)^-$**	12.80560		1	GaL ⇌ GaOHL + H $log_{10}(\beta)$ = -2.9 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Ga + OH + L ⇌ GaOHL $log_{10}(\beta)$ = 10.88342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.80560
$Rb^+ + (citrate)^{3-} \rightleftharpoons$ **$Rb(citrate)^{2-}$**	1.13073		1	Original data for β: $log_{10}(\beta)$ = 0.49, at I = 0.1 M.
$Sr^{2+} + (citrate)^{3-} \rightleftharpoons$ **$Sr(citrate)^-$**	4.41		1	
$H^+ + Sr^{2+} + (citrate)^{3-} \rightleftharpoons$ **$SrH(citrate)$ *(aq)***	9.216		1	Sr + HL ⇌ SrHL $log_{10}(\beta)$ = 2.82 H + L ⇌ HL $log_{10}(\beta)$ = 6.396 Sr + H + L ⇌ SrHL $log_{10}(\beta)$ = 9.216
$2\ H^+ + Sr^{2+} + (citrate)^{3-} \rightleftharpoons$ **$SrH_2(citrate)^+$**	12.53623		1	Sr + H_2L ⇌ SrH_2L $log_{10}(\beta)$ = 0.9 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 10.14120 I = 0.1 M Sr + 2 H + L ⇌ SrH_2L $log_{10}(\beta)$ = 11.04120 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.53623
$Y^{3+} + (citrate)^{3-} \rightleftharpoons$ **$Y(citrate)$ *(aq)***	9.42		1	
$Pd^{2+} + (citrate)^{3-} \rightleftharpoons$ **$Pd(citrate)^-$**	4.67896	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.46, at I = 1.0 M. Original data for ΔH at I = 1.0 M.
$Cd^{2+} + (citrate)^{3-} \rightleftharpoons$ **$Cd(citrate)^-$**	5.00145	8E+3	1	Original data for β: $log_{10}(\beta)$ = 3.72, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cd^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$Cd(citrate)_2^{4-}$**	5.94073	2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 5.3, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + Cd^{2+} + $(citrate)^{3-}$ ⇌ **CdH(citrate)** ***(aq)***	9.33030	3.3E+3	1	Cd + HL ⇌ CdHL $\log_{10}(\beta)$ = 2.18 I = 0.1 M ΔH = 0 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 5.75527 I = 0.1 M ΔH = 3.3E+3 Cd + H + L ⇌ CdHL $\log_{10}(\beta)$ = 7.83527 I = 0.1 M ΔH = 3.3E+3 I = 0 M: $\log_{10}(\beta)$ = 9.33030
2 H^{+} + Cd^{2+} + $(citrate)^{3-}$ ⇌ **CdH_2(citrate)$^{+}$**	12.73623		1	Cd + H_2L ⇌ CdH_2L $\log_{10}(\beta)$ = 1.1 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 10.14120 I = 0.1 M Cd + 2 H + L ⇌ CdH_2L $\log_{10}(\beta)$ = 11.24120 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 12.73623
Cs^{+} + $(citrate)^{3-}$ ⇌ **Cs(citrate)$^{2-}$**	0.96073		1	Original data for β: $\log_{10}(\beta)$ = 0.32, at I = 0.1 M.
Ba^{2+} + $(citrate)^{3-}$ ⇌ **Ba(citrate)$^{-}$**	4.15		1	
H^{+} + Ba^{2+} + $(citrate)^{3-}$ ⇌ **BaH(citrate)** ***(aq)***	9.086		1	Ba + HL ⇌ BaHL $\log_{10}(\beta)$ = 2.69 H + L ⇌ HL $\log_{10}(\beta)$ = 6.396 Ba + H + L ⇌ BaHL $\log_{10}(\beta)$ = 9.086
2 H^{+} + Ba^{2+} + $(citrate)^{3-}$ ⇌ **BaH_2(citrate)$^{+}$**	12.33623		1	Ba + H_2L ⇌ BaH_2L $\log_{10}(\beta)$ = 0.7 I = 0.1 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 10.14120 I = 0.1 M Ba + 2 H + L ⇌ BaH_2L $\log_{10}(\beta)$ = 10.84120 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 12.33623
La^{3+} + $(citrate)^{3-}$ ⇌ **La(citrate)** ***(aq)***	9.18		1	
Ce^{3+} + $(citrate)^{3-}$ ⇌ **Ce(citrate)** ***(aq)***	9.33218		1	Original data for β: $\log_{10}(\beta)$ = 7.41, at I = 0.1 M.
Pr^{3+} + $(citrate)^{3-}$ ⇌ **Pr(citrate)** ***(aq)***	9.5		1	
Nd^{3+} + $(citrate)^{3-}$ ⇌ **Nd(citrate)** ***(aq)***	9.51		1	
Pm^{3+} + $(citrate)^{3-}$ ⇌ **Pm(citrate)** ***(aq)***	9.63218		1	Original data for β: $\log_{10}(\beta)$ = 7.71, at I = 0.1 M.
Sm^{3+} + $(citrate)^{3-}$ ⇌ **Sm(citrate)** ***(aq)***	9.59		1	
Eu^{3+} + $(citrate)^{3-}$ ⇌ **Eu(citrate)** ***(aq)***	9.46		1	
Gd^{3+} + $(citrate)^{3-}$ ⇌ **Gd(citrate)** ***(aq)***	9.38		1	
Tb^{3+} + $(citrate)^{3-}$ ⇌ **Tb(citrate)** ***(aq)***	9.30		1	
Dy^{3+} + $(citrate)^{3-}$ ⇌ **Dy(citrate)** ***(aq)***	9.34		1	
Ho^{3+} + $(citrate)^{3-}$ ⇌ **Ho(citrate)** ***(aq)***	9.39		1	
Er^{3+} + $(citrate)^{3-}$ ⇌ **Er(citrate)** ***(aq)***	9.41		1	
Tm^{3+} + $(citrate)^{3-}$ ⇌ **Tm(citrate)** ***(aq)***	9.55		1	
Yb^{3+} + $(citrate)^{3-}$ ⇌ **Yb(citrate)** ***(aq)***	9.65		1	
Lu^{3+} + $(citrate)^{3-}$ ⇌ **Lu(citrate)** ***(aq)***	9.67		1	
Hg(II)$^{2+}$ + $(citrate)^{3-}$ ⇌ **Hg(II)(citrate)$^{-}$**	12.18145		1	Original data for β: $\log_{10}(\beta)$ = 10.9, at I = 0.1 M.
Pb(II)$^{2+}$ + $(citrate)^{3-}$ ⇌ **Pb(II)(citrate)$^{-}$**	5.65896		1	Original data for β: $\log_{10}(\beta)$ = 4.44, at I = 1.0 M.
Pb(II)$^{2+}$ + 2 $(citrate)^{3-}$ ⇌ **Pb(II)(citrate)$_2^{4-}$**	6.52948		1	Original data for β: $\log_{10}(\beta)$ = 5.92, at I = 1.0 M.
H^{+} + Pb(II)$^{2+}$ + $(citrate)^{3-}$ ⇌ **Pb(II)H(citrate)** ***(aq)***	10.18864		1	Pb(II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 2.98 I = 1.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 5.78652 I = 1.0 M Pb(II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 8.76652 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 10.18864

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + Pb(II)^{2+} + (citrate)^{3-} \rightleftharpoons$ **$Pb(II)H_2(citrate)^+$**	13.26332		1	$Pb(II) + H_2L \rightleftharpoons Pb(II)H_2L$ $log_{10}(\beta) = 1.7$ I = 1.0 M $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta) = 10.14120$ I = 1.0 M $Pb(II) + 2\ H + L \rightleftharpoons Pb(II)H_2L$ $log_{10}(\beta) = 11.84120$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 13.26332$
$H^+ + Pb(II)^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$Pb(II)H(citrate)_2^{3-}$**	12.03212		1	$Pb(II)L_2 + H \rightleftharpoons Pb(II)HL_2$ $log_{10}(\beta) = 4.69$ I = 1.0 M $Pb(II) + 2\ L \rightleftharpoons Pb(II)L_2$ $log_{10}(\beta) = 5.92$ I = 1.0 M $Pb(II) + H + 2\ L \rightleftharpoons Pb(II)HL2$ $log_{10}(\beta) = 10.61$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 12.03212$
$2\ Pb(II)^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$Pb(II)_2(citrate)_2^{2-}$**	12.93476		1	Original data for β: $log_{10}(\beta) = 10.70$, at I = 1.0 M.
$2\ Pb(II)^{2+} + (OH)^- + 2\ (citrate)^{3-} \rightleftharpoons$ **$Pb(II)_2(OH)(citrate)_2^{3-}$**	18.58844		1	$Pb(II)L_2 + OH \rightleftharpoons Pb(II)_2OHL_2$ $log_{10}(\beta) = 6.06$ I = 1.0 M $2\ Pb(II) + 2\ L \rightleftharpoons Pb(II)_2L_2$ $log_{10}(\beta) = 10.7$ I = 1.0 M $2\ Pb(II) + OH + 2\ L \rightleftharpoons Pb(II)_2OHL_2$ $log_{10}(\beta) = 16.76$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 18.58844$
$2\ Pb(II)^{2+} + 2\ (OH)^- + 2\ (citrate)^{3-} \rightleftharpoons$ **$Pb(II)_2(OH)_2(citrate)_2^{4-}$**	25.42896		1	$Pb(II)_2OHL_2 + OH \rightleftharpoons Pb(II)_2(OH)_2L_2$ $log_{10}(\beta) = 7.45$ I = 1.0 M $2\ Pb(II) + OH + 2\ L \rightleftharpoons Pb(II)_2OHL_2$ $log_{10}(\beta) = 16.76$ I = 1.0 M $2\ Pb(II) + 2\ OH + 2\ L \rightleftharpoons Pb(II)_2(OH)_2L_2$ $log_{10}(\beta) = 24.21$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 25.42896$
$(U(VI)O_2)^{2+} + (citrate)^{3-} \rightleftharpoons$ **$(U(VI)O_2)(citrate)^-$**	8.68145		1	Original data for β: $log_{10}(\beta) = 7.4$, at I = 0.1 M.
$2\ (U(VI)O_2)^{2+} + 2\ (citrate)^{3-} \rightleftharpoons$ **$(U(VI)O_2)_2(citrate)_2^{2-}$**	21.21933		1	Original data for β: $log_{10}(\beta) = 18.87$, at I = 0.1 M.
$H^+ + (NH_3)$ *(aq)* $+ (citrate)^{3-} \rightleftharpoons$ **$H(NH_3)(citrate)^{2-}$**	10.90762		1	$NH_4 + L \rightleftharpoons NH_4L$ $log_{10}(\beta) = 0.95$ I = 0.15 M (Original data for β at T = 37°C) $NH_3 + H \rightleftharpoons NH_4$ $log_{10}(\beta) = 9.244$ I = 0.15 M $H + NH_3 + L \rightleftharpoons NH_4L$ $log_{10}(\beta) = 10.194$ I = 0.15 M I = 0 M: $log_{10}(\beta) = 10.90762$
$2\ H^+ + (H_2SiO_4)^{2-} + (citrate)^{3-} \rightleftharpoons$ **$(H_4SiO_4)(citrate)^{3-}$**	23.15000		1	$H_4SiO_4 + L \rightleftharpoons H_4SiO_4L$ $log_{10}(\beta) = 0.11$ I = 0.5 M $2\ H + H_2SiO_4 \rightleftharpoons H_4SiO_4$ $log_{10}(\beta) = 22.23484$ I = 0.5 M $2\ H + H_2SiO_4 \rightleftharpoons H_4SiO_4L$ $log_{10}(\beta) = 22.34484$ I = 0.5 M I = 0 M: $log_{10}(\beta) = 23.15000$

2.2.31. HEDTA

The ligand in its neutral form is N-(2-hydroxyethyl)ethylenedinitrilotriacetic acid (HEDTA; $C_{10}H_{18}N_2O_7$). The ligand L as it is present in the database is the anion $C_{10}H_{15}N_2O_7^{3-}$. Its molecular weight is 275.237. Its structural formula is shown on the right.
Do not mix up this one with EDTA (next section).



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (HEDTA)^{3-} \rightleftharpoons$ **$H(HEDTA)^{2-}$**	10.42573	-2.7E+4	1	Original data for β: $log_{10}(\beta)$ = 9.70, at I = 0.1 M when a Na^+-salt is the background electrolyte; $log_{10}(\beta)$ = 9.87 (also at I = 0.1 M) when a K^+-salt is the background electrolyte. The average log-value (9.785) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
$2\ H^+ + (HEDTA)^{3-} \rightleftharpoons$ **$H_2(HEDTA)^-$**	16.23288	-3.9E+4	1	$HL + H \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 5.38 I = 0.1 M ΔH = -1.2E+4 (Original data for ΔH at I = 0.1 M) $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 9.785 I = 0.1 M ΔH = -2.7E+4 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 15.165 I = 0.1 M ΔH = -3.9E+4 I = 0 M: $log_{10}(\beta)$ = 16.23288
$3\ H^+ + (HEDTA)^{3-} \rightleftharpoons$ **$H_3(HEDTA)$ *(aq)***	19.06645	-3.44E+4	1	$H_2L + H \rightleftharpoons H_3L$ $log_{10}(\beta)$ = 2.62 I = 0.1 M ΔH = 4.6E+3 (Original data for ΔH at I = 0.1 M) $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 15.165 I = 0.1 M ΔH = -3.9E+4 $3\ H + L \rightleftharpoons H_3L$ $log_{10}(\beta)$ = 17.785 I = 0.1 M ΔH = -3.44E+4 I = 0 M: $log_{10}(\beta)$ = 19.06645
$4\ H^+ + (HEDTA)^{3-} \rightleftharpoons$ **$H_4(HEDTA)^+$**	20.66645		1	$H_3L + H \rightleftharpoons H_4L$ $log_{10}(\beta)$ = 1.6 I = 1.0 M $3\ H + L \rightleftharpoons H_3L$ $log_{10}(\beta)$ = 17.84749 I = 1.0 M $4\ H + L \rightleftharpoons H_4L$ $log_{10}(\beta)$ = 19.44749 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 20.66645

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Mg^{2+} + $(HEDTA)^{3-}$ ⇌ **$Mg(HEDTA)^{-}$**	8.28145	1.4E+4	1	Original data for β: $log_{10}(\beta)$ = 7.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M
Al^{3+} + $(HEDTA)^{3-}$ ⇌ **Al(HEDTA) *(aq)***	16.32218	3.7E+4	1	Original data for β: $log_{10}(\beta)$ = 14.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Al^{3+} + $(HEDTA)^{3-}$ ⇌ **$AlH(HEDTA)^{+}$**	18.46218		1	AlL + H ⇌ AlHL $log_{10}(\beta)$ = 2.14 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 14.4 I = 0.1 M Al + L + H ⇌ AlHL $log_{10}(\beta)$ = 16.54 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.46218
Al^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Al(HEDTA)(OH)^{-}$**	25.21560		1	AlL ⇌ AlOHL + H $log_{10}(\beta)$ = -4.89 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 14.4 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + L + OH ⇌ AlOHL $log_{10}(\beta)$ = 23.29342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.21560
Al^{3+} + 2 $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Al(HEDTA)(OH)_2^{2-}$**	29.59544		1	AlOHL ⇌ $Al(OH)_2L$ + H $log_{10}(\beta)$ = -9.19 I = 0.1 M Al + L + OH ⇌ AlOHL $log_{10}(\beta)$ = 23.29342 I = 0.1 M OH + H ⇌ H2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + L + 2 OH ⇌ $Al(OH)_2L$ $log_{10}(\beta)$ = 27.88684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 29.59544
Ca^{2+} + $(HEDTA)^{3-}$ ⇌ **$Ca(HEDTA)^{-}$**	9.38145	-2.7E+4	1	Original data for β: $log_{10}(\beta)$ = 8.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Sc^{3+} + $(HEDTA)^{3-}$ ⇌ **Sc(HEDTA) *(aq)***	19.22218		1	Original data for β: $log_{10}(\beta)$ = 17.3, at I = 0.1 M.
$Mn(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **$Mn(II)(HEDTA)^{-}$**	12.38145	-2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 11.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Fe(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **$Fe(II)(HEDTA)^{-}$**	13.48145	-2.5E+4	1	Original data for β: $log_{10}(\beta)$ = 12.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M
H^{+} + $Fe(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **Fe(II)H(HEDTA) *(aq)***	16.40003	-3.1E+4	1	Fe(II) + HL ⇌ Fe(II)HL $log_{10}(\beta)$ = 5.12 I = 0.1 M ΔH = -4E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.785 I = 0.1 M ΔH = -2.7E+4 Fe(II) + H + L ⇌ Fe(II)HL $log_{10}(\beta)$ = 14.905 I = 0.1 M ΔH = -3.1E+4 I = 0 M: $log_{10}(\beta)$ = 16.40003
$Fe(III)^{3+}$ + $(HEDTA)^{3-}$ ⇌ **Fe(III)(HEDTA) *(aq)***	21.62218		1	Original data for β: $log_{10}(\beta)$ = 19.7, at I = 0.1 M.
$Fe(III)^{3+}$ + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Fe(III)(HEDTA)(OH)^{-}$**	31.52560		1	Fe(III)L ⇌ Fe(III)OHL + H $log_{10}(\beta)$ = -3.88 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 19.7 I = 0.1 M Fe(III) + L + OH ⇌ Fe(III)OHL $log_{10}(\beta)$ = 29.60342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 31.52560
$Fe(III)^{3+}$ + 2 $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Fe(III)(HEDTA)(OH)_2^{2-}$**	36.26544		1	Fe(III)OHL ⇌ $Fe(III)(OH)_2L$ + H $log_{10}(\beta)$ = -8.83 I = 0.1 M Fe(III) + L + OH ⇌ Fe(III)OHL $log_{10}(\beta)$ = 29.60342 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(III) + L + 2 OH ⇌ $Fe(III)(OH)_2L$ $log_{10}(\beta)$ = 34.55684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 36.26544

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Fe(III)$^{3+}$ + 3 (OH)$^{-}$ + (HEDTA)$^{3-}$ ⇌ **Fe(III)(HEDTA)(OH)$_3^{3-}$**	39.62171		1	Fe(III)(OH)$_2$L ⇌ Fe(III)(OH)$_3$L + H log$_{10}$(β) = -10.00 I = 0.1 M Fe(III) + 2 OH + L ⇌ Fe(III)(OH)$_2$L log$_{10}$(β) = 34.55684 I = 0.1 M OH + H ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Fe(III) + 3 OH +L ⇌ Fe(III)(OH)$_3$L log$_{10}$(β) = 38.34026 I = 0.1 M I = 0 M: log$_{10}$(β) = 39.62171
2 Fe(III)$^{3+}$ + 2 (OH)$^{-}$ + 2 (HEDTA)$^{3-}$ ⇌ **Fe(III)$_2$(HEDTA)$_2$(OH)$_2^{2-}$**	65.22804		1	2 Fe(III)OHL ⇌ Fe(III)$_2$(OH)$_2$L$_2$ log$_{10}$(β) = 2.38 I = 1.0 M 2 Fe(III) + 2 OH + 2 L ⇌ 2 Fe(III)OHL log$_{10}$(β) = 59.39432 I = 1.0 M 2 Fe(III) + 2 OH + 2 L ⇌ Fe(III)$_2$(OH)$_2$L$_2$ log$_{10}$(β) = 61.77432 I = 1.0 M I = 0 M: log$_{10}$(β) = 65.22804
Co(II)$^{2+}$ + (HEDTA)$^{3-}$ ⇌ **Co(II)(HEDTA)$^{-}$**	15.78145	-2.7E+4	1	Original data for β: log$_{10}$(β) = 14.5, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Co(II)$^{2+}$ + (HEDTA)$^{3-}$ ⇌ **Co(II)H(HEDTA) *(aq)***	18.23503		1	Co(II)L + H ⇌ Co(II)HL log$_{10}$(β) = 2.24 I = 0.1 M Co(II) + L ⇌ Co(II)L log$_{10}$(β) = 14.5 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL log$_{10}$(β) = 16.74 I = 0.1 M I = 0 M: log$_{10}$(β) = 18.23503
Co(III)$^{3+}$ + (HEDTA)$^{3-}$ ⇌ **Co(III)(HEDTA) *(aq)***	39.12218		1	Original data for β: log$_{10}$(β) = 37.2, at I = 0.1 M.
Ni^{2+} + (HEDTA)$^{3-}$ ⇌ **Ni(HEDTA)$^{-}$**	18.38145	-4.3E+4	1	Original data for β: log$_{10}$(β) = 17.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Ni^{2+} + (HEDTA)$^{3-}$ ⇌ **NiH(HEDTA) *(aq)***	21.22461		1	NiL + H ⇌ NiHL log$_{10}$(β) = 2.54 I = 1.0 M Ni + L ⇌ NiL log$_{10}$(β) = 17.16249 I = 1.0 M Ni + H + L ⇌ NiHL log$_{10}$(β) = 19.80249 I = 1.0 M I = 0 M: log$_{10}$(β) = 21.22461
Cu(II)$^{2+}$ + (HEDTA)$^{3-}$ ⇌ **Cu(II)(HEDTA)$^{-}$**	18.68145	-3.9E+4	1	Original data for β: log$_{10}$(β) = 17.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Cu(II)$^{2+}$ + (HEDTA)$^{3-}$ ⇌ **Cu(II)H(HEDTA) *(aq)***	21.34503		1	Cu(II)L + H ⇌ Cu(II)HL log$_{10}$(β) = 2.45 I = 0.1 M Cu(II) + L ⇌ Cu(II)L log$_{10}$(β) = 17.4 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL log$_{10}$(β) = 19.85 I = 0.1 M I = 0 M: log$_{10}$(β) = 21.34503
Zn^{2+} + (HEDTA)$^{3-}$ ⇌ **Zn(HEDTA)$^{-}$**	15.88145	-3.5E+4	1	Original data for β: log$_{10}$(β) = 14.6, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ga^{3+} + (HEDTA)$^{3-}$ ⇌ **Ga(HEDTA) *(aq)***	20.02218		1	Original data for β: log$_{10}$(β) = 18.1, at I = 0.1 M.
Ga^{3+} + (OH)$^{-}$ + (HEDTA)$^{3-}$ ⇌ **Ga(HEDTA)(OH)$^{-}$**	29.42560		1	GaL ⇌ GaOHL + H log$_{10}$(β) = -4.38 I = 0.1 M Ga + L ⇌ GaL log$_{10}$(β) = 18.1 I = 0.1 M OH + H ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Ga + L + OH ⇌ GaOHL log$_{10}$(β) = 27.50342 I = 0.1 M I = 0 M: log$_{10}$(β) = 29.42560
Sr^{2+} + (HEDTA)$^{3-}$ v **Sr(HEDTA)$^{-}$**	8.08145	-2.1E+4	1	Original data for β: log$_{10}$(β) = 6.8, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Y^{3+} + (HEDTA)$^{3-}$ ⇌ **Y(HEDTA) *(aq)***	16.64218	-1.0E+4	1	Original data for β: log$_{10}$(β) = 14.72, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Y^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Y(HEDTA)(OH)^{-}$**	21.40218		1	YL + OH ⇌ YOHL $log_{10}(\beta)$ = 4.76 I = 0.1 M (Original data for β at T = 20°C) Y + L ⇌ YL $log_{10}(\beta)$ = 14.72 I = 0.1 M Y + OH + L ⇌ YOHL $log_{10}(\beta)$ = 19.48 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.40218
Ag^{+} + $(HEDTA)^{3-}$ ⇌ **$Ag(HEDTA)^{2-}$**	7.31073		1	Original data for β: $log_{10}(\beta)$ = 6.67, at I = 0.1 M.
Cd^{2+} + $(HEDTA)^{3-}$ ⇌ **$Cd(HEDTA)^{-}$**	14.98145	-4.3E+4	1	Original data for β: $log_{10}(\beta)$ = 13.7, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Cd^{2+} + $(HEDTA)^{3-}$ ⇌ **CdH(HEDTA) *(aq)***	17.55752		1	CdL + H ⇌ CdHL $log_{10}(\beta)$ = 2.30 I = 1.0 M Cd + L ⇌ CdL $log_{10}(\beta)$ = 13.76249 I = 1.0 M Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 16.06249 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 17.55752
In^{3+} + $(HEDTA)^{3-}$ ⇌ **In(HEDTA) *(aq)***	22.12218		1	Original data for β at I = 0.1 M at 20°C.
Ba^{2+} + $(HEDTA)^{3-}$ ⇌ **$Ba(HEDTA)^{-}$**	7.48145	-2.2E+4	1	Original data for β: $log_{10}(\beta)$ = 6.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
La^{3+} + $(HEDTA)^{3-}$ ⇌ **La(HEDTA) *(aq)***	15.40218	-1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 13.48, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
La^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$La(HEDTA)(OH)^{-}$**	18.86218		1	LaL + OH ⇌ LaOHL $log_{10}(\beta)$ = 3.46 I = 0.1 M (Original data for β at T = 20°C) La + L ⇌ LaL $log_{10}(\beta)$ = 13.48 I = 0.1 M La + OH + L ⇌ LaOHL $log_{10}(\beta)$ = 16.94 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.86218
Ce^{3+} + $(HEDTA)^{3-}$ ⇌ **Ce(HEDTA) *(aq)***	16.01218	-2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 14.09, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Pr^{3+} + $(HEDTA)^{3-}$ ⇌ **Pr(HEDTA) *(aq)***	16.53218	-2.3E+4	1	Original data for β: $log_{10}(\beta)$ = 14.61, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Pr^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Pr(HEDTA)(OH)^{-}$**	20.32218		1	PrL + OH ⇌ PrOHL $log_{10}(\beta)$ = 3.69 I = 0.1 M (Original data for β at T = 20°C) Pr + L ⇌ PrL $log_{10}(\beta)$ = 14.61 I = 0.1 M Pr + OH + L ⇌ PrOHL $log_{10}(\beta)$ = 18.30 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.32218
Nd^{3+} + $(HEDTA)^{3-}$ ⇌ **Nd(HEDTA) *(aq)***	16.80218	-2.5E+4	1	Original data for β: $log_{10}(\beta)$ = 14.88, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Nd^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **$Nd(HEDTA)(OH)^{-}$**	20.39218		1	NdL + OH ⇌ NdOHL $log_{10}(\beta)$ = 3.59 I = 0.1 M (Original data for β at T = 20°C) Nd + L ⇌ NdL $log_{10}(\beta)$ = 14.88 I = 0.1 M Nd + OH + L ⇌ NdOHL $log_{10}(\beta)$ = 18.47 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.39218
Sm^{3+} + $(HEDTA)^{3-}$ ⇌ **Sm(HEDTA) *(aq)***	17.23218	-2.9E+4	1	Original data for β: $log_{10}(\beta)$ = 15.31, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

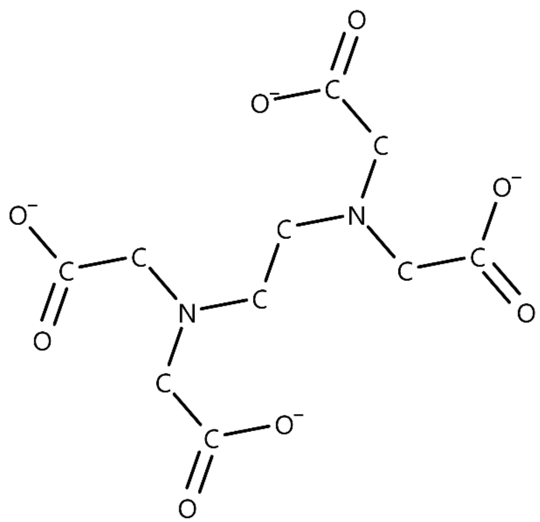
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Sm^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **Sm(HEDTA)(OH)**$^{-}$	20.93218		1	SmL + OH ⇌ SmOHL $log_{10}(\beta)$ = 3.70 I = 0.1 M (Original data for β at T = 20°C) Sm + L ⇌ SmL $log_{10}(\beta)$ = 15.31 I = 0.1 M Sm + OH + L ⇌ SmOHL $log_{10}(\beta)$ = 19.01 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.93218
Eu^{3+} + $(HEDTA)^{3-}$ ⇌ **Eu(HEDTA)** ***(aq)***	17.26218	-2.9E+4	1	Original data for β: $log_{10}(\beta)$ = 15.34, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Eu^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **Eu(HEDTA)(OH)**$^{-}$	21.29218		1	EuL + OH ⇌ EuOHL $log_{10}(\beta)$ = 4.03 I = 0.1 M (Original data for β at T = 20°C) Eu + L ⇌ EuL $log_{10}(\beta)$ = 15.34 I = 0.1 M Eu + OH + L ⇌ EuOHL $log_{10}(\beta)$ = 19.37 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.29218
Gd^{3+} + $(HEDTA)^{3-}$ ⇌ **Gd(HEDTA)** ***(aq)***	17.12218	-2.8E+4	1	Original data for β: $log_{10}(\beta)$ = 15.20, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Gd^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **Gd(HEDTA)(OH)**$^{-}$	21.10218		1	GdL + OH ⇌ GdOHL $log_{10}(\beta)$ = 3.98 I = 0.1 M (Original data for β at T = 20°C) Gd + L ⇌ GdL $log_{10}(\beta)$ = 15.20 I = 0.1 M Gd + OH + L ⇌ GdOHL $log_{10}(\beta)$ = 19.18 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.10218
Tb^{3+} + $(HEDTA)^{3-}$ ⇌ **Tb(HEDTA)** ***(aq)***	17.20218	-2.4E+4	1	Original data for β: $log_{10}(\beta)$ = 15.28, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Tb^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **Tb(HEDTA)(OH)**$^{-}$	21.72218		1	TbL + OH ⇌ TbOHL $log_{10}(\beta)$ = 4.52 I = 0.1 M (Original data for β at T = 20°C) Tb + L ⇌ TbL $log_{10}(\beta)$ = 15.28 I = 0.1 M Tb + OH + L ⇌ TbOHL $log_{10}(\beta)$ = 19.80 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.72218
Dy^{3+} + $(HEDTA)^{3-}$ ⇌ **Dy(HEDTA)** ***(aq)***	17.18218	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 15.26, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Dy^{3+} + $(OH)^{-}$ + $(HEDTA)^{3-}$ ⇌ **Dy(HEDTA)(OH)**$^{-}$	22.06218		1	DyL + OH ⇌ DyOHL $log_{10}(\beta)$ = 4.88 I = 0.1 M (Original data for β at T = 20°C) Dy + L ⇌ DyL $log_{10}(\beta)$ = 15.26 I = 0.1 M Dy + OH + L ⇌ DyOHL $log_{10}(\beta)$ = 20.14 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.06218
Ho^{3+} + $(HEDTA)^{3-}$ ⇌ **Ho(HEDTA)** ***(aq)***	17.20218	-1.4E+4	1	Original data for β: $log_{10}(\beta)$ = 15.28, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ho^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Ho(HEDTA)(OH)**$^-$	22.32218		1	HoL + OH ⇌ HoOHL $log_{10}(\beta)$ = 5.12 I = 0.1 M (Original data for β at T = 20°C) Ho + L ⇌ HoL $log_{10}(\beta)$ = 15.28 I = 0.1 M Ho + OH + L ⇌ HoOHL $log_{10}(\beta)$ = 20.40 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.32218
Er^{3+} + $(HEDTA)^{3-}$ ⇌ **Er(HEDTA)** ***(aq)***	17.30218	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 15.38, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Er^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Er(HEDTA)(OH)**$^-$	22.44218		1	ErL + OH ⇌ ErOHL $log_{10}(\beta)$ = 5.14 I = 0.1 M (Original data for β at T = 20°C) Er + L ⇌ ErL $log_{10}(\beta)$ = 15.38 I = 0.1 M Er + OH + L ⇌ ErOHL $log_{10}(\beta)$ = 20.52 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.44218
Tm^{3+} + $(HEDTA)^{3-}$ ⇌ **Tm(HEDTA)** ***(aq)***	17.48218	-7.5E+3	1	Original data for β: $log_{10}(\beta)$ = 15.56, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Tm^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Tm(HEDTA)(OH)**$^-$	22.59218		1	TmL + OH ⇌ TmOHL $log_{10}(\beta)$ = 5.11 I = 0.1 M (Original data for β at T = 20°C) Tm + L ⇌ Tm L $log_{10}(\beta)$ = 15.56 I = 0.1 M Tm + OH + L ⇌ TmOHL $log_{10}(\beta)$ = 20.67 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.59218
Yb^{3+} + $(HEDTA)^{3-}$ ⇌ **Yb(HEDTA)** ***(aq)***	17.75218	-8.7E+3	1	Original data for β: $log_{10}(\beta)$ = 15.83, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Yb^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Yb(HEDTA)(OH)**$^-$	22.96218		1	YbL + OH ⇌ YbOHL $log_{10}(\beta)$ = 5.14 I = 0.1 M (Original data for β at T = 20°C) Yb + L ⇌ YbL $log_{10}(\beta)$ = 15.38 I = 0.1 M Yb + OH + L ⇌ YbOHL $log_{10}(\beta)$ = 20.52 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.44218
Lu^{3+} + $(HEDTA)^{3-}$ ⇌ **Lu(HEDTA)** ***(aq)***	17.85218	-9.2E+3	1	Original data for β: $log_{10}(\beta)$ = 15.93, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Lu^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Lu(HEDTA)(OH)**$^-$	22.98218		1	LuL + OH ⇌ LuOHL $log_{10}(\beta)$ = 5.21 I = 0.1 M (Original data for β at T = 20°C) Lu + L ⇌ LuL $log_{10}(\beta)$ = 15.83 I = 0.1 M Lu + OH + L ⇌ LuOHL $log_{10}(\beta)$ = 21.04 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.98218
$Hg(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **Hg(II)(HEDTA)**$^-$	21.38145	-8.36E+4	1	Original data for β: $log_{10}(\beta)$ = 20.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Hg(II)^{2+}$ + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **Hg(II)(HEDTA)(OH)**$^{2-}$	26.55130		1	Hg(II)L ⇌ Hg(II)OHL + H $log_{10}(\beta)$ = -8.4 I = 0.1 M Hg(II) + L ⇌ Hg(II)L $log_{10}(\beta)$ = 20.1 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Hg(II) + OH + L ⇌ Hg(II)OHL $log_{10}(\beta)$ = 25.48342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.55130

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **$Pb(II)(HEDTA)^{-}$**	16.88145	-5.27E+4	1	Original data for β: $log_{10}(\beta)$ = 15.6, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + $Pb(II)^{2+}$ + $(HEDTA)^{3-}$ ⇌ **Pb(II)H(HEDTA) *(aq)***	19.22461		1	Pb(II)L + H ⇌ Pb(II)HL $log_{10}(\beta)$ = 2.14 I = 1.0 M Pb(II) + L ⇌ Pb(II)L $log_{10}(\beta)$ = 15.66249 I = 1.0 M Pb(II) + L + H ⇌ Pb(II)HL $log_{10}(\beta)$ = 17.80249 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 19.22461
Bi^{3+} + $(HEDTA)^{3-}$ ⇌ **Bi(HEDTA) *(aq)***	24.12844		1	Original data for β: $log_{10}(\beta)$ = 22.3, at I = 1.0 M.
Bi^{3+} + $(OH)^-$ + $(HEDTA)^{3-}$ ⇌ **$Bi(OH)(HEDTA)^-$**	32.47228		1	BiL ⇌ BiOHL + H $log_{10}(\beta)$ = -5.45 I = 1.0 M Bi + L ⇌ BiL $log_{10}(\beta)$ = 22.3 I = 1.0 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Bi + OH + L ⇌ BiOHL $log_{10}(\beta)$ = 30.64384 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 32.47228

2.2.32. EDTA

The ligand in its neutral form is ethylenedinitrilotetraacetic acid (EDTA; $C_{10}H_{16}N_2O_8$). The ligand L as it is present in the database is the anion $C_{10}H_{12}N_2O_8^{4-}$. Its molecular weight is 288.212. Its structural formula is shown on the right.
Do not mix up this one with HEDTA (previous section).



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(EDTA)^{4-}$ ⇌ **$H(EDTA)^{3-}$**	10.948	-2.1E+4	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + $(EDTA)^{4-}$ ⇌ **$H_2(EDTA)^{2-}$**	17.221	-3.6E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 6.273 ΔH = -1.5E+4 H + L ⇌ HL $log_{10}(\beta)$ = 10.948 ΔH = -2.1E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 17.221 ΔH = -3.6E+4
3 H^+ + $(EDTA)^{4-}$ ⇌ **$H_3(EDTA)^{-}$**	20.33815	-2.89E+4	1	H_2L + H ⇌ H_3L $log_{10}(\beta)$ = 2.69 I = 0.1 M ΔH = 7.1E+3 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 15.72597 I = 0.1 M ΔH = -3.6E+4 3 H + L ⇌ H_3L $log_{10}(\beta)$ = 18.41597 I = 0.1 M ΔH = -2.89E+4 I = 0 M: $log_{10}(\beta)$ = 20.33815
4 H^+ + $(EDTA)^{4-}$ ⇌ **$H_4(EDTA)$ *(aq)***	22.55172	-2.79E+4	1	H_3L + H ⇌ H_4L $log_{10}(\beta)$ = 2.00 I = 0.1 M ΔH = 1E+3 (Original data for ΔH at I = 0.1 M) 3 H + L ⇌ H_3L $log_{10}(\beta)$ = 18.41597 I = 0.1 M ΔH = -2.89E+4 4 H + L ⇌ H_4L $log_{10}(\beta)$ = 20.41597 I = 0.1 M ΔH = -2.79E+4 I = 0 M: $log_{10}(\beta)$ = 22.55172
5 H^+ + $(EDTA)^{4-}$ ⇌ **$H_5(EDTA)^{+}$**	24.05172	-2.59E+4	1	H_4L + H ⇌ H_5L $log_{10}(\beta)$ = 1.5 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M and 20°C) 4 H + L ⇌ H_4L $log_{10}(\beta)$ = 20.41597 I = 0.1 M ΔH = -2.79E+4 5 H + L ⇌ H_5L $log_{10}(\beta)$ = 21.91597 I = 0.1 M ΔH = -2.59E+4 I = 0 M: $log_{10}(\beta)$ = 24.05172
6 H^+ + $(EDTA)^{4-}$ ⇌ **$H_6(EDTA)^{2+}$**	23.94230	-2.50E+4	1	H_5L + H ⇌ H_6L $log_{10}(\beta)$ = 0.0 I = 1.0 M ΔH = 8E+2 (Original data for ΔH at I = 0.1 M) 5 H + L ⇌ H_5L $log_{10}(\beta)$ = 22.02012 I = 1.0 M ΔH = -2.59E+4 6 H + L ⇌ H_6L $log_{10}(\beta)$ = 22.02012 I = 1.0 M ΔH = -2.51E+4 I = 0 M: $log_{10}(\beta)$ = 23.94230
Li^+ + $(EDTA)^{4-}$ ⇌ **$Li(EDTA)^{3-}$**	3.80430	4E+2	1	Original data for β: $log_{10}(\beta)$ = 2.95, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Be^{2+} + $(EDTA)^{4-}$ ⇌ **$Be(EDTA)^{2-}$**	11.40860	4.1E+4	1	Original data for β: $log_{10}(\beta)$ = 9.7, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Na^+ + $(EDTA)^{4-}$ ⇌ **$Na(EDTA)^{3-}$**	2.71430	-5.8E+3	1	Original data for β: $log_{10}(\beta)$ = 1.86, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Na^+ + $(EDTA)^{4-}$ ⇌ **$NaH(EDTA)^{2-}$**	11.168		4	
Mg^{2+} + $(EDTA)^{4-}$ ⇌ **$Mg(EDTA)^{2-}$**	10.58360	1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 8.79, at I = 0.1 M when K^+ is the background electrolyte; $log_{10}(\beta)$ = 8.96 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (8.875) was converted to I = 0 M.
H^+ + Mg^{2+} + $(EDTA)^{4-}$ ⇌ **$MgH(EDTA)^{-}$**	15.01075		1	MgL + H ⇌ MgHL $log_{10}(\beta)$ = 4.0 I = 0.1 M Mg + L ⇌ MgL $log_{10}(\beta)$ = 8.875 I = 0.1 M Mg + H + L ⇌ MgHL $log_{10}(\beta)$ = 12.875 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.01075
Al^{3+} + $(EDTA)^{4-}$ ⇌ **$Al(EDTA)^{-}$**	18.96290	5.27E+4	1	Original data for β: $log_{10}(\beta)$ = 16.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Al^{3+} + (EDTA)^{4-} \rightleftharpoons$ **AlH(EDTA)** ***(aq)***	21.77648	3.67E+4	1	AlL + H ⇌ AlHL $\log_{10}(\beta)$ = 2.6 I = 0.1 M ΔH = -1.6E+4 (Original data for ΔH at I = 0.1 M and 20°C) Al + L ⇌ AlL $\log_{10}(\beta)$ = 16.4 I = 0.1 M ΔH = 5.27E+4 Al + H + L ⇌ AlHL $\log_{10}(\beta)$ = 19.0 I = 0.1 M ΔH = 3.67E+4 I = 0 M: $\log_{10}(\beta)$ = 21.77648
$Al^{3+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Al(EDTA)(OH)^{2-}$**	26.63275	1.689E+4	1	AlL ⇌ AlOHL + H $\log_{10}(\beta)$ = -5.9 I = 0.1 M ΔH = 2E+4 (Original data for ΔH at I = 0.1 M and 20°C) Al + L ⇌ AlL $\log_{10}(\beta)$ = 16.4 I = 0.1 M ΔH = 5.27E+4 OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Al + OH + L ⇌ AlOHL $\log_{10}(\beta)$ = 24.28342 I = 0.1 M ΔH = 1.689E+4 I = 0 M: $\log_{10}(\beta)$ = 26.63275
$Al^{3+} + 2\ (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Al(EDTA)(OH)_2^{3-}$**	29.67902		1	AlOHL ⇌ $Al(OH)_2L$ + H $\log_{10}(\beta)$ = -10.31 I = 0.1 M Al + OH + L ⇌ AlOHL $\log_{10}(\beta)$ = 24.28342 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + 2 OH + L ⇌ $Al(OH)_2L$ $\log_{10}(\beta)$ = 27.75684 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 29.67902
$K^+ + (EDTA)^{4-} \rightleftharpoons$ **$K(EDTA)^{3-}$**	1.65430	0	1	Original data for β: $\log_{10}(\beta)$ = 0.8, at I = 0.1 M.
$Ca^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Ca(EDTA)^{2-}$**	12.43860	-2.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 10.65, at I = 0.1 M when K^+ is the background electrolyte; $\log_{10}(\beta)$ = 10.81 (also at I = 0.1 M) when a tetraalkyl ammonium salt is the background electrolyte. The average log-value (10.73) was converted to I = 0 M.
$H^+ + Ca^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$CaH(EDTA)^-$**	15.96575		1	CaL + H ⇌ CaHL $\log_{10}(\beta)$ = 3.1 I = 0.1 M Ca + L ⇌ CaL $\log_{10}(\beta)$ = 10.73 I = 0.1 M Ca + H + L ⇌ CaHL $\log_{10}(\beta)$ = 13.83 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 15.96575
$Sc^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Sc(EDTA)^-$**	25.66290		1	Original data for β: $\log_{10}(\beta)$ = 23.1, at I = 0.1 M at 20°C.
$H^+ + Sc^{3+} + (EDTA)^{4-} \rightleftharpoons$ **ScH(EDTA)** ***(aq)***	27.87648		1	ScL + H ⇌ ScHL $\log_{10}(\beta)$ = 2.0 I = 0.1 M (Original data for β at T = 20°C) Sc + L ⇌ ScL $\log_{10}(\beta)$ = 23.1 I = 0.1 M Sc + H + L ⇌ ScHL $\log_{10}(\beta)$ = 25.1 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 27.87648
$Sc^{3+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Sc(EDTA)(OH)^{2-}$**	28.57275		1	ScL ⇌ Sc(OH)L + H $\log_{10}(\beta)$ = -10.66 I = 0.1 M (Original data for β at T = 20°C) OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Sc + L ⇌ ScL $\log_{10}(\beta)$ = 23.1 I = 0.1 M Sc + L + OH ⇌ Sc(OH)L $\log_{10}(\beta)$ = 26.22342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.57275
$Cr(III)^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Cr(III)(EDTA)^-$**	25.96290		1	Original data for β: $\log_{10}(\beta)$ = 23.4, at I = 0.1 M at 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $Cr(III)^{3+}$ + $(EDTA)^{4-}$ ⇌ **Cr(III)H(EDTA) *(aq)***	27.87648		1	Cr(III)L + H ⇌ Cr(III)HL $log_{10}(\beta)$ = 1.7 I = 0.1 M Cr(III) + L ⇌ Cr(III)L $log_{10}(\beta)$ = 23.4 I = 0.1 M Cr(III) + H + L ⇌ Cr(III)HL $log_{10}(\beta)$ = 25.1 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 27.87648
$Cr(III)^{3+}$ + $(OH)^-$ + $(EDTA)^{4-}$ ⇌ **$Cr(III)(EDTA)(OH)^{2-}$**	32.16275		1	Cr(III)L ⇌ Cr(III)OHL + H $log_{10}(\beta)$ = -7.37 I = 0.1 M Cr(III) + L ⇌ Cr(III)L $log_{10}(\beta)$ = 23.4 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Cr(III) + L + OH ⇌ Cr(III)OHL $log_{10}(\beta)$ = 29.81342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.16275
$Mn(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Mn(II)(EDTA)^{2-}$**	15.59860	-1.9E+4	1	Original data for β: $log_{10}(\beta)$ = 13.89, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
H^+ + $Mn(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Mn(II)H(EDTA)^-$**	19.12575	-2.4E+4	1	Mn(II)L + H ⇌ Mn(II)HL $log_{10}(\beta)$ = 3.1 I = 0.1 M (Original data for ΔH at I = 0.1 M) Mn(II) + L ⇌ Mn(II)L $log_{10}(\beta)$ = 13.89 I = 0.1 M Mn(II) + H + L ⇌ Mn(II)HL $log_{10}(\beta)$ = 16.99 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.12575
$Fe(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Fe(II)(EDTA)^{2-}$**	16.00860	-1.6E+4	1	Original data for β: $log_{10}(\beta)$ = 14.30, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + $Fe(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Fe(II)H(EDTA)^-$**	19.04945	-2.5E+4	1	Fe(II) + HL ⇌ Fe(II)HL $log_{10}(\beta)$ = 6.82 I = 0.1 M ΔH = -4E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.09370 I = 0.1 M ΔH = -2.1E+4 Fe(II) + H + L ⇌ Fe(II)HL $log_{10}(\beta)$ = 16.91370 I = 0.1 M ΔH = -2.5E+4 I = 0 M: $log_{10}(\beta)$ = 19.04945
$Fe(II)^{2+}$ + $(OH)^-$ + $(EDTA)^{4-}$ ⇌ **$Fe(II)(EDTA)(OH)^{3-}$**	20.4		3	
$Fe(II)^{2+}$ + 2 $(OH)^-$ + $(EDTA)^{4-}$ ⇌ **$Fe(II)(EDTA)(OH)_2^{4-}$**	23.7		3	
$Fe(III)^{3+}$ + $(EDTA)^{4-}$ ⇌ **$Fe(III)(EDTA)^-$**	27.66290	-1.1E+4	1	Original data for β: $log_{10}(\beta)$ = 25.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + $Fe(III)^{3+}$ + $(EDTA)^{4-}$ ⇌ **Fe(III)H(EDTA) *(aq)***	29.17648	-1.14E+4	1	Fe(III)L + H ⇌ Fe(III)HL $log_{10}(\beta)$ = 1.3 I = 0.1 M ΔH = -4E+2 (Original data for ΔH at I = 0.1 M) Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 25.1 I = 0.1 M ΔH = -1.1E+4 Fe(III) + L + H ⇌ Fe(III)HL $log_{10}(\beta)$ = 26.4 I = 0.1 M ΔH = -1.14E+4 I = 0 M: $log_{10}(\beta)$ = 29.17648

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Fe(III)^{3+}$ + $(OH)^{-}$ + $(EDTA)^{4-}$ ⇌ **$Fe(III)(EDTA)(OH)^{2-}$**	33.84275	-2.581E+4	1	Fe(III)L ⇌ Fe(III)OHL + H $log_{10}(\beta)$ = -7.39 I = 0.1 M ΔH = 4.1E+4 (Original data for ΔH at I = 1.0 M) Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 25.1 I = 0.1 M ΔH = -1.1E+4 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581e+4 Fe(III) + L + OH ⇌ Fe(III)OHL $log_{10}(\beta)$ = 31.49342 I = 0.1 M ΔH = -2.581e+4 I = 0 M: $log_{10}(\beta)$ = 33.84275
$Fe(III)^{3+}$ + 2 $(OH)^{-}$ + $(EDTA)^{4-}$ ⇌ **$Fe(III)(EDTA)(OH)_2^{3-}$**	37.7		3	
2 $Fe(III)^{3+}$ + 2 $(OH)^{-}$ + 2 $(EDTA)^{4-}$ ⇌ **$Fe(III)_2(EDTA)_2(OH)_2^{4-}$**	69.67286	-1.1362E+5	1	2 Fe(III)OHL ⇌ $Fe(III)_2(OH)_2L_2$ $log_{10}(\beta)$ = 2.8 I = 1.0 M ΔH = -6.2E+4 (Original data for ΔH at I = 1.0 M) 2 Fe(III) + 2 OH + 2 L ⇌ 2 Fe(III)OHL $log_{10}(\beta)$ = 63.21598 I = 1.0 M ΔH = -5.162E+4 2 Fe(III) + 2 OH + 2 L ⇌ $Fe(III)_2(OH)_2L_2$ $log_{10}(\beta)$ = 66.01598 I = 1.0 M ΔH = -1.1362E+5 I = 0 M: $log_{10}(\beta)$ = 69.67286
$Co(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Co(II)(EDTA)^{2-}$**	18.15860	-1.5E+4	1	Original data for β: $log_{10}(\beta)$ = 16.45, at I = 0.1 M.
H^{+} + $Co(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Co(II)H(EDTA)^{-}$**	21.58575	-2.29E+4	1	Co(II)L + H ⇌ Co(II)HL $log_{10}(\beta)$ = 3.0 I = 0.1 M ΔH = -7.9E+3 (Original data for ΔH at I = 0.1 M) Co(II) + L ⇌ Co(II)L $log_{10}(\beta)$ = 16.45 I = 0.1 M ΔH = -1.5E+4 Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 19.45 I = 0.1 M ΔH = -2.29E+4 I = 0 M: $log_{10}(\beta)$ = 21.58575
2 H^{+} + $Co(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Co(II)H_2(EDTA)$ *(aq)***	23.48891		1	Co(II)HL + H ⇌ $Co(II)H_2L$ $log_{10}(\beta)$ = 1.7 I = 1.0 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 19.55415 I = 1.0 M Co(II) + 2 H + L ⇌ $Co(II)H_2L$ $log_{10}(\beta)$ = 21.25415 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 23.48891
$Co(III)^{3+}$ + $(EDTA)^{4-}$ ⇌ **$Co(III)(EDTA)^{-}$**	43.96290		1	Original data for β: $log_{10}(\beta)$ = 41.4, at I = 0.1 M.
H^{+} + $Co(III)^{3+}$ + $(EDTA)^{4-}$ ⇌ **$Co(III)H(EDTA)$ *(aq)***	47.15648		1	Co(III)L + H ⇌ Co(III)HL $log_{10}(\beta)$ = 2.98 I = 0.1 M (Original data for β at T = 20°C) Co(III) + L ⇌ Co(III)L $log_{10}(\beta)$ = 41.4 I = 0.1 M Co(III) + H + L ⇌ Co(III)HL $log_{10}(\beta)$ = 44.38 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 47.15648
Ni^{2+} + $(EDTA)^{4-}$ ⇌ **$Ni(EDTA)^{2-}$**	20.10860	-3.0E+4	1	Original data for β: $log_{10}(\beta)$ = 18.4, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Ni^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{NiH(EDTA)^-}$	23.63575	-3.75E+4	1	NiL + H ⇌ NiHL $log_{10}(\beta)$ = 3.1 I = 0.1 M ΔH = -7.5E+3 (Original data for ΔH at I = 0.1 M) Ni + L ⇌ NiL $log_{10}(\beta)$ = 18.4 I = 0.1 M ΔH = -3.0E+4 Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 21.5 I = 0.1 M ΔH = -3.75E+4 I = 0 M: $log_{10}(\beta)$ = 23.63575
$2\ H^+ + Ni^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{NiH_2(EDTA)}$ ***(aq)***	24.73891		1	NiHL + H ⇌ NiH_2L $log_{10}(\beta)$ = 0.9 I = 1.0 M Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 21.60415 I = 1.0 M Ni + 2 H + L ⇌ NiH_2L $log_{10}(\beta)$ = 22.50415 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 24.73891
$Ni^{2+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons \mathbf{Ni(EDTA)(OH)^{3-}}$	21.56487	-3.941E+04	1	NiL ⇌ NiOHL + H $log_{10}(\beta)$ = -11.9 I = 0.1 M ΔH = 4.64E+4 (Original data for ΔH at I = 1.0 M) Ni + L ⇌ NiL $log_{10}(\beta)$ = 18.4 I = 0.1 M ΔH = -3E+4 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Ni + L + OH ⇌ NiOHL $log_{10}(\beta)$ = 20.28342 I = 0.1 M ΔH = -3.941E+04 I = 0 M: $log_{10}(\beta)$ = 21.56487
$Cu(II)^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Cu(II)(EDTA)^{2-}}$	20.48860	-3.3E+4	1	Original data for β: $log_{10}(\beta)$ = 18.78, at I = 0.1 M.
$H^+ + Cu(II)^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Cu(II)H(EDTA)^-}$	24.01575	-4.13E+4	1	Cu(II)L + H ⇌ Cu(II)HL $log_{10}(\beta)$ = 3.1 I = 0.1 M ΔH = -8.3E+3 (Original data for ΔH at I = 0.1 M) Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 18.78 I = 0.1 M ΔH = -3.3E+4 Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 21.88 I = 0.1 M ΔH = -4.13E+4 I = 0 M: $log_{10}(\beta)$ = 24.01575
$2\ H^+ + Cu(II)^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Cu(II)H_2(EDTA)}$ ***(aq)***	26.22933		1	Cu(II)HL + H ⇌ $Cu(II)H_2L$ $log_{10}(\beta)$ = 2.0 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 21.88 I = 0.1 M Cu(II) + 2 H + L ⇌ $Cu(II)H_2L$ $log_{10}(\beta)$ = 23.88 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.22933
$Cu(II)^{2+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons \mathbf{Cu(II)(EDTA)(OH)^{3-}}$	22.44487	-5.881E+4	1	Cu(II)L ⇌ Cu(II)OHL + H $log_{10}(\beta)$ = -11.4 I = 0.1 M ΔH = 3E+4 (Original data for ΔH at I = 1.0 M) Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 18.78 I = 0.1 M ΔH = -3.3E+4 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cu(II) + L + OH ⇌ Cu(II)OHL $log_{10}(\beta)$ = 21.16342 I = 0.1 M ΔH = -5.881E+4 I = 0 M: $log_{10}(\beta)$ = 22.44487
$Zn^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Zn(EDTA)^{2-}}$	18.0	-1.9E+4	1	Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Zn^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$ZnH(EDTA)^-$**	21.42715	-2.82E+4	1	ZnL + H ⇌ ZnHL $\log_{10}(\beta)$ = 3.0 I = 0.1 M ΔH = -9.2E+3 (Original data for ΔH at I = 0.1 M) Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 16.29140 I = 0.1 M ΔH = -1.9E+4 Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 19.29140 I = 0.1 M ΔH = -2.82E+4 I = 0 M: $\log_{10}(\beta)$ = 21.42715
$2\ H^+ + Zn^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$ZnH_2(EDTA)$ *(aq)***	22.83031		1	ZnHL + H ⇌ ZnH_2L $\log_{10}(\beta)$ = 1.2 I = 1.0 M Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 19.39555 I = 1.0 M Zn + 2 H + L ⇌ ZnH_2L $\log_{10}(\beta)$ = 20.59555 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 22.83031
$Zn^{2+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Zn(EDTA)(OH)^{3-}$**	19.75627	-3.981E+4	1	ZnL ⇌ ZnOHL + H $\log_{10}(\beta)$ = -11.6 I = 0.1 M ΔH = 3.5E+4 (Original data for ΔH at I = 1.0 M) Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 16.29140 I = 0.1 M ΔH = -1.9E+4 OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Zn + L + OH ⇌ ZnOHL $\log_{10}(\beta)$ = 18.47482 I = 0.1 M ΔH = -3.981E+4 I = 0 M: $\log_{10}(\beta)$ = 19.75627
$Ga^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Ga(EDTA)^-$**	24.26290		1	Original data for β: $\log_{10}(\beta)$ = 21.7, at I = 0.1 M.
$H^+ + Ga^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$GaH(EDTA)$ *(aq)***	26.17648		1	GaL + H ⇌ GaHL $\log_{10}(\beta)$ = 1.7 I = 0.1 M Ga + L ⇌ GaL $\log_{10}(\beta)$ = 21.7 I = 0.1 M Ga + H + L ⇌ GaHL $\log_{10}(\beta)$ = 23.4 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 26.17648
$Ga^{3+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Ga(EDTA)(OH)^{2-}$**	32.25275		1	GaL ⇌ GaOHL + H $\log_{10}(\beta)$ = -5.58 I = 0.1 M Ga + L ⇌ GaL $\log_{10}(\beta)$ = 21.7 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Ga + L + OH ⇌ GaOHL $\log_{10}(\beta)$ = 29.90342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 32.25275
$Rb^+ + (EDTA)^{4-} \rightleftharpoons$ **$Rb(EDTA)^{3-}$**	1.45430		1	Original data for β: $\log_{10}(\beta)$ = 0.6, at I = 0.1 M.
$Sr^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Sr(EDTA)^{2-}$**	10.42860	-1.7E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.72, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Sr^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$SrH(EDTA)^-$**	14.78575		1	SrL + H ⇌ SrHL $\log_{10}(\beta)$ = 3.93 I = 0.1 M (Original data for β at T = 20°C) Sr + L ⇌ SrL $\log_{10}(\beta)$ = 8.72 I = 0.1 M Sr + H + L ⇌ SrHL $\log_{10}(\beta)$ = 12.65 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 14.78575
$Y^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Y(EDTA)^-$**	20.64290	-2E+3	1	Original data for β: $\log_{10}(\beta)$ = 18.08, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Zr^{4+} + (EDTA)^{4-} \rightleftharpoons$ **$Zr(EDTA)$ *(aq)***	32.8	-2E+3	1	
$Zr^{4+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Zr(OH)(EDTA)^-$**	40.38342		1	ZrL ⇌ ZrOHL + H $\log_{10}(\beta)$ = -6.2 I = 0.1 M Zr + L ⇌ ZrL $\log_{10}(\beta)$ = 29.38280 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Zr + OH + L ⇌ ZrOHL $\log_{10}(\beta)$ = 36.96622 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 40.38342

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ Zr^{4+} + 2\ (OH)^{-} + 2\ (EDTA)^{4-} \rightleftharpoons \mathbf{Zr_2(OH)_2(EDTA)_2^{2-}}$	84.05327		1	$2\ ZrOHL \rightleftharpoons Zr_2(OH)_2L_2$ $log_{10}(\beta) = 3.5$ I = 0.1 M $2\ Zr + 2\ OH + 2\ L \rightleftharpoons 2\ ZrOHL$ $log_{10}(\beta) = 73.93244$ I = 0.1 M $2\ Zr + 2\ OH + 2\ L \rightleftharpoons Zr_2(OH)_2L_2$ $log_{10}(\beta) = 77.43244$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 84.05327$
$Pd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Pd(EDTA)^{2-}}$	27.30860		1	Original data for β: $log_{10}(\beta) = 25.6$, at I = 0.1 M at 20°C.
$H^{+} + Pd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{PdH(EDTA)^{-}}$	30.72492		1	$PdL + H \rightleftharpoons PdHL$ $log_{10}(\beta) = 3.01$ I = 1.0 M (Original data for β at T = 20°C) $Pd + L \rightleftharpoons PdL$ $log_{10}(\beta) = 25.68332$ I = 1.0 M $Pd + H + L \rightleftharpoons PdHL$ $log_{10}(\beta) = 28.69332$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 30.72492$
$2\ H^{+} + Pd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{PdH_2(EDTA)}$ ***(aq)***	33.23808		1	$PdHL + H \rightleftharpoons PdH_2L$ $log_{10}(\beta) = 2.31$ I = 1.0 M (Original data for β at T = 20°C) $Pd + H + L \rightleftharpoons PdHL$ $log_{10}(\beta) = 28.69332$ I = 1.0 M $Pd + 2\ H + L \rightleftharpoons PdH_2L$ $log_{10}(\beta) = 31.00332$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 33.23808$
$3\ H^{+} + Pd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{PdH_3(EDTA)^{+}}$	34.13808		1	$PdH_2L + H \rightleftharpoons PdH_3L$ $log_{10}(\beta) = 0.9$ I = 1.0 M (Original data for β at T = 20°C) $Pd + 2\ H + L \rightleftharpoons PdH_2L$ $log_{10}(\beta) = 31.00332$ I = 1.0 M $Pd + 3\ H + L \rightleftharpoons PdH_3L$ $log_{10}(\beta) = 31.90332$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 34.13808$
$Ag^{+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Ag(EDTA)^{3-}}$	8.05430	-3.1E+4	1	Original data for β: $log_{10}(\beta) = 7.20$, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
$H^{+} + Ag^{+} + (EDTA)^{4-} \rightleftharpoons \mathbf{AgH(EDTA)^{2-}}$	14.73503		1	$AgL + H \rightleftharpoons AgHL$ $log_{10}(\beta) = 6.04$ I = 0.1 M $Ag + L \rightleftharpoons AgL$ $log_{10}(\beta) = 7.20$ I = 0.1 M $Ag + H + L \rightleftharpoons AgHL$ $log_{10}(\beta) = 13.24$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 14.73503$
$2\ Ag^{+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Ag_2(EDTA)^{2-}}$	9.02212		1	Original data for β: $log_{10}(\beta) = 7.6$, at I = 1.0 M.
$Cd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{Cd(EDTA)^{2-}}$	18.1	-3.6E+4	1	
$H^{+} + Cd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{CdH(EDTA)^{-}}$	21.42715	-3.7E+4	1	$CdL + H \rightleftharpoons CdHL$ $log_{10}(\beta) = 2.9$ I = 0.1 M ΔH = -1E+3 (Original data for ΔH at I = 0.1 M) $Cd + L \rightleftharpoons CdL$ $log_{10}(\beta) = 16.39140$ I = 0.1 M ΔH = -3.6E+4 $Cd + H + L \rightleftharpoons CdHL$ $log_{10}(\beta) = 19.29140$ I = 0.1 M ΔH = -3.7E+4 I = 0 M: $log_{10}(\beta) = 21.42715$
$2\ H^{+} + Cd^{2+} + (EDTA)^{4-} \rightleftharpoons \mathbf{CdH_2(EDTA)}$ ***(aq)***	23.23031		1	$CdHL + H \rightleftharpoons CdH_2L$ $log_{10}(\beta) = 1.6$ I = 1.0 M $Cd + H + L \rightleftharpoons CdHL$ $log_{10}(\beta) = 19.39555$ I = 1.0 M $Cd + 2\ H + L \rightleftharpoons CdH_2L$ $log_{10}(\beta) = 20.99555$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 23.23031$

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + $(OH)^-$ + $(EDTA)^{4-}$ ⇌ **$Cd(EDTA)(OH)^{3-}$**	18.28752	-4.121E+4	1	CdL ⇌ CdOHL + H $\log_{10}(\beta)$ = -13.2 I = 1.0 M ΔH = 5.06E+4 (Original data for ΔH at I = 1.0 M) Cd + L ⇌ CdL $\log_{10}(\beta)$ = 16.47472 I = 1.0 M ΔH = -3.6E+4 OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.79384 I = 1.0 M ΔH = -5.581E+4 Cd + OH + L ⇌ CdOHL $\log_{10}(\beta)$ = 17.06856 I = 1.0 M ΔH = -4.121E+4 I = 0 M: $\log_{10}(\beta)$ = 18.28752
In^{3+} + $(EDTA)^{4-}$ ⇌ **$In(EDTA)^-$**	27.56290	-3.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 25.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
H^+ + In^{3+} + $(EDTA)^{4-}$ ⇌ **InH(EDTA) *(aq)***	28.53129		1	InL + H ⇌ InHL $\log_{10}(\beta)$ = 0.7 I = 0.5 M In + L ⇌ InL $\log_{10}(\beta)$ = 24.34224 I = 0.5 M In + H + L ⇌ InHL $\log_{10}(\beta)$ = 25.04224 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 28.53129
In^{3+} + $(OH)^-$ + $(EDTA)^{4-}$ ⇌ **$In(OH)(EDTA)^{2-}$**	32.70275		1	InL ⇌ InOHL + H $\log_{10}(\beta)$ = -8.43 I = 0.1 M In + L ⇌ InL $\log_{10}(\beta)$ = 25.0 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M In + L + OH ⇌ InOHL $\log_{10}(\beta)$ = 30.35342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 32.70275
$Sn(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Sn(II)(EDTA)^{2-}$**	19.92528		1	Original data for β: $\log_{10}(\beta)$ = 18.3, at I = 1.0 M at 20°C.
H^+ + $Sn(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Sn(II)H(EDTA)^-$**	22.83160		1	Sn(II)L + H ⇌ Sn(II)HL $\log_{10}(\beta)$ = 2.5 I = 1.0 M (Original data for β at T = 20°C) Sn + L ⇌ SnL $\log_{10}(\beta)$ = 18.3 I = 1.0 M Sn + H + L ⇌ SnHL $\log_{10}(\beta)$ = 20.8 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 22.83160
2 H^+ + $Sn(II)^{2+}$ + $(EDTA)^{4-}$ ⇌ **$Sn(II)H_2(EDTA)$ *(aq)***	24.53476		1	Sn(II)HL + H ⇌ $Sn(II)H_2L$ $\log_{10}(\beta)$ = 1.5 I = 1.0 M (Original data for β at T = 20°C) Sn + H + L ⇌ SnHL $\log_{10}(\beta)$ = 20.8 I = 1.0 M Sn + 2 H + L ⇌ SnH_2L $\log_{10}(\beta)$ = 22.3 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 24.53476
Cs^+ + $(EDTA)^{4-}$ ⇌ **$Cs(EDTA)^{3-}$**	1.0543		1	Original data for β: $\log_{10}(\beta)$ = 0.2, at I = 0.1 M.
Ba^{2+} + $(EDTA)^{4-}$ ⇌ **$Ba(EDTA)^{2-}$**	9.5886	-2.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 7.88, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Ba^{2+} + $(EDTA)^{4-}$ ⇌ **$BaH(EDTA)^-$**	14.6		3	
La^{3+} + $(EDTA)^{4-}$ ⇌ **$La(EDTA)^-$**	17.92290	-1.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 15.36, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + La^{3+} + $(EDTA)^{4-}$ ⇌ **LaH(EDTA) *(aq)***	20.37648		1	LaL + H ⇌ LaHL $\log_{10}(\beta)$ = 2.24 I = 0.1 M La + L ⇌ LaL $\log_{10}(\beta)$ = 15.36 I = 0.1 M La + H + L ⇌ LaHL $\log_{10}(\beta)$ = 17.60 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.37648
Ce^{3+} + $(EDTA)^{4-}$ ⇌ **$Ce(EDTA)^-$**	18.49290	-1.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 15.93, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

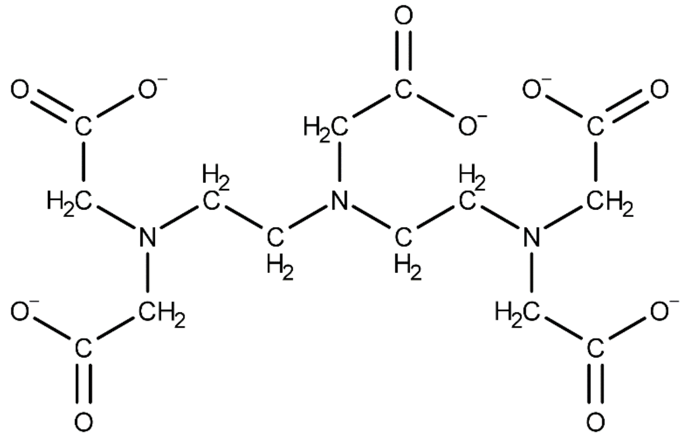
Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Ce^{3+} + (EDTA)^{4-}$ ⇌ **CeH(EDTA)** ***(aq)***	20.39606		1	CeL + H ⇌ CeHL $log_{10}(β)$ = 1.7 I = 1.0 M Ce + L ⇌ CeL $log_{10}(β)$ = 16.05498 I = 1.0 M Ce + H + L ⇌ CeHL $log_{10}(β)$ = 17.75498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 20.39606
$Pr^{3+} + (EDTA)^{4-}$ ⇌ **Pr(EDTA)**$^-$	18.86290	-1.3E+4	1	Original data for β: $log_{10}(β)$ = 16.30, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Pr^{3+} + (EDTA)^{4-}$ ⇌ **PrH(EDTA)** ***(aq)***	20.66606		1	PrL + H ⇌ PrHL $log_{10}(β)$ = 1.6 I = 1.0 M Pr + L ⇌ PrL $log_{10}(β)$ = 16.42498 I = 1.0 M Pr + H + L ⇌ PrHL $log_{10}(β)$ = 18.02498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 20.66606
$Nd^{3+} + (EDTA)^{4-}$ ⇌ **Nd(EDTA)**$^-$	19.07290	-1.5E+4	1	Original data for β: $log_{10}(β)$ = 16.51, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Nd^{3+} + (EDTA)^{4-}$ ⇌ **NdH(EDTA)** ***(aq)***	20.77606		1	NdL + H ⇌ NdHL $log_{10}(β)$ = 1.5 I = 1.0 M Nd + L ⇌ NdL $log_{10}(β)$ = 16.63498 I = 1.0 M Nd + H + L ⇌ NdHL $log_{10}(β)$ = 18.13498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 20.77606
$Pm^{3+} + (EDTA)^{4-}$ ⇌ **Pm(EDTA)**$^-$	19.46290		1	Original data for β: $log_{10}(β)$ = 16.9, at I = 0.1 M.
$Sm^{3+} + (EDTA)^{4-}$ ⇌ **Sm(EDTA)**$^-$	19.62290	-1.4E+4	1	Original data for β: $log_{10}(β)$ = 17.06, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Sm^{3+} + (EDTA)^{4-}$ ⇌ **SmH(EDTA)** ***(aq)***	21.32606		1	SmL + H ⇌ SmHL $log_{10}(β)$ = 1.5 I = 1.0 M Sm + L ⇌ SmL $log_{10}(β)$ = 17.18498 I = 1.0 M Sm + H + L ⇌ SmHL $log_{10}(β)$ = 18.68498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 21.32606
$Eu^{3+} + (EDTA)^{4-}$ ⇌ **Eu(EDTA)**$^-$	19.81290	-1.0E+4	1	Original data for β: $log_{10}(β)$ = 17.25, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Eu^{3+} + (EDTA)^{4-}$ ⇌ **EuH(EDTA)** ***(aq)***	21.41606		1	EuL + H ⇌ EuHL $log_{10}(β)$ = 1.4 I = 1.0 M Eu + L ⇌ EuL $log_{10}(β)$ = 17.37498 I = 1.0 M Eu + H + L ⇌ EuHL $log_{10}(β)$ = 18.77498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 21.41606
$Gd^{3+} + (EDTA)^{4-}$ ⇌ **Gd(EDTA)**$^-$	19.91290	-6.6E+3	1	Original data for β: $log_{10}(β)$ = 17.35, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Gd^{3+} + (EDTA)^{4-}$ ⇌ **GdH(EDTA)** ***(aq)***	21.41606		1	GdL + H ⇌ GdHL $log_{10}(β)$ = 1.3 I = 1.0 M Gd + L ⇌ GdL $log_{10}(β)$ = 17.47498 I = 1.0 M Gd + H + L ⇌ GdHL $log_{10}(β)$ = 18.77498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 21.41606
$Tb^{3+} + (EDTA)^{4-}$ ⇌ **Tb(EDTA)**$^-$	20.43290	-4.6E+3	1	Original data for β: $log_{10}(β)$ = 17.87, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Tb^{3+} + (EDTA)^{4-}$ ⇌ **TbH(EDTA)** ***(aq)***	21.53606		1	TbL + H ⇌ TbHL $log_{10}(β)$ = 0.9 I = 1.0 M Tb + L ⇌ TbL $log_{10}(β)$ = 17.99498 I = 1.0 M Tb + H + L ⇌ TbHL $log_{10}(β)$ = 18.89498 I = 1.0 M I = 0 M: $log_{10}(β)$ = 21.53606
$Dy^{3+} + (EDTA)^{4-}$ ⇌ **Dy(EDTA)**$^-$	20.86290	-5.0E+3	1	Original data for β: $log_{10}(β)$ = 18.30, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Dy^{3+} + (EDTA)^{4-} \rightleftharpoons$ **DyH(EDTA)** ***(aq)***	21.76606		1	DyL + H ⇌ DyHL $\log_{10}(\beta)$ = 0.7 I = 1.0 M Dy + L ⇌ DyL $\log_{10}(\beta)$ = 18.42498 I = 1.0 M Dy + H + L ⇌ DyHL $\log_{10}(\beta)$ = 19.12498 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 21.76606
$Ho^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Ho(EDTA)^-$**	21.12290	-5.8E+3	1	Original data for β: $\log_{10}(\beta)$ = 18.56, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Ho^{3+} + (EDTA)^{4-} \rightleftharpoons$ **HoH(EDTA)** ***(aq)***	21.82606		1	HoL + H ⇌ HoHL $\log_{10}(\beta)$ = 0.5 I = 1.0 M Ho + L ⇌ HoL $\log_{10}(\beta)$ = 18.68498 I = 1.0 M Ho + H + L ⇌ HoHL $\log_{10}(\beta)$ = 19.18498 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 21.82606
$Er^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Er(EDTA)^-$**	21.45290	-7.1E+3	1	Original data for β: $\log_{10}(\beta)$ = 18.89, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Tm^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Tm(EDTA)^-$**	21.88290	-7.9E+3	1	Original data for β: $\log_{10}(\beta)$ = 19.32, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Yb^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Yb(EDTA)^-$**	22.05290	-9.6E+3	1	Original data for β: $\log_{10}(\beta)$ = 19.49, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Lu^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Lu(EDTA)^-$**	22.30290	-1.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 19.74, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Hf^{4+} + (EDTA)^{4-} \rightleftharpoons$ **Hf(EDTA)** ***(aq)***	33.7	-8E+2	1	
$Hg(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Hg(II)(EDTA)^{2-}$**	23.20860	-7.9E+4	1	Original data for β: $\log_{10}(\beta)$ = 21.5, at I = 0.1 M. Original data for ΔH at I = 0.1 M and 20°C.
$H^+ + Hg(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Hg(II)H(EDTA)^-$**	26.83575	-8.1E+4	1	Hg(II)L + H ⇌ Hg(II)HL $\log_{10}(\beta)$ = 3.2 I = 0.1 M ΔH = -2E+3 (Original data for ΔH at I = 0.1 M) Hg(II) + L ⇌ Hg(II)L $\log_{10}(\beta)$ = 21.5 I = 0.1 M ΔH = -7.9E+4 Hg(II) + H + L ⇌ Hg(II)HL $\log_{10}(\beta)$ = 24.7 I = 0.1 M ΔH = -8.1E+4 I = 0 M: $\log_{10}(\beta)$ = 26.83575
$2\ H^+ + Hg(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Hg(II)H_2(EDTA)$** ***(aq)***	29.13891		1	Hg(II)HL + H ⇌ $Hg(II)H_2L$ $\log_{10}(\beta)$ = 2.1 I = 1.0 M Hg(II) + H + L ⇌ Hg(II)HL $\log_{10}(\beta)$ = 24.80415 I = 1.0 M Hg(II) + 2 H + L ⇌ $Hg(II)H_2L$ $\log_{10}(\beta)$ = 26.90415 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 29.13891
$Hg(II)^{2+} + (OH)^- + (EDTA)^{4-} \rightleftharpoons$ **$Hg(II)(EDTA)(OH)^{3-}$**	27.66487		1	Hg(II)L ⇌ Hg(II)OHL + H $\log_{10}(\beta)$ = -8.9 I = 0.1 M Hg(II) + L ⇌ Hg(II)L $\log_{10}(\beta)$ = 21.5 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Hg(II) + L + OH ⇌ Hg(II)(OH)L $\log_{10}(\beta)$ = 26.38342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 27.66487
$Pb(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Pb(II)(EDTA)^{2-}$**	19.70860	-5.48E+4	1	Original data for β: $\log_{10}(\beta)$ = 18.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Pb(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Pb(II)H(EDTA)^-$**	22.53575		1	Pb(II)L + H ⇌ Pb(II)HL $\log_{10}(\beta)$ = 2.4 I = 0.1 M Pb + L ⇌ PbL $\log_{10}(\beta)$ = 18.0 I = 0.1 M Pb + H + L ⇌ PbHL $\log_{10}(\beta)$ = 20.4 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 22.53575

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^{+} + Pb(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Pb(II)H_2(EDTA)$ *(aq)***	24.43891		1	Pb(II)HL + H ⇌ Pb(II)H_2L $log_{10}(\beta)$ = 1.7 I = 1.0 M Pb + H + L ⇌ PbHL $log_{10}(\beta)$ = 20.50415 I = 1.0 M Pb + 2 H + L ⇌ PbH_2L $log_{10}(\beta)$ = 22.20415 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 24.43891
$3\ H^{+} + Pb(II)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$Pb(II)H_3(EDTA)^{+}$**	25.63891		1	Pb(II)H_2L + H ⇌ Pb(II)H_3L $log_{10}(\beta)$ = 1.2 I = 1.0 M Pb + 2 H + L ⇌ PbH_2L $log_{10}(\beta)$ = 22.20415 I = 1.0 M Pb + 3 H + L ⇌ PbH_3L $log_{10}(\beta)$ = 23.40415 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 25.63891
$Bi^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$Bi(EDTA)^{-}$**	28.93792		1	Original data for β: $log_{10}(\beta)$ = 26.5, at I = 1.0 M.
$H^{+} + Bi^{3+} + (EDTA)^{4-} \rightleftharpoons$ **$BiH(EDTA)$ *(aq)***	30.55150		1	BiL + H ⇌ BiHL $log_{10}(\beta)$ = 1.4 I = 0.1 M Bi + L ⇌ BiL $log_{10}(\beta)$ = 26.37502 I = 0.1 M Bi + H + L ⇌ BiHL $log_{10}(\beta)$ = 27.77502 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 30.55150
$Bi^{3+} + (OH)^{-} + (EDTA)^{4-} \rightleftharpoons$ **$Bi(OH)(EDTA)^{2-}$**	31.90777		1	BiL ⇌ BiOHL + H $log_{10}(\beta)$ = -10.6 I = 0.1 M Bi + L ⇌ BiL $log_{10}(\beta)$ = 26.37502 I = 0.1 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Bi + L + OH ⇌ BiOHL $log_{10}(\beta)$ = 29.55844 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 31.90777
$(U(VI)O_2)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)(EDTA)^{2-}$**	10.90528		1	Original data for β: $log_{10}(\beta)$ = 9.28, at I = 1.0 M.
$H^{+} + (U(VI)O_2)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)H(EDTA)^{-}$**	19.62945		1	(UO_2) + HL ⇌ (UO_2)HL $log_{10}(\beta)$ = 7.40 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 10.09370 I = 0.1 M (UO_2) + H + L ⇌ (UO_2)HL $log_{10}(\beta)$ = 17.49370 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.62945
$2\ (U(VI)O_2)^{2+} + (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)_2(EDTA)$ *(aq)***	20.43290		1	Original data for β: $log_{10}(\beta)$ = 17.87, at I = 0.1 M.
$2\ (U(VI)O_2)^{2+} + (OH)^{-} + (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)_2(EDTA)(OH)^{-}$**	29.41674		1	$(UO_2)_2$L ⇌ $(UO_2)_2$(OH)L + H $log_{10}(\beta)$ = -4.81 I = 1.0 M 2 (UO_2) + L ⇌ $(UO_2)_2$L $log_{10}(\beta)$ = 17.99498 I = 1.0 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M 2 (UO_2) + L + OH ⇌ $(UO_2)_2$(OH)L $log_{10}(\beta)$ = 26.97882 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 29.41674
$2\ (U(VI)O_2)^{2+} + 2\ (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)_2(EDTA)_2^{4-}$**	29.33290		1	$(UO_2)_2$L + L ⇌ $(UO_2)_2L_2$ $log_{10}(\beta)$ = 8.90 I = 1.0 M 2 (UO_2) + L ⇌ $(UO_2)_2$L $log_{10}(\beta)$ = 17.99498 I = 1.0 M 2 (UO_2) + 2 L ⇌ $(UO_2)_2L_2$ $log_{10}(\beta)$ = 26.89498 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 29.33290
$4\ (U(VI)O_2)^{2+} + 4\ (OH)^{-} + 2\ (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)_4(OH)_4(EDTA)_2^{4-}$**	74.17224		1	4 (UO_2) + 2 L ⇌ $(UO_2)_4(OH)_4L_2$ + 4 H $log_{10}(\beta)$ = 15.34 I = 1.0 M 4 OH + 4 H ⇌ 4 H_2O $log_{10}(\beta)$ = 55.17536 I = 1.0 M 4 (UO_2) + 2 L + 4 (OH) ⇌ $(UO_2)_4(OH)_4L_2$ $log_{10}(\beta)$ = 70.51536 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 74.17224
$6\ (U(VI)O_2)^{2+} + 4\ (OH)^{-} + 3\ (EDTA)^{4-} \rightleftharpoons$ **$(U(VI)O_2)_6(OH)_4(EDTA)_3^{4-}$**	95.57016		1	6 (UO_2) + 3 L ⇌ $(UO_2)_6(OH)_4L_3$ + 4 H $log_{10}(\beta)$ = 34.3 I = 1.0 M 4 OH + 4 H ⇌ 4 H_2O $log_{10}(\beta)$ = 55.17536 I = 1.0 M 6 (UO_2) + 3 L + 4 (OH) ⇌ $(UO_2)_6(OH)_4L_3$ $log_{10}(\beta)$ = 89.47536 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 95.57016

2.2.33. DTPA

The ligand in its neutral form is 2-[Bis[2-[bis(carboxymethyl)amino]ethyl]amino]acetic acid (DTPA; $C_{14}H_{23}N_2O_{10}$). The ligand L as it is present in the database is the anion $C_{14}H_{18}N_2O_{10}^{5-}$. Its molecular weight is 388.309. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + (DTPA)^{5-} \rightleftharpoons$ **$H(DTPA)^{4-}$**	11.46455	-3.3E+4	1	Original data for β: $log_{10}(\beta)$ = 9.90 or 10.50 or 10.79, depending on the background electrolytes (Na/K/N(alkyl)$_4$), all at I = 0.1 M. The average log-value (10.39667) was converted to I = 0 M. Original data for ΔH at I = 0.1 M.
$2\ H^+ + (DTPA)^{5-} \rightleftharpoons$ **$H_2(DTPA)^{3-}$**	20.71885	-5.0E+4	1	$HL + H \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 8.40 I = 0.1 M ΔH = -1.7E+4 (Original data for ΔH at I = 0.1 M) $H + L \rightleftharpoons HL$ $log_{10}(\beta)$ = 10.39667 I = 0.1 M ΔH = -3.3E+4 $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 18.79667 I = 0.1 M ΔH = -5.0E+4 I = 0 M: $log_{10}(\beta)$ = 20.71885
$3\ H^+ + (DTPA)^{5-} \rightleftharpoons$ **$H_3(DTPA)^{2-}$**	25.63957	-5.62E+4	1	$H_2L + H \rightleftharpoons H_3L$ $log_{10}(\beta)$ = 4.28 I = 0.1 M ΔH = -6.2E+3 (Original data for ΔH at I = 0.1 M) $2\ H + L \rightleftharpoons H_2L$ $log_{10}(\beta)$ = 18.79667 I = 0.1 M ΔH = -5.0E+4 $3\ H + L \rightleftharpoons H_3L$ $log_{10}(\beta)$ = 23.07667 I = 0.1 M ΔH = -5.62E+4 I = 0 M: $log_{10}(\beta)$ = 25.63957

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
4 H^+ + $(DTPA)^{5-}$ ⇌ **$H_4(DTPA)^-$**	28.76672	-5.72E+4	1	H_3L + H ⇌ H_4L log10(β) = 2.70 I = 0.1 M ΔH = -1E+3 (Original data for ΔH at I = 0.1 M) 3 H + L ⇌ H_3L log10(β) = 23.07667 I = 0.1 M ΔH = -5.62E+4 4 H + L ⇌ H_4L log10(β) = 25.77667 I = 0.1 M ΔH = -5.72E+4 I = 0 M: log10(β) = 28.76672
5 H^+ + $(DTPA)^{5-}$ ⇌ **$H_5(DTPA)$ *(aq)***	30.98030	-5.52E+4	1	H_4L + H ⇌ H_5L $log_{10}(\beta)$ = 2.0 I = 0.1 M ΔH = 2E+3 (Original data for ΔH at I = 0.1 M) 4 H + L ⇌ H_4L $log_{10}(\beta)$ = 25.77667 I = 0.1 M ΔH = -5.72E+4 5 H + L ⇌ H_5L $log_{10}(\beta)$ = 27.77667 I = 0.1 M ΔH = -5.52E+4 I = 0 M: $log_{10}(\beta)$ = 30.98030
6 H^+ + $(DTPA)^{5-}$ ⇌ **$H_6(DTPA)^+$**	32.58030		1	H_5L + H ⇌ H_6L $log_{10}(\beta)$ = 1.6 I = 0.1 M 5 H + L ⇌ H_5L $log_{10}(\beta)$ = 27.77667 I = 0.1 M 6 H + L ⇌ H_6L $log_{10}(\beta)$ = 29.37667 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.58030
7 H^+ + $(DTPA)^{5-}$ ⇌ **$H_7(DTPA)^{2+}$**	33.06672		1	H_6L + H ⇌ H_7L $log_{10}(\beta)$ = 0.7 I = 0.1 M 6 H + L ⇌ H_6L $log_{10}(\beta)$ = 29.37667 I = 0.1 M 7 H + L ⇌ H_8L $log_{10}(\beta)$ = 30.07667 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 33.06672
8 H^+ + $(DTPA)^{5-}$ ⇌ **$H_8(DTPA)^{3+}$**	32.53957		1	H_7L + H ⇌ H_8L $log_{10}(\beta)$ = -0.1 I = 0.1 M 7 H + L ⇌ H_7L $log_{10}(\beta)$ = 30.07667 I = 0.1 M 8 H + L ⇌ H_8L $log_{10}(\beta)$ = 29.97667 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.53957
Li^+ + $(DTPA)^{5-}$ ⇌ **$Li(DTPA)^{4-}$**	4.16788		1	Original data for β: $log_{10}(\beta)$ = 3.1, at I = 0.1 M.
Mg^{2+} + $(DTPA)^{5-}$ ⇌ **$Mg(DTPA)^{3-}$**	11.40575	1.2E+4	1	Original data for β: $log_{10}(\beta)$ = 9.27, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Mg^{2+} + $(DTPA)^{5-}$ ⇌ **$MgH(DTPA)^{2-}$**	18.89648		1	MgL + H ⇌ MgHL $log_{10}(\beta)$ = 6.85 I = 0.1 M Mg + L ⇌ MgL $log_{10}(\beta)$ = 9.27 I = 0.1 M Mg + H + L ⇌ MgHL $log_{10}(\beta)$ = 16.12 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.89648
2 Mg^{2+} + $(DTPA)^{5-}$ ⇌ **$Mg_2(DTPA)^-$**	14.90300		1	MgL + M ⇌ Mg_2L $log_{10}(\beta)$ = 2.07 I = 0.15 M (Original data for β at T = 37°C) Mg + L ⇌ MgL $log_{10}(\beta)$ = 9.02701 I = 0.15 M 2 Mg + L ⇌ Mg_2L $log_{10}(\beta)$ = 11.09701 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 14.90300
Al^{3+} + $(DTPA)^{5-}$ ⇌ **$Al(DTPA)^{2-}$**	21.80363	3.0E+4	1	Original data for β: $log_{10}(\beta)$ = 18.6, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Al^{3+} + $(DTPA)^{5-}$ ⇌ **$AlH(DTPA)^-$**	26.53078		1	AlL + H ⇌ AlHL $log_{10}(\beta)$ = 4.3 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 18.6 I = 0.1 M Al + H + L ⇌ AlHL $log_{10}(\beta)$ = 22.9 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.53078

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Al^{3+} + $(OH)^{-}$ + $(DTPA)^{5-}$ ⇌ **$Al(DTPA)(OH)^{3-}$**	27.95990		1	AlL ⇌ Al(OH)L + H $\log_{10}(\beta)$ = -7.2 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 18.6 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L $\log_{10}(\beta)$ = 25.18342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 27.95990
K^{+} + $(DTPA)^{5-}$ ⇌ **$K(DTPA)^{4-}$**	1.96788		1	Original data for β: $\log_{10}(\beta)$ = 0.9, at I = 0.1 M and 20°C.
Ca^{2+} + $(DTPA)^{5-}$ ⇌ **$Ca(DTPA)^{3-}$**	12.88575	-2.4E+4	1	Original data for β: $\log_{10}(\beta)$ = 10.75, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Ca^{2+} + $(DTPA)^{5-}$ ⇌ **$CaH(DTPA)^{2-}$**	19.63648		1	CaL + H ⇌ CaHL $\log_{10}(\beta)$ = 6.11 I = 0.1 M Ca + L ⇌ CaL $\log_{10}(\beta)$ = 10.75 I = 0.1 M Ca + H + L ⇌ CaHL $\log_{10}(\beta)$ = 16.86 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.63648
2 Ca^{2+} + $(DTPA)^{5-}$ ⇌ **$Ca_2(DTPA)^{-}$**	15.76720		1	CaL + Ca ⇌ M_2L $\log_{10}(\beta)$ = 1.6 I = 0.1 M Ca + L ⇌ CaL $\log_{10}(\beta)$ = 10.75 I = 0.1 M 2 Ca + L ⇌ Ca_2L $\log_{10}(\beta)$ = 12.35 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 15.76720
Sc^{3+} + $(DTPA)^{5-}$ ⇌ **$Sc(DTPA)^{2-}$**	27.10363	-3.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 23.9, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Mn(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Mn(II)(DTPA)^{3-}$**	17.33575	-3.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 15.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + $Mn(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Mn(II)H(DTPA)^{2-}$**	22.42648		1	Mn(II)L + H ⇌ Mn(II)HL $\log_{10}(\beta)$ = 4.45 I = 0.1 M Mn(II) + L ⇌ Mn(II)L $\log_{10}(\beta)$ = 15.2 I = 0.1 M Mn(II) + H + L ⇌ Mn(II)HL $\log_{10}(\beta)$ = 19.65 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 22.42648
2 $Mn(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Mn(II)_2(DTPA)^{-}$**	20.70720		1	Mn(II)L + M ⇌ $Mn(II)_2L$ $\log_{10}(\beta)$ = 2.09 I = 0.1 M (Original data for β at T = 20°C) Mn(II) + L ⇌ Mn(II)L $\log_{10}(\beta)$ = 15.2 I = 0.1 M 2 Mn(II) + L ⇌ $Mn(II)_2L$ $\log_{10}(\beta)$ = 17.29 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.70720
$Fe(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Fe(II)(DTPA)^{3-}$**	18.33575	-3.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 16.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + $Fe(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Fe(II)H(DTPA)^{2-}$**	24.27648		1	Fe(II)L + H ⇌ Fe(II)HL $\log_{10}(\beta)$ = 5.30 I = 0.1 M Fe(II) + L ⇌ Fe(II)L $\log_{10}(\beta)$ = 16.2 I = 0.1 M Fe(II) + H + L ⇌ Fe(II)HL $\log_{10}(\beta)$ = 21.5 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 24.27648
$Fe(II)^{2+}$ + $(OH)^{-}$ + $(DTPA)^{5-}$ ⇌ **$Fe(II)(DTPA)(OH)^{4-}$**	22.70845		1	Fe(II)L ⇌ Fe(II)(OH)L + H $\log_{10}(\beta)$ = -8.77 I = 0.1 M Fe(II) + L ⇌ Fe(II)L $\log_{10}(\beta)$ = 16.2 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Fe(II) + OH + L ⇌ Fe(II)(OH)L $\log_{10}(\beta)$ = 21.21342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 22.70845

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Fe(II)^{2+} + 2\ (OH)^{-} + (DTPA)^{5-} \rightleftharpoons$ **$Fe(II)(DTPA)(OH)_2^{5-}$**	26.22757		1	$Fe(II)OHL \rightleftharpoons Fe(II)(OH)_2L + H$ $log_{10}(\beta)$ = -9.41 I = 0.1 M $Fe(II) + OH + L \rightleftharpoons Fe(II)OHL$ $log_{10}(\beta)$ = 21.21342 I = 0.1 M $OH + H \rightleftharpoons H_2O$ $log_{10}(\beta)$ = 13.78342 I = 0.1 M $Fe(II) + 2\ OH + L \rightleftharpoons Fe(II)(OH)_2L$ $log_{10}(\beta)$ = 25.58684 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.22757
$2\ Fe(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Fe(II)_2(DTPA)^{-}$**	22.59720		1	$Fe(II)L + Fe(II) \rightleftharpoons Fe(II)_2L$ $log_{10}(\beta)$ = 2.98 I = 0.1 M (Original data for β at T = 20°C) $Fe(II) + L \rightleftharpoons Fe(II)L$ $log_{10}(\beta)$ = 16.2 I = 0.1 M $2\ Fe(II) + L \rightleftharpoons Fe(II)_2L$ $log_{10}(\beta)$ = 19.18 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 22.59720
$Fe(III)^{3+} + (DTPA)^{5-} \rightleftharpoons$ **$Fe(III)(DTPA)^{2-}$**	30.90363		1	Original data for β: $log_{10}(\beta)$ = 27.7, at I = 0.1 M.
$H^{+} + Fe(III)^{3+} + (DTPA)^{5-} \rightleftharpoons$ **$Fe(III)H(DTPA)^{-}$**	34.89078		1	$Fe(III)L + H \rightleftharpoons Fe(III)HL$ $log_{10}(\beta)$ = 3.56 I = 0.1 M $Fe(III) + L \rightleftharpoons Fe(III)L$ $log_{10}(\beta)$ = 27.7 I = 0.1 M $Fe(III) + H + L \rightleftharpoons Fe(III)HL$ $log_{10}(\beta)$ = 31.26 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 34.89078
$Fe(III)^{3+} + (OH)^{-} + (DTPA)^{5-} \rightleftharpoons$ **$Fe(III)(DTPA)(OH)^{3-}$**	34.59990		1	$Fe(III)L \rightleftharpoons Fe(III)(OH)L + H$ $log_{10}(\beta)$ = -9.66 I = 0.1 M $Fe(III) + L \rightleftharpoons Fe(III)L$ $log_{10}(\beta)$ = 27.7 I = 0.1 M $OH + H \rightleftharpoons H_2O$ $log_{10}(\beta)$ = 13.78342 I = 0.1 M $Fe(III) + OH + L \rightleftharpoons Fe(III)(OH)L$ $log_{10}(\beta)$ = 31.82342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 34.59990
$Co(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Co(II)(DTPA)^{3-}$**	20.93575	-3.9E+4	1	Original data for β: $log_{10}(\beta)$ = 18.8, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^{+} + Co(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Co(II)H(DTPA)^{2-}$**	26.51648		1	$Co(II)L + H \rightleftharpoons Co(II)HL$ $log_{10}(\beta)$ = 4.94 I = 0.1 M $Co(II) + L \rightleftharpoons Co(II)L$ $log_{10}(\beta)$ = 18.8 I = 0.1 M $Co(II) + H + L \rightleftharpoons Co(II)HL$ $log_{10}(\beta)$ = 23.74 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 26.51648
$2\ Co(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Co(II)_2(DTPA)^{-}$**	25.95720		1	$Co(II)L + Co(II) \rightleftharpoons Co(II)_2L$ $log_{10}(\beta)$ = 3.74 I = 0.1 M $Co(II) + L \rightleftharpoons Co(II)L$ $log_{10}(\beta)$ = 18.8 I = 0.1 M $2\ Co(II) + L \rightleftharpoons Co(II)_2L$ $log_{10}(\beta)$ = 22.54 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 25.95720
$Ni^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Ni(DTPA)^{3-}$**	22.23575	-4.68E+4	1	Original data for β: $log_{10}(\beta)$ = 20.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^{+} + Ni^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$NiH(DTPA)^{2-}$**	28.51648		1	$NiL + H \rightleftharpoons NiHL$ $log_{10}(\beta)$ = 5.64 I = 0.1 M $Ni + L \rightleftharpoons NiL$ $log_{10}(\beta)$ = 20.1 I = 0.1 M $Ni + H + L \rightleftharpoons NiHL$ $log_{10}(\beta)$ = 25.74 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 28.51648
$2\ Ni^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Ni_2(DTPA)^{-}$**	29.10720		1	$NiL + Ni \rightleftharpoons Ni_2L$ $log_{10}(\beta)$ = 5.59 I = 0.1 M $Ni + L \rightleftharpoons NiL$ $log_{10}(\beta)$ = 20.1 I = 0.1 M $2\ Ni + L \rightleftharpoons Ni_2L$ $log_{10}(\beta)$ = 25.69 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 29.10720
$Cu(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Cu(II)(DTPA)^{3-}$**	23.33575	-5.60E+4	1	Original data for β: $log_{10}(\beta)$ = 21.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + Cu(II)^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Cu(II)H(DTPA)^{2-}}$	28.77648		1	Cu(II)L + H ⇌ Cu(II)HL $\log_{10}(\beta)$ = 4.80 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 21.2 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 26.0 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.77648
$2\ H^{+} + Cu(II)^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Cu(II)H_2(DTPA)^{-}}$	32.16363		1	Cu(II)HL + H ⇌ $Cu(II)H_2L$ $\log_{10}(\beta)$ = 2.96 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 26.0 I = 0.1 M Cu(II) + 2 H + L ⇌ $Cu(II)H_2L$ $\log_{10}(\beta)$ = 28.96 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 32.16363
$2\ Cu(II)^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Cu(II)_2(DTPA)^{-}}$	31.40720		1	Cu(II)L + Cu(II) ⇌ $Cu(II)_2L$ $\log_{10}(\beta)$ = 6.79 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 21.2 I = 0.1 M 2 Cu(II) + L ⇌ $Cu(II)_2L$ $\log_{10}(\beta)$ = 27.99 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 31.40720
$Zn^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Zn(DTPA)^{3-}}$	20.33575	-4.43E+4	1	Original data for β: $\log_{10}(\beta)$ = 18.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^{+} + Zn^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{ZnH(DTPA)^{2-}}$	26.57648		1	ZnL + H ⇌ ZnHL $\log_{10}(\beta)$ = 5.60 I = 0.1 M Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 18.2 I = 0.1 M Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 23.8 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 26.57648
$2\ Zn^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Zn_2(DTPA)^{-}}$	26.09720		1	ZnL + Zn ⇌ Zn_2L $\log_{10}(\beta)$ = 4.48 I = 0.1 M Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 18.2 I = 0.1 M 2 Zn + L ⇌ Zn_2L $\log_{10}(\beta)$ = 22.68 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 26.09720
$Ga^{3+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Ga(DTPA)^{2-}}$	27.50363		1	Original data for β: $\log_{10}(\beta)$ = 24.3, at I = 0.1 M.
$H^{+} + Ga^{3+} + (DTPA)^{5-} \rightleftharpoons \mathbf{GaH(DTPA)^{-}}$	32.04078		1	GaL + H ⇌ GaHL $\log_{10}(\beta)$ = 4.11 I = 0.1 M Ga + L ⇌ GaL $\log_{10}(\beta)$ = 24.3 I = 0.1 M Ga + H + L ⇌ GaHL $\log_{10}(\beta)$ = 28.41 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 32.04078
$Ga^{3+} + (OH)^{-} + (DTPA)^{5-} \rightleftharpoons \mathbf{Ga(DTPA)(OH)^{3-}}$	33.34990		1	GaL ⇌ Ga(OH)L + H $\log_{10}(\beta)$ = -7.51 I = 0.1 M Ga + L ⇌ GaL $\log_{10}(\beta)$ = 24.3 I = 0.1 M OH + H ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Ga + OH + L ⇌ Ga(OH)L $\log_{10}(\beta)$ = 30.57342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 33.34990
$Sr^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Sr(DTPA)^{3-}}$	11.92575	-2.9E+4	1	Original data for β: $\log_{10}(\beta)$ = 9.79, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^{+} + Sr^{2+} + (DTPA)^{5-} \rightleftharpoons \mathbf{SrH(DTPA)^{2-}}$	17.96648		1	SrL + H ⇌ SrHL $\log_{10}(\beta)$ = 5.4 I = 0.1 M Sr + L ⇌ SrL $\log_{10}(\beta)$ = 9.79 I = 0.1 M Sr + H + L ⇌ SrHL $\log_{10}(\beta)$ = 15.19 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 17.96648
$Y^{3+} + (DTPA)^{5-} \rightleftharpoons \mathbf{Y(DTPA)^{2-}}$	25.25363	-2.7E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.05, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Y^{3+} + (DTPA)^{5-} \rightleftharpoons$ **$YH(DTPA)^-$**	27.59078		1	$YL + H \rightleftharpoons YHL$ $\log_{10}(\beta) = 1.91$ I = 0.1 M (Original data for β at T = 20°C) $Y + L \rightleftharpoons YL$ $\log_{10}(\beta) = 22.05$ I = 0.1 M $Y + H + L \rightleftharpoons YHL$ $\log_{10}(\beta) = 23.96$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 27.59078$
$Zr^{4+} + (DTPA)^{5-} \rightleftharpoons$ **$Zr(DTPA)^-$**	40.07150		1	Original data for β: $\log_{10}(\beta) = 35.8$, at I = 0.1 M and 20°C.
$Zr^{4+} + (OH)^- + (DTPA)^{5-} \rightleftharpoons$ **$Zr(DTPA)(OH)^{2-}$**	47.76218		1	$ZrL \rightleftharpoons Zr(OH)L + H$ $\log_{10}(\beta) = -5.9$ I = 1.0 M (Original data for β at T = 20°C) $Zr + L \rightleftharpoons ZrL$ $\log_{10}(\beta) = 36.0083$ I = 1.0 M $OH + H \rightleftharpoons H_2O$ $\log_{10}(\beta) = 13.79384$ I = 1.0 M $Zr + OH + L \rightleftharpoons Zr(OH)L$ $\log_{10}(\beta) = 43.90214$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 47.76218$
$Pd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Pd(DTPA)^{3-}$**	31.73160		1	Original data for β: $\log_{10}(\beta) = 29.7$, at I = 1.0 M and 20 °C.
$H^+ + Pd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$PdH(DTPA)^{2-}$**	35.83108		1	$PdL + H \rightleftharpoons PdHL$ $\log_{10}(\beta) = 3.49$ I = 1.0 M (Original data for β at T = 20°C) $Pd + L \rightleftharpoons PdL$ $\log_{10}(\beta) = 29.7$ I = 1.0 M $Pd + H + L \rightleftharpoons PdHL$ $\log_{10}(\beta) = 33.19$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 35.83108$
$2 H^+ + Pd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$PdH_2(DTPA)^-$**	38.86266		1	$PdHL + H \rightleftharpoons PdH_2L$ $\log_{10}(\beta) = 2.93$ I = 1.0 M (Original data for β at T = 20°C) $Pd + H + L \rightleftharpoons PdHL$ $\log_{10}(\beta) = 33.19$ I = 1.0 M $Pd + 2 H + L \rightleftharpoons PdH_2L$ $\log_{10}(\beta) = 36.12$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 38.86266$
$3 H^+ + Pd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$PdH_3(DTPA)$ *(aq)***	41.93056		1	$PdH_2L + H \rightleftharpoons PdH_3L$ $\log_{10}(\beta) = 2.56$ I = 1.0 M (Original data for β at T = 20°C) $Pd + 2 H + NL \rightleftharpoons PdH_2L$ $\log_{10}(\beta) = 36.12$ I = 1.0 M $Pd + 3 H + L \rightleftharpoons PdH_3L$ $\log_{10}(\beta) = 38.68$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 41.93056$
$4 H^+ + Pd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$PdH_4(DTPA)^+$**	43.86056		1	$PdH_3L + H \rightleftharpoons PdH_4L$ $\log_{10}(\beta) = 1.93$ I = 1.0 M (Original data for β at T = 20°C) $Pd + 3 H + NL \rightleftharpoons PdH_3L$ $\log_{10}(\beta) = 38.68$ I = 1.0 M $Pd + 4 H + L \rightleftharpoons PdH_4L$ $\log_{10}(\beta) = 40.61$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 43.86056$
$Ag^+ + (DTPA)^{5-} \rightleftharpoons$ **$Ag(DTPA)^{4-}$**	9.73788		1	Original data for β: $\log_{10}(\beta) = 8.67$, at I = 0.1 M.
$H^+ + Ag^+ + (DTPA)^{5-} \rightleftharpoons$ **$AgH(DTPA)^{3-}$**	18.45218		1	$AgL + H \rightleftharpoons AgHL$ $\log_{10}(\beta) = 7.86$ I = 0.1 M $Ag + L \rightleftharpoons AgL$ $\log_{10}(\beta) = 8.67$ I = 0.1 M $Ag + H + L \rightleftharpoons AgHL$ $\log_{10}(\beta) = 16.53$ I = 0.1 M I = 0 M: $\log_{10}(\beta) = 18.45218$

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + Ag^+ + (DTPA)^{5-} \rightleftharpoons$ **$AgH_2(DTPA)^{2-}$**	24.16290		1	$AgHL + H \rightleftharpoons AgH_2L$ $log_{10}(\beta)$ = 5.07 I = 1.0 M $Ag + H + L \rightleftharpoons AgHL$ $log_{10}(\beta)$ = 16.53 I = 1.0 M $Ag + 2\ H + L \rightleftharpoons AgH_2L$ $log_{10}(\beta)$ = 21.60 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 24.16290
$Cd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Cd(DTPA)^{3-}$**	21.13575	-5.18E+4	1	Original data for β: $log_{10}(\beta)$ = 19.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Cd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$CdH(DTPA)^{2-}$**	25.94648		1	$CdL + H \rightleftharpoons CdHL$ $log_{10}(\beta)$ = 4.17 I = 0.1 M $Cd + L \rightleftharpoons CdL$ $log_{10}(\beta)$ = 19.0 I = 0.1 M $Cd + H + L \rightleftharpoons CdHL$ $log_{10}(\beta)$ = 23.17 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 25.94648
$2\ Cd^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Cd_2(DTPA)^-$**	24.71720		1	$CdL + Cd \rightleftharpoons Cd_2L$ $log_{10}(\beta)$ = 2.3 I = 0.1 M $Cd + L \rightleftharpoons CdL$ $log_{10}(\beta)$ = 19.0 I = 0.1 M $2\ Cd + L \rightleftharpoons Cd_2L$ $log_{10}(\beta)$ = 21.3 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 24.71720
$In^{3+} + (DTPA)^{5-} \rightleftharpoons$ **$In(DTPA)^{2-}$**	32.70363		1	Original data for β: $log_{10}(\beta)$ = 29.5, at I = 0.1 M.
$In^{3+} + (OH)^- + (DTPA)^{5-} \rightleftharpoons$ **$In(DTPA)(OH)^{3-}$**	34.15990		1	$InL \rightleftharpoons In(OH)L + H$ $log_{10}(\beta)$ = -11.9 I = 0.1 M (Original data for β at T = 20°C) $In + L \rightleftharpoons InL$ $log_{10}(\beta)$ = 29.5 I = 0.1 M $OH + H \rightleftharpoons H_2O$ $log_{10}(\beta)$ = 13.78342 I = 0.1 M $In + OH + L \rightleftharpoons In(OH)L$ $log_{10}(\beta)$ = 31.38342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 34.15990
$Sn(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Sn(II)(DTPA)^{3-}$**	22.73160		1	Original data for β: $log_{10}(\beta)$ = 20.7, at I = 1.0 M and 20°C.
$H^+ + Sn(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Sn(II)H(DTPA)^{2-}$**	27.44108		1	$Sn(II)L + H \rightleftharpoons Sn(II)HL$ $log_{10}(\beta)$ = 4.1 I = 1.0 M (Original data for β at T = 20°C) $Sn(II) + L \rightleftharpoons Sn(II)L$ $log_{10}(\beta)$ = 20.7 I = 1.0 M $Sn(II) + H + L \rightleftharpoons Sn(II)HL$ $log_{10}(\beta)$ = 24.8 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 27.44108
$2\ H^+ + Sn(II)^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Sn(II)H_2(DTPA)^-$**	30.34740		1	$Sn(II)HL + H \rightleftharpoons Sn(II)H_2L$ $log_{10}(\beta)$ = 2.5 I = 1.0 M (Original data for β at T = 20°C) $Sn(II) + H + L \rightleftharpoons Sn(II)HL$ $log_{10}(\beta)$ = 24.8 I = 1.0 M $Sn(II) + 2\ H + L \rightleftharpoons Sn(II)H_2L$ $log_{10}(\beta)$ = 27.3 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 30.34740
$Ba^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$Ba(DTPA)^{3-}$**	10.87575	-2.9E+4	1	Original data for β: $log_{10}(\beta)$ = 8.74, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Ba^{2+} + (DTPA)^{5-} \rightleftharpoons$ **$BaH(DTPA)^{2-}$**	16.85648		1	$BaL + H \rightleftharpoons BaHL$ $log_{10}(\beta)$ = 5.34 I = 0.1 M $Ba + L \rightleftharpoons BaL$ $log_{10}(\beta)$ = 8.74 I = 0.1 M $Ba + H + L \rightleftharpoons BaHL$ $log_{10}(\beta)$ = 14.08 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.85648
$La^{3+} + (DTPA)^{5-} \rightleftharpoons$ **$La(DTPA)^{2-}$**	22.69363	-2.2E+4	1	Original data for β: $log_{10}(\beta)$ = 19.49, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + La^{3+} + $(DTPA)^{5-}$ ⇌ **$LaH(DTPA)^{-}$**	25.72078		1	LaL + H ⇌ LaHL $\log_{10}(\beta)$ = 2.6 I = 0.1 M (Original data for β at T = 20°C) La + L ⇌ LaL $\log_{10}(\beta)$ = 19.49 I = 0.1 M La + H + L ⇌ LaHL $\log_{10}(\beta)$ = 22.09 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 25.72078
Ce^{3+} + $(DTPA)^{5-}$ ⇌ **$Ce(DTPA)^{2-}$**	23.63363	-2.4E+4	1	Original data for β: $\log_{10}(\beta)$ = 20.43, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Pr^{3+} + $(DTPA)^{5-}$ ⇌ **$Pr(DTPA)^{2-}$**	24.30363	-2.6E+4	1	Original data for β: $\log_{10}(\beta)$ = 21.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Pr^{3+} + $(DTPA)^{5-}$ ⇌ **$PrH(DTPA)^{-}$**	27.11078		1	PrL + H ⇌ PrHL $\log_{10}(\beta)$ = 2.38 I = 0.1 M (Original data for β at T = 20°C) Pr + L ⇌ PrL $\log_{10}(\beta)$ = 21.1 I = 0.1 M Pr + H + L ⇌ PrHL $\log_{10}(\beta)$ = 23.48 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 27.11078
Nd^{3+} + $(DTPA)^{5-}$ ⇌ **$Nd(DTPA)^{2-}$**	24.82363	-3.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 21.62, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Nd^{3+} + $(DTPA)^{5-}$ ⇌ **$NdH(DTPA)^{-}$**	27.64078		1	NdL + H ⇌ NdHL $\log_{10}(\beta)$ = 2.39 I = 0.1 M (Original data for β at T = 20°C) Nd + L ⇌ NdL $\log_{10}(\beta)$ = 21.62 I = 0.1 M Nd + H + L ⇌ NdHL $\log_{10}(\beta)$ = 24.01 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 27.64078
2 Nd^{3+} + $(DTPA)^{5-}$ ⇌ **$Nd_2(DTPA)^{+}$**	30.46508		1	Original data for β: $\log_{10}(\beta)$ = 25.98, at I = 0.1 M and 20°C.
Sm^{3+} + $(DTPA)^{5-}$ ⇌ **$Sm(DTPA)^{2-}$**	25.55363	-3.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.35, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Sm^{3+} + $(DTPA)^{5-}$ ⇌ **$SmH(DTPA)^{-}$**	28.18078		1	SmL + H ⇌ SmHL $\log_{10}(\beta)$ = 2.2 I = 0.1 M (Original data for β at T = 20°C) Sm + L ⇌ SmL $\log_{10}(\beta)$ = 22.35 I = 0.1 M Sm + H + L ⇌ SmHL $\log_{10}(\beta)$ = 24.55 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.18078
2 Sm^{3+} + $(DTPA)^{5-}$ ⇌ **$Sm_2(DTPA)^{+}$**	30.03508		1	Original data for β: $\log_{10}(\beta)$ = 25.55, at I = 0.1 M and 20°C.
Eu^{3+} + $(DTPA)^{5-}$ ⇌ **$Eu(DTPA)^{2-}$**	25.59363	-3.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.39, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^{+} + Eu^{3+} + $(DTPA)^{5-}$ ⇌ **$EuH(DTPA)^{-}$**	28.17078		1	EuL + H ⇌ EuHL $\log_{10}(\beta)$ = 2.15 I = 0.1 M (Original data for β at T = 20°C) Eu + L ⇌ EuL $\log_{10}(\beta)$ = 22.39 I = 0.1 M Eu + H + L ⇌ EuHL $\log_{10}(\beta)$ = 24.54 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.17078
2 Eu^{3+} + $(DTPA)^{5-}$ ⇌ **$Eu_2(DTPA)^{+}$**	30.03508		1	Original data for β: $\log_{10}(\beta)$ = 25.55, at I = 0.1 M and 20°C.
Gd^{3+} + $(DTPA)^{5-}$ ⇌ **$Gd(DTPA)^{2-}$**	25.59363	-3.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.39, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

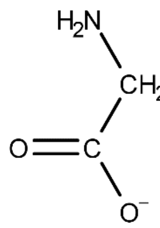
Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^+ + Gd^{3+} + (DTPA)^{5-} \rightleftharpoons$ **GdH(DTPA)**$^-$	28.41078		1	GdL + H ⇌ GdHL $\log_{10}(\beta)$ = 2.39 I = 0.1 M (Original data for β at T = 20°C) Gd + L ⇌ GdL $\log_{10}(\beta)$ = 22.39 I = 0.1 M Gd + H + L ⇌ GdHL $\log_{10}(\beta)$ = 24.78 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.41078
$Tb^{3+} + (DTPA)^{5-} \rightleftharpoons$ **Tb(DTPA)**$^{2-}$	25.92363	-3.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.72, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Tb^{3+} + (DTPA)^{5-} \rightleftharpoons$ **TbH(DTPA)**$^-$	28.49078		1	TbL + H ⇌ TbHL $\log_{10}(\beta)$ = 2.14 I = 0.1 M (Original data for β at T = 20°C) Tb + L ⇌ TbL $\log_{10}(\beta)$ = 22.72 I = 0.1 M Tb + H + L ⇌ TbHL $\log_{10}(\beta)$ = 24.86 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.49078
$Dy^{3+} + (DTPA)^{5-} \rightleftharpoons$ **Dy(DTPA)**$^{2-}$	26.03363	-3.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.83, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Dy^{3+} + (DTPA)^{5-} \rightleftharpoons$ **DyH(DTPA)**$^-$	28.65078		1	DyL + H ⇌ DyHL $\log_{10}(\beta)$ = 2.19 I = 0.1 M (Original data for β at T = 20°C) Dy + L ⇌ DyL $\log_{10}(\beta)$ = 22.83 I = 0.1 M Dy + H + L ⇌ DyHL $\log_{10}(\beta)$ = 25.02 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.65078
$Ho^{3+} + (DTPA)^{5-} \rightleftharpoons$ **Ho(DTPA)**$^{2-}$	25.99363	-3.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.79, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Ho^{3+} + (DTPA)^{5-} \rightleftharpoons$ **HoH(DTPA)**$^-$	28.67078		1	HoL + H ⇌ HoHL $\log_{10}(\beta)$ = 2.25 I = 0.1 M (Original data for β at T = 20°C) Ho + L ⇌ HoL $\log_{10}(\beta)$ = 22.79 I = 0.1 M Ho + H + L ⇌ HoHL $\log_{10}(\beta)$ = 25.04 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.67078
$Er^{3+} + (DTPA)^{5-} \rightleftharpoons$ **Er(DTPA)**$^{2-}$	25.95363	-3.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.75, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$H^+ + Er^{3+} + (DTPA)^{5-} \rightleftharpoons$ **ErH(DTPA)**$^-$	28.38078		1	ErL + H ⇌ ErHL $\log_{10}(\beta)$ = 2.00 I = 0.1 M (Original data for β at T = 20°C) Er + L ⇌ ErL $\log_{10}(\beta)$ = 22.75 I = 0.1 M Er + H + L ⇌ ErHL $\log_{10}(\beta)$ = 24.75 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.38078
$Tm^{3+} + (DTPA)^{5-} \rightleftharpoons$ **Tm(DTPA)**$^{2-}$	25.93363	-2.6E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.73, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + Tm^{3+} + $(DTPA)^{5-}$ ⇌ **$TmH(DTPA)^-$**	28.26078		1	TmL + H ⇌ TmHL $\log_{10}(\beta)$ = 1.90 I = 0.1 M (Original data for β at T = 20°C) Tm + L ⇌ TmL $\log_{10}(\beta)$ = 22.73 I = 0.1 M Tm + H + L ⇌ TmHL $\log_{10}(\beta)$ = 24.63 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.26078
Yb^{3+} + $(DTPA)^{5-}$ ⇌ **$Yb(DTPA)^{2-}$**	25.84363	-2.5E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.64, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Yb^{3+} + $(DTPA)^{5-}$ ⇌ **$YbH(DTPA)^-$**	28.57078		1	YbL + H ⇌ YbHL $\log_{10}(\beta)$ = 2.30 I = 0.1 M (Original data for β at T = 20°C) Yb + L ⇌ YbL $\log_{10}(\beta)$ = 22.64 I = 0.1 M Yb + H + L ⇌ YbHL $\log_{10}(\beta)$ = 24.94 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.57078
Lu^{3+} + $(DTPA)^{5-}$ ⇌ **$Lu(DTPA)^{2-}$**	25.66363	-2.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 22.46, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + Lu^{3+} + $(DTPA)^{5-}$ ⇌ **$LuH(DTPA)^-$**	28.27078		1	LuL + H ⇌ LuHL $\log_{10}(\beta)$ = 2.18 I = 0.1 M (Original data for β at T = 20°C) Lu + L ⇌ LuL $\log_{10}(\beta)$ = 22.46 I = 0.1 M Lu + H + L ⇌ LuHL $\log_{10}(\beta)$ = 24.64 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 28.27078
Hf^{4+} + $(DTPA)^{5-}$ ⇌ **$Hf(DTPA)^-$**	39.67150		1	Original data for β: $\log_{10}(\beta)$ = 35.4, at I = 0.1 M and 20°C.
$Hg(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Hg(II)(DTPA)^{3-}$**	28.53575	-9.87E+4	1	Original data for β: $\log_{10}(\beta)$ = 26.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + $Hg(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Hg(II)H(DTPA)^{2-}$**	33.41648		1	Hg(II)L + H ⇌ Hg(II)HL $\log_{10}(\beta)$ = 4.24 I = 0.1 M (Original data for β at T = 20°C) Hg(II) + L ⇌ Hg(II)L $\log_{10}(\beta)$ = 26.4 I = 0.1 M Hg(II) + H + L ⇌ Hg(II)HL $\log_{10}(\beta)$ = 30.64 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 33.41648
$Pb(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Pb(II)(DTPA)^{3-}$**	20.93575	-7.86E+4	1	Original data for β: $\log_{10}(\beta)$ = 18.8, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
H^+ + $Pb(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Pb(II)H(DTPA)^{2-}$**	26.09648		1	Pb(II)L + H ⇌ Pb(II)HL $\log_{10}(\beta)$ = 4.52 I = 0.1 M (Original data for β at T = 20°C) Pb(II) + L ⇌ Pb(II)L $\log_{10}(\beta)$ = 18.8 I = 0.1 M Pb(II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 23.32 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 26.09648
2 $Pb(II)^{2+}$ + $(DTPA)^{5-}$ ⇌ **$Pb(II)_2(DTPA)^-$**	25.62720		1	Pb(II)L + Pb(II) ⇌ $Pb(II)_2L$ $\log_{10}(\beta)$ = 3.41 I = 0.1 M (Original data for β at T = 20°C) Pb(II) + L ⇌ Pb(II)L $\log_{10}(\beta)$ = 18.8 I = 0.1 M Pb(II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 22.21 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ =

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Bi^{3+} + $(DTPA)^{5-}$ ⇌ **$Bi(DTPA)^{2-}$**	33.90363		1	Original data for β: $log_{10}(\beta)$ = 30.7, at I = 0.1 M.
H^+ + Bi^{3+} + $(DTPA)^{5-}$ ⇌ **$BiH(DTPA)^-$**	36.73078		1	BiL + H ⇌ BiHL $log_{10}(\beta)$ = 2.40 I = 0.1 M Bi + L ⇌ BiL $log_{10}(\beta)$ = 30.7 I = 0.1 M Bi + H + L ⇌ BiHL $log_{10}(\beta)$ = 33.1 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 36.73078
2 H^+ + Bi^{3+} + $(DTPA)^{5-}$ ⇌ **$BiH_2(DTPA)$ *(aq)***	38.74435		1	BiHL + H ⇌ BiH_2L $log_{10}(\beta)$ = 1.8 I = 0.1 M Bi + H + L ⇌ BiHL $log_{10}(\beta)$ = 33.1 I = 0.1 M Bi + 2 H + L ⇌ BiH_2L $log_{10}(\beta)$ = 34.9 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 38.74435
Bi^{3+} + $(OH)^-$ + $(DTPA)^{5-}$ ⇌ **$Bi(DTPA)(OH)^{3-}$**	35.99115		1	BiL ⇌ Bi(OH)L + H $log_{10}(\beta)$ = -11.3 I = 1.0 M (Original data for β at T = 20°C) Bi + L ⇌ BiL $log_{10}(\beta)$ = 30.85623 I = 1.0 M OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.79384 I = 1.0 M Bi + OH + L ⇌ Bi(OH)L $log_{10}(\beta)$ = 33.35007 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 35.99115

2.2.34. Glycine

The ligand in its neutral form is 2-aminoethanoic acid (glycine; $C_2H_5NO_2$). The ligand L as it is present in the database is the anion $C_2H_4NO_2^-$. Its molecular weight is 74.059. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(glycine)^-$ ⇌ **H(glycine) *(aq)***	9.778	-4.435E+4	1	
2 H^+ + $(glycine)^-$ ⇌ **$H_2(glycine)^+$**	12.128	-4.835E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.350 ΔH = -4.0E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.778 ΔH = -4.435E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 12.128 ΔH = -4.835E+4
Na^+ + $(glycine)^-$ ⇌ **Na(glycine) *(aq)***	-0.6		1	
Mg^{2+} + $(glycine)^-$ ⇌ **$Mg(glycine)^+$**	2.08	2.5E+4	1	Original data for ΔH at I = 0.1 M.
2 Mg^{2+} + $(glycine)^-$ ⇌ **$Mg(glycine)_2$ *(aq)***	2.26		1	Original data for β: $log_{10}(\beta)$ = 2.26, at I = 3.0 M.

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Mg^{2+} + H^{+} + (glycine)$^{-}$ ⇌ **MgH(glycine)$^{2+}$**	10.15800		1	Mg + HL ⇌ MgHL log$_{10}$(β) = 0.38 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 9.56442 I = 0.1 M Mg + H + L ⇌ MgHL log$_{10}$(β) = 9.94442 I = 0.1 M I = 0 M: log$_{10}$(β) = 10.15800
Al^{3+} + (glycine)$^{-}$ ⇌ **Al(glycine)$^{2+}$**	6.55073		1	Original data for β: log$_{10}$(β) = 5.91, at I = 0.1 M.
Al^{3+} + (OH)$^{-}$ + (glycine)$^{-}$ ⇌ **Al(OH)(glycine)$^{+}$**	15.93130		1	AlL ⇌ Al(OH)L + H log$_{10}$(β) = -4.83 I = 0.1 M Al + L ⇌ AlL log$_{10}$(β) = 5.91000 I = 0.1 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L log$_{10}$(β) = 14.86342 I = 0.1 M I = 0 M: log$_{10}$(β) = 15.93130
2 Al^{3+} + (OH)$^{-}$ + (glycine)$^{-}$ ⇌ **Al$_2$(OH)(glycine)$^{4+}$**	18.56057		1	Al(OH)L + Al ⇌ Al$_2$(OH)L log$_{10}$(β) = 3.27 I = 0.1 M Al + OH + L ⇌ Al(OH)L log$_{10}$(β) = 14.86342 I = 0.1 M 2 Al + OH + L ⇌ Al$_2$(OH)L log$_{10}$(β) = 18.13342 I = 0.1 M I = 0 M: log$_{10}$(β) = 18.56057
Ca^{2+} + (glycine)$^{-}$ ⇌ **Ca(glycine)$^{+}$**	1.39	-4E+3	1	
Ca^{2+} + H^{+} + (glycine)$^{-}$ ⇌ **CaH(glycine)$^{2+}$**	10.07800	-3.635E+4	1	Ca + HL ⇌ CaHL log$_{10}$(β) = 0.30 I = 0.1 M ΔH = 8E+3 H + L ⇌ HL log$_{10}$(β) = 9.56442 I = 0.1 M ΔH = -4.435E+4 Ca + H + L ⇌ CaHL log$_{10}$(β) = 9.86442 I = 0.1 M ΔH = -3.635E+4 I = 0 M: log$_{10}$(β) = 10.07800
Mn(II)$^{2+}$ + (glycine)$^{-}$ ⇌ **Mn(II)(glycine)$^{+}$**	3.19	-1E+3	1	
Mn(II)$^{2+}$ + 2 (glycine)$^{-}$ ⇌ **Mn(II)(glycine)$_2$ *(aq)***	5.44073		1	Original data for β: log$_{10}$(β) = 4.8, at I = 0.1 M.
Fe(II)$^{2+}$ + (glycine)$^{-}$ ⇌ **Fe(II)(glycine)$^{+}$**	4.31	-1.5E+4	1	
Fe(II)$^{2+}$ + 2 (glycine)$^{-}$ ⇌ **Fe(II)(glycine)$_2$ *(aq)***	8.29073		1	Original data for β: log$_{10}$(β) = 7.65, at I = 0.1 M.
Fe(II)$^{2+}$ + 3 (glycine)$^{-}$ ⇌ **Fe(II)(glycine)$_3^{-}$**	9.47948		1	Original data for β: log$_{10}$(β) = 8.87, at I = 1.0 M.
Fe(III)$^{3+}$ + (glycine)$^{-}$ ⇌ **Fe(III)(glycine)$^{2+}$**	9.37516		1	Original data for β: log$_{10}$(β) = 8.57, at I = 0.5 M.
Fe(III)$^{3+}$ + H^{+} + (glycine)$^{-}$ ⇌ **Fe(III)H(glycine)$^{3+}$**	11.54800		1	Fe(III) + HL ⇌ Fe(III)HL log$_{10}$(β) = 1.77 I = 0.5 M H + L ⇌ HL log$_{10}$(β) = 9.50961 I = 0.5 M Fe(III) + H + L ⇌ Fe(III)HL log$_{10}$(β) = 11.27961 I = 0.5 M I = 0 M: log$_{10}$(β) = 11.54800
Fe(III)$^{3+}$ + 2 H^{+} + 2 (glycine)$^{-}$ ⇌ **Fe(III)H$_2$(glycine)$_2^{3+}$**	23.25600		1	Fe(III) + 2 HL ⇌ Fe(III)H$_2$L$_2$ log$_{10}$(β) = 3.7 I = 3.0 M 2 H + 2 L ⇌ 2 HL log$_{10}$(β) = 20.09646 I = 3.0 M Fe(III) + 2 H + 2 L ⇌ Fe(III)H$_2$L$_2$ log$_{10}$(β) = 23.79646 I = 3.0 M I = 0 M: log$_{10}$(β) = 23.25600
Co(II)$^{2+}$ + (glycine)$^{-}$ ⇌ **Co(II)(glycine)$^{+}$**	5.07	-1.2E+4	1	
Co(II)$^{2+}$ + 2 (glycine)$^{-}$ ⇌ **Co(II)(glycine)$_2$ *(aq)***	9.07	-2.6E+4	1	
Co(II)$^{2+}$ + 3 (glycine)$^{-}$ ⇌ **Co(II)(glycine)$_3^{-}$**	11.6	-4.1E+4	1	
Co(II)$^{2+}$ + (OH)$^{-}$ + (glycine)$^{-}$ ⇌ **Co(II)(OH)(glycine) *(aq)***	8.97700		1	Co(II)L ⇌ Co (II)(OH)L + H log$_{10}$(β) = -10.09 I = 0.1 M Co(II) + L ⇌ Co(II)L log$_{10}$(β) = 4.64285 I = 0.1 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Co(II) + OH + L ⇌ Co(II)(OH)L log$_{10}$(β) = 8.33627 I = 0.1 M I = 0 M: log$_{10}$(β) = 8.97700
Ni^{2+} + (glycine)$^{-}$ ⇌ **Ni(glycine)$^{+}$**	6.15	-1.8E+4	1	
Ni^{2+} + 2 (glycine)$^{-}$ ⇌ **Ni(glycine)$_2$ *(aq)***	11.12	-3.8E+4	1	
Ni^{2+} + 3 (glycine)$^{-}$ ⇌ **Ni(glycine)$_3^{-}$**	14.6	-6.23E+4	1	

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Cu(I)$^{+}$ + 2 (glycine)$^{-}$ ⇌ **Cu(I)(glycine)$_2^{-}$**	10.31358		1	Original data for β: log$_{10}$(β) = 10.1, at I = 0.1 M.
Cu(II)$^{2+}$ + (glycine)$^{-}$ ⇌ **Cu(II)(glycine)$^{+}$**	8.56	-2.5E+4	1	
Cu(II)$^{2+}$ + 2 (glycine)$^{-}$ ⇌ **Cu(II)(glycine)$_2$ *(aq)***	15.7	-5.43E+4	1	
Zn^{2+} + (glycine)$^{-}$ ⇌ **Zn(glycine)$^{+}$**	5.38	-1.1E+4	1	
Zn^{2+} + 2 (glycine)$^{-}$ ⇌ **Zn(glycine)$_2$ *(aq)***	9.81	-2.5E+4	1	
Zn^{2+} + 3 (glycine)$^{-}$ ⇌ **Zn(glycine)$_3^{-}$**	12.3	-3.9E+4	1	
Zn^{2+} + (OH)$^{-}$ + (glycine)$^{-}$ ⇌ **Zn(OH)(glycine) *(aq)***	10.47700		1	ZnL ⇌ Zn(OH)L + H log$_{10}$(β) = -8.9 I = 0.15 M (Original data for β at T = 37°C) Zn + L ⇌ ZnL log$_{10}$(β) = 4.90425 I = 0.15 M H + OH ⇌ H_2O log$_{10}$(β) = 13.75913 I = 0.15 M Zn + OH + L ⇌ Zn(OH)L log$_{10}$(β) = 9.76338 I = 0.15 M I = 0 M: log$_{10}$(β) = 10.47700
Ga^{3+} + (glycine)$^{-}$ ⇌ **Ga(glycine)$^{2-}$**	8.78931		1	Original data for β: log$_{10}$(β) = 9.60, at I = 3.0 M.
Ga^{3+} + H^{+} + (glycine)$^{-}$ ⇌ **GaH(glycine)$^{3+}$**	11.88800		1	Ga + HL ⇌ GaHL log$_{10}$(β) = 2.11 I = 3.0 M H + L ⇌ HL log$_{10}$(β) = 10.04823 I = 3.0 M Ga + H + L ⇌ GaHL log$_{10}$(β) = 12.15823 I = 3.0 M I = 0 M: log$_{10}$(β) = 11.88800
Sr^{2+} + (glycine)$^{-}$ ⇌ **Sr(glycine)$^{+}$**	0.91		1	
Y^{3+} + (glycine)$^{-}$ ⇌ **Y(glycine)$^{2+}$**	4.14073		1	Original data for β: log$_{10}$(β) = 3.5, at I = 0.1 M.
Pd^{2+} + H^{+} + (glycine)$^{-}$ ⇌ **PdH(glycine)$^{2+}$**	15.17800		1	Pd + HL ⇌ PdHL log$_{10}$(β) = 5.4 I = 1.0 M (Original data for β at T = 20°C) H + L ⇌ HL log$_{10}$(β) = 9.57484 I = 1.0 M Pd + H + L ⇌ PdHL log$_{10}$(β) = 14.97484 I = 1.0 M I = 0 M: log$_{10}$(β) = 15.17800
Pd^{2+} + 2 H^{+} + 2 (glycine)$^{-}$ ⇌ **PdH$_2$(glycine)$_2^{2+}$**	27.75600		1	Pd + 2 HL ⇌ PdH_2L_2 log$_{10}$(β) = 8.2 I = 1.0 M (Original data for β at T = 20°C) 2 H + 2 L ⇌ H_2L_2 log$_{10}$(β) = 19.14968 I = 1.0 M Pd + 2 H + 2 L ⇌ PdH_2L_2 log$_{10}$(β) = 27.34968 I = 1.0 M I = 0 M: log$_{10}$(β) = 27.75600
Ag^{+} + (glycine)$^{-}$ ⇌ **Ag(glycine) *(aq)***	3.51	-1.9E+4	1	Original data for ΔH at I = 0.5 M.
Ag^{+} + 2 (glycine)$^{-}$ ⇌ **Ag(glycine)$_2^{-}$**	6.89	-4.81E+4	1	Original data for ΔH at I = 0.5 M.
Ag^{+} + H^{+} + (glycine)$^{-}$ ⇌ **AgH(glycine)$^{+}$**	9.878		1	Ag + HL ⇌ AgHL log$_{10}$(β) = 0.1 I = 3.0 M H + L ⇌ HL log$_{10}$(β) = 10.04823 I = 3.0 M Ag + H + L ⇌ AgHL log$_{10}$(β) = 10.14823 I = 3.0 M I = 0 M: log$_{10}$(β) = 9.878
Ag^{+} + (OH)$^{-}$ + (glycine)$^{-}$ ⇌ **Ag(OH)(glycine)$^{-}$**	8.01723		1	AgL ⇌ Ag(OH)L + H log$_{10}$(β) = -9.76 I = 3.0 M Ag + L ⇌ AgL log$_{10}$(β) = 3.78023 I = 3.0 M H + OH ⇌ H_2O log$_{10}$(β) = 14.26723 I = 3.0 M Ag + OH + L ⇌ Ag(OH)L log$_{10}$(β) = 8.28746 I = 3.0 M I = 0 M: log$_{10}$(β) = 8.01723
Cd^{2+} + (glycine)$^{-}$ ⇌ **Cd(glycine)$^{+}$**	4.69	-8.7E+3	1	

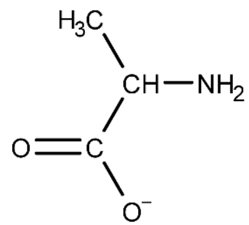
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + 2 $(glycine)^{-}$ ⇌ **$Cd(glycine)_2$ *(aq)***	8.40	-2.2E+4	1	
Cd^{2+} + 3 $(glycine)^{-}$ ⇌ **$Cd(glycine)_3^{-}$**	10.7	-3.5E+4	1	
Ba^{2+} + $(glycine)^{-}$ ⇌ **$Ba(glycine)^{+}$**	0.77		1	
La^{3+} + $(glycine)^{-}$ ⇌ **$La(glycine)^{2+}$**	3.74073		1	Original data for β: $log_{10}(\beta)$ = 3.1, at I = 0.1 M.
Ce^{3+} + H^{+} + $(glycine)^{-}$ ⇌ **$CeH(glycine)^{3+}$**	10.318	-3.235E+04	1	Ce + HL ⇌ CeHL $log_{10}(\beta)$ = 0.53 I = 2.0 M ΔH = 1.2E+4 (Original data for β at T = 20°C; original data for ΔH at I = 2.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.79244 I = 2.0 M ΔH = -4.435E+4 Ce + H + L ⇌ CeHL $log_{10}(\beta)$ = 10.32244 I = 2.0 M ΔH = -3.235E+04 I = 0 M: $log_{10}(\beta)$ = 10.30800
Pr^{3+} + $(glycine)^{-}$ ⇌ **$Pr(glycine)^{2+}$**	3.94073		1	Original data for β: $log_{10}(\beta)$ = 3.3, at I = 0.1 M.
Nd^{3+} + $(glycine)^{-}$ ⇌ **$Nd(glycine)^{2+}$**	3.90073		1	Original data for β: $log_{10}(\beta)$ = 3.26, at I = 0.1 M.
Nd^{3+} + H^{+} + $(glycine)^{-}$ ⇌ **$NdH(glycine)^{3+}$**	10.70800		1	Nd + HL ⇌ NdHL $log_{10}(\beta)$ = 0.93 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 9.56442 I = 0.1 M Nd + H + L ⇌ NdHL $log_{10}(\beta)$ = 10.49442 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.708
Nd^{3+} + $(OH)^{-}$ + $(glycine)^{-}$ ⇌ **$Nd(OH)(glycine)^{+}$**	9.89130		1	NdL ⇌ Nd(OH)L + H $log_{10}(\beta)$ = -8.22 I = 0.1 M Nd + L ⇌ NdL $log_{10}(\beta)$ = 3.26 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Nd + OH + L ⇌ Nd(OH)L $log_{10}(\beta)$ = 8.82342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 9.89130
Pm^{3+} + H^{+} + $(glycine)^{-}$ ⇌ **$PmH(glycine)^{3+}$**	10.44800	-2.835E+04	1	Pm + HL ⇌ PmHL $log_{10}(\beta)$ = 0.67 I = 2.0 M ΔH = 1.6E+4 (Original data for β at T = 20°C; original data for ΔH at I = 2.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.79244 I = 2.0 M ΔH = -4.435E+4 Pm + H + L ⇌ PmHL $log_{10}(\beta)$ = 10.46244 I = 2.0 M ΔH = -2.835E+04 I = 0 M: $log_{10}(\beta)$ = 10.44800
Sm^{3+} + $(glycine)^{-}$ ⇌ **$Sm(glycine)^{2+}$**	4.14073		1	Original data for β: $log_{10}(\beta)$ = 3.5, at I = 0.1 M.
Eu^{3+} + $(glycine)^{-}$ ⇌ **$Eu(glycine)^{2+}$**	4.14073		1	Original data for β: $log_{10}(\beta)$ = 3.5, at I = 0.1 M.
Eu^{3+} + H^{+} + $(glycine)^{-}$ ⇌ **$EuH(glycine)^{3+}$**	10.51800	-3.235E+04	1	Eu + HL ⇌ EuHL $log_{10}(\beta)$ = 0.74 I = 2.0 M ΔH = 1.2E+4 (Original data for ΔH at I = 2.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.79244 I = 2.0 M ΔH = -4.435E+4 Eu + H + L ⇌ EuHL $log_{10}(\beta)$ = 10.53244 I = 2.0 M ΔH = -3.235E+04 I = 0 M: $log_{10}(\beta)$ = 10.51800
Gd^{3+} + $(glycine)^{-}$ ⇌ **$Gd(glycine)^{2+}$**	4.04073		1	Original data for β: $log_{10}(\beta)$ = 3.4, at I = 0.1 M.
Gd^{3+} + H^{+} + $(glycine)^{-}$ ⇌ **$GdH(glycine)^{3+}$**	10.50800		1	Gd + HL ⇌ GdHL $log_{10}(\beta)$ = 0.73 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 9.56442 I = 0.1 M Gd + H + L ⇌ GdHL $log_{10}(\beta)$ = 10.29442 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.508
Tb^{3+} + $(glycine)^{-}$ ⇌ **$Tb(glycine)^{2+}$**	4.24073		1	Original data for β: $log_{10}(\beta)$ = 3.6, at I = 0.1 M.
Dy^{3+} + $(glycine)^{-}$ ⇌ **$Dy(glycine)^{2+}$**	4.24073		1	Original data for β: $log_{10}(\beta)$ = 3.6, at I = 0.1 M.
Ho^{3+} + $(glycine)^{-}$ ⇌ **$Ho(glycine)^{2+}$**	4.34073		1	Original data for β: $log_{10}(\beta)$ = 3.7, at I = 0.1 M.
Er^{3+} + $(glycine)^{-}$ ⇌ **$Er(glycine)^{2+}$**	4.34073		1	Original data for β: $log_{10}(\beta)$ = 3.7, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Yb^{3+} + $(glycine)^-$ ⇌ **$Yb(glycine)^{2+}$**	4.54073		1	Original data for β: $log_{10}(\beta)$ = 3.9, at I = 0.1 M.
Lu^{3+} + $(glycine)^-$ ⇌ **$Lu(glycine)^{2+}$**	4.54073		1	Original data for β: $log_{10}(\beta)$ = 3.9, at I = 0.1 M.
$Hg(II)^{2+}$ + $(glycine)^-$ ⇌ **$Hg(II)(glycine)^+$**	10.83678		1	Original data for β: $log_{10}(\beta)$ = 10.3, at I = 0.5 M and 20°C.
$Hg(II)^{2+}$ + 2 $(glycine)^-$ ⇌ **$Hg(II)(glycine)_2$ *(aq)***	20.00516	-8.84E+4	1	Original data for β: $log_{10}(\beta)$ = 19.2, at I = 0.5 M and 20°C. ΔH can be calculated as follows: $Hg(II)Cl_2$ + 2 L = $Hg(II)L_2$ + 2 Cl ΔH = -3.7E+4 Hg(II) + 2 Cl = $Hg(II)Cl_2$ ΔH = -5.14E+4 Hg(II) + 2 L = $Hg(II)L_2$ ΔH = -8.84E+4
$Hg(II)Cl_2$ *(aq)* + $(glycine)^-$ ⇌ **Hg(II)Cl(glycine) *(aq)*** + Cl^-	17.42	-7.64E+4	1	$Hg(II)Cl_2$ + L ⇌ Hg(II)ClL + Cl $log_{10}(\beta)$ = 3.42 ΔH = -2.5E+4 Hg(II) + 2 Cl ⇌ $Hg(II)Cl_2$ $log_{10}(\beta)$ = 14 ΔH = -5.14E+04 Hg(II) + Cl + L ⇌ Hg(II)ClL $log_{10}(\beta)$ = 17.42 ΔH = -7.64E+04
$Pb(II)^{2+}$ + $(glycine)^-$ ⇌ **$Pb(II)(glycine)^+$**	5.14715	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 4.72, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Pb(II)^{2+}$ + 2 $(glycine)^-$ ⇌ **$Pb(II)(glycine)_2$ *(aq)***	8.34073		1	Original data for β: $log_{10}(\beta)$ = 7.7, at I = 0.1 M.
$Pb(II)^{2+}$ + H^+ + $(glycine)^-$ ⇌ **$Pb(II)H(glycine)^{2+}$**	11.27800	-1.935E+4	1	Pb(II) + HL ⇌ Pb(II)HL $log_{10}(\beta)$ = 1.5 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 3.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.56442 I = 0.1 M ΔH = -4.835E+4 Pb(II) + H + L ⇌ Pb(II)HL $log_{10}(\beta)$ = 11.06442 I = 0.1 M ΔH = -1.935E+4 I = 0 M: $log_{10}(\beta)$ = 11.27800
$Pb(II)^{2+}$ + 2 H^+ + 2 $(glycine)^-$ ⇌ **$Pb(II)H_2(glycine)_2^{2+}$**	21.05600		1	Pb(II) + 2 HL ⇌ $Pb(II)H_2L_2$ $log_{10}(\beta)$ = 1.5 I = 1.0 M 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 19.14968 I = 1.0 M Pb(II) + 2 H + 2 L ⇌ $Pb(II)H_2L_2$ $log_{10}(\beta)$ = 20.64968 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 21.05600
$Pb(II)^{2+}$ + 3 H^+ + 3 $(glycine)^-$ ⇌ **$Pb(II)H_3(glycine)_3^{2+}$**	31.40400		1	Pb(II) + 3 HL ⇌ $Pb(II)H_3L_3$ $log_{10}(\beta)$ = 2.07 I = 3.0 M 3 H + 3 L ⇌ 3 HL $log_{10}(\beta)$ = 30.14469 I = 3.0 M Pb(II) + 3 H + 3 L ⇌ $Pb(II)H_3L_3$ $log_{10}(\beta)$ = 32.21469 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 31.40400
$Pb(II)^{2+}$ + $(OH)^-$ + $(glycine)^-$ ⇌ **Pb(II)(OH)(glycine) *(aq)***	11.50415	-1.048E+5	1	Pb(II)L ⇌ Pb(II)(OH)L + H $log_{10}(\beta)$ = -7.64 I = 3.0 M ΔH = -2.9E+4 (Original data for ΔH at I = 2.0 M) Pb(II) + L ⇌ Pb(II)L $log_{10}(\beta)$ = 5.68761 I = 3.0 M ΔH = -2.0E+4 H + OH ⇌ H_2O $log_{10}(\beta)$ = 14.26723 I = 3.0 M ΔH = -5.581E+4 Pb(II) + OH + L ⇌ Pb(II)(OH)L $log_{10}(\beta)$ = 12.31484 I = 3.0 M ΔH = -1.0481E+05 I = 0 M: $log_{10}(\beta)$ = 11.50415
$Pb(II)^{2+}$ + H^+ + 2 $(glycine)^-$ ⇌ **$Pb(II)H(glycine)_2^+$**	14.75916		1	$Pb(II)H_2L_2$ ⇌ $Pb(II)HL_2$ + H $log_{10}(\beta)$ = -6.5 I = 1.0 M Pb(II) + 2 H + 2 L ⇌ $Pb(II)H_2L_2$ $log_{10}(\beta)$ = 20.64968 I = 1.0 M Pb(II) + H + 2 L ⇌ $Pb(II)HL_2$ $log_{10}(\beta)$ = 14.14968 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 14.75916
Bi^{3+} + $(glycine)^-$ ⇌ **$Bi(glycine)^{2+}$**	10.80516		1	Original data for β: $log_{10}(\beta)$ = 10.0, at I = 0.5 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Bi^{3+} + $(OH)^-$ + $(glycine)^-$ ⇌ **$Bi(OH)(glycine)^+$**	21.14194		1	BiL + OH = M(OH)L $log_{10}(\beta)$ = 9.8 I = 0.5 M Bi + L = BiL $log_{10}(\beta)$ = 10.0 I = 0.5 M Bi + OH + L = BiL $log_{10}(\beta)$ = 19.8 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 21.14194
$(U(VI)O_2)^{2+}$ + H^+ + $(glycine)^-$ ⇌ **$(U(VI)O_2)H(glycine)^{2+}$**	11.20800	-4.535E+4	1	(UO_2) + HL ⇌ $(UO_2)HL$ $log_{10}(\beta)$ = 1.43 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.56442 I = 0.1 M ΔH = -4.835E+4 (UO_2) + H + L ⇌ $(UO_2)HL$ $log_{10}(\beta)$ = 10.99442 I = 0.1 M ΔH = -4.535E+4 I = 0 M: $log_{10}(\beta)$ = 11.2800
$(U(VI)O_2)^{2+}$ + 2 H^+ + 2 $(glycine)^-$ ⇌ **$(U(VI)O_2)H_2(glycine)_2^{2+}$**	21.75600	-8.57E+4	1	(UO_2) + 2 HL ⇌ $(UO_2)H_2L_2$ $log_{10}(\beta)$ = 2.20 I = 1.0 M ΔH = 4.6E+3 (Original data for ΔH at I = 1.0 M) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 19.14968 I = 1.0 M ΔH = -8.87E+4 (UO_2) + H + L ⇌ $(UO_2)HL$ $log_{10}(\beta)$ = 21.34968 I = 1.0 M ΔH = -8.57E+4 I = 0 M: $log_{10}(\beta)$ = 21.75600

2.2.35. Alanine

The ligand in its neutral form is L-2-aminopropanoic acid (alanine; $C_3H_7NO_2$). The ligand L as it is present in the database is the anion $C_3H_6NO_2^-$. Its molecular weight is 88.086. Its structural formula is shown on the right.



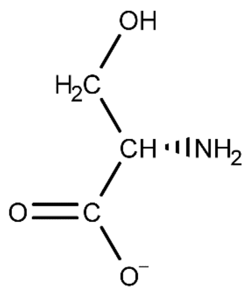
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(alanine)^-$ ⇌ **H(alanine) *(aq)***	9.868	-4.522E+04	1	
2 H^+ + $(alanine)^-$ ⇌ **$H_2(alanine)^+$**	12.212	-4.722E+04	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.344 ΔH = -2.0E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.868 ΔH = -4.522E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 12.212 ΔH = -4.722E+4
Mg^{2+} + $(alanine)^-$ ⇌ **$Mg(alanine)^+$**	1.96		1	
Ca^{2+} + $(alanine)^-$ ⇌ **$Ca(alanine)^+$**	1.30	4E+3	1	
Ca^{2+} + H^+ + $(alanine)^-$ ⇌ **$CaH(alanine)^{2+}$**	10.218	-3.722E+04	1	Ca + HL ⇌ CaHL $log_{10}(\beta)$ = 0.35 ΔH = 8.0E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.868 ΔH = -4.522E+4 Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 10.218 ΔH = -3.722E+4
$Mn(II)^{2+}$ + $(alanine)^-$ ⇌ **$Mn(II)(alanine)^+$**	2.87715		1	Original data for β: $log_{10}(\beta)$ = 2.45, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Mn(II)^{2+}$ + 2 $(alanine)^-$ ⇌ **$Mn(II)(alanine)_2$ *(aq)***	4.99073		1	Original data for β: $log_{10}(\beta)$ = 4.35, at I = 0.1 M.
$Fe(II)^{2+}$ + $(alanine)^-$ ⇌ **$Fe(II)(alanine)^+$**	3.94632		1	Original data for β: $log_{10}(\beta)$ = 3.54, at I = 1.0 M and 20°C.
$Fe(III)^{3+}$ + $(alanine)^-$ ⇌ **$Fe(III)(alanine)^{2+}$**	9.68516		1	Original data for β: $log_{10}(\beta)$ = 8.88, at I = 0.5 M.
$Fe(III)^{3+}$ + $(OH)^-$ + $(alanine)^-$ ⇌ **$Fe(III)(OH)(alanine)^+$**	21.70055		1	Fe(III)L ⇌ Fe(III)(OH)L + H $log_{10}(\beta)$ = -2.17 I = 0.5 M Fe(III) + L ⇌ Fe(III)L $log_{10}(\beta)$ = 8.8 I = 0.5 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.72861 I = 0.5 M Fe(III) + OH + L ⇌ Fe(III)(OH)L $log_{10}(\beta)$ = 20.35861 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 21.70055
$Co(II)^{2+}$ + $(alanine)^-$ ⇌ **$Co(II)(alanine)^+$**	4.71	-5.4E+3	1	Original data for ΔH at I = 0.1 M.
$Co(II)^{2+}$ + 2 $(alanine)^-$ ⇌ **$Co(II)(alanine)_2$ *(aq)***	8.40	-1.5E+4	1	Original data for ΔH at I = 0.1 M.
$Co(II)^{2+}$ + 3 $(alanine)^-$ ⇌ **$Co(II)(alanine)_3^-$**	10.34073		1	Original data for β: $log_{10}(\beta)$ = 9.7, at I = 0.1 M.
Ni^{2+} + $(alanine)^-$ ⇌ **$Ni(alanine)^+$**	5.82	-1.4E+4	1	Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 $(alanine)^-$ ⇌ **$Ni(alanine)_2$ *(aq)***	10.51	-3.0E+4	1	Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 $(alanine)^-$ ⇌ **$Ni(alanine)_3^-$**	13.45073	-5.64E+4	1	Original data for ΔH at I = 1.0 M.
$Cu(I)^+$ + 2 $(alanine)^-$ ⇌ **$Cu(I)(alanine)_2^-$**	9.86839		1	Original data for β: $log_{10}(\beta)$ = 9.6, at I = 0.5 M.
$Cu(II)^{2+}$ + $(alanine)^-$ ⇌ **$Cu(II)(alanine)^+$**	8.55	-2.2E+4	1	Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(alanine)^-$ ⇌ **$Cu(II)(alanine)_2$ *(aq)***	15.5	-4.93E+4	1	Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + H^+ + $(alanine)^-$ ⇌ **$Cu(II)H(alanine)^{2+}$**	12.14180		1	Cu(II)L + H ⇌ Cu(II)HL $log_{10}(\beta)$ = 2.77 I = 5.0 M Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 10.19360 I = 5.0 M Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 12.96360 I = 5.0 M I = 0 M: $log_{10}(\beta)$ = 12.14180
Zn^{2+} + $(alanine)^-$ ⇌ **$Zn(alanine)^+$**	4.95	-6.6E+3	1	Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 $(alanine)^-$ ⇌ **$Zn(alanine)_2$ *(aq)***	9.23	-1.7E+4	1	Original data for ΔH at I = 0.1 M.
Zn^{2+} + 3 $(alanine)^-$ ⇌ **$Zn(alanine)_3^-$**	11.40516		1	Original data for β: $log_{10}(\beta)$ = 10.6, at I = 0.5 M.
Zn^{2+} + $(OH)^-$ + $(alanine)^-$ ⇌ **Zn(OH)(alanine) *(aq)***	10.74700		1	ZnL ⇌ Zn(OH)L + H $log_{10}(\beta)$ = -8.2 I = 0.1 M Zn + L ⇌ ZnL $log_{10}(\beta)$ = 4.52285 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Zn + OH + L ⇌ Zn(OH)L $log_{10}(\beta)$ = 10.10627 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.74700
Sr^{2+} + $(alanine)^-$ ⇌ **$Sr(alanine)^+$**	0.74		1	
Pd^{2+} + H^+ + $(alanine)^-$ ⇌ **$PdH(alanine)^{2+}$**	15.06800		1	Pd + HL ⇌ PdHL $log_{10}(\beta)$ = 5.2 I = 1.0 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 9.66484 I = 1.0 M Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 14.86484 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 15.06800
Pd^{2+} + 2 H^+ + 2 $(alanine)^-$ ⇌ **$PdH_2(alanine)_2^{2+}$**	27.93600		1	Pd + 2 HL ⇌ PdH_2L_2 $log_{10}(\beta)$ = 8.2 I = 1.0 M (Original data for β at T = 20°C) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 19.32968 I = 1.0 M Pd + 2 H + 2 L ⇌ PdH_2L_2 $log_{10}(\beta)$ = 27.52968 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 27.93600
Ag^+ + $(alanine)^-$ ⇌ **Ag(alanine) *(aq)***	3.64		1	
Ag^+ + 2 $(alanine)^-$ ⇌ **$Ag(alanine)_2^-$**	7.18		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + (alanine)$^-$ ⇌ **Cd(alanine)$^+$**	4.40715		1	Original data for β: $log_{10}(\beta)$ = 3.98, at I = 0.1 M.
Cd^{2+} + 2 (alanine)$^-$ ⇌ **Cd(alanine)$_2$ *(aq)***	7.99073		1	Original data for β: $log_{10}(\beta)$ = 7.35, at I = 0.1 M.
Cd^{2+} + 3 (alanine)$^-$ ⇌ **Cd(alanine)$_3^-$**	10.57073		1	Original data for β: $log_{10}(\beta)$ = 9.93, at I = 0.1 M.
Ba^{2+} + (alanine)$^-$ ⇌ **Ba(alanine)$^+$**	0.77		1	
Nd^{3+} + H^+ + (alanine)$^-$ ⇌ **NdH(alanine)$^{3+}$**	10.50800		1	Nd + HL ⇌ NdHL $log_{10}(\beta)$ = 0.64 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 9.65442 I = 0.1 M Nd + H + L ⇌ NdHL $log_{10}(\beta)$ = 10.29442 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.50800
Eu^{3+} + H^+ + (alanine)$^-$ ⇌ **EuH(alanine)$^{3+}$**	10.60800		1	Eu + HL ⇌ EuHL $log_{10}(\beta)$ = 0.74 I = 2.0 M H + L ⇌ HL $log_{10}(\beta)$ = 9.88244 I = 2.0 M Eu + H + L ⇌ EuHL $log_{10}(\beta)$ = 10.62244 I = 2.0 M I = 0 M: $log_{10}(\beta)$ = 10.60800
Pb(II)$^{2+}$ + (alanine)$^-$ ⇌ **Pb(II)(alanine)$^+$**	4.62954		1	Original data for β: $log_{10}(\beta)$ = 5.17, at I = 3.0 M.
Pb(II)$^{2+}$ + 2 (alanine)$^-$ ⇌ **Pb(II)(alanine)$_2$ *(aq)***	7.31931		1	Original data for β: $log_{10}(\beta)$ = 8.13, at I = 3.0 M.
Pb(II)$^{2+}$ + H^+ + (alanine)$^-$ ⇌ **Pb(II)H(alanine)$^{2+}$**	11.14800		1	Pb(II) + HL ⇌ Pb(II)HL $log_{10}(\beta)$ = 1.28 I = 3.0 M H + L ⇌ HL $log_{10}(\beta)$ = 10.13823 I = 3.0 M Pb(II) + H + L ⇌ Pb(II)HL $log_{10}(\beta)$ = 11.41823 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 11.14800

2.2.36. Serine

The ligand in its neutral form is L-2-amino-3-hydroxypropanoic acid (serine; $C_3H_7NO_3$). The ligand L as it is present in the database is the anion $C_3H_6NO_3^-$. Its molecular weight is 104.085. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + (serine)$^-$ ⇌ **H(serine) *(aq)***	9.209	-4.30E+4	1	Original data for ΔH at I = 0.1 M.

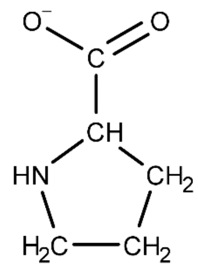
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + $(serine)^-$ ⇌ **$H_2(serine)^+$**	11.396	-4.6E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.187 ΔH = -3.0E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.209 ΔH = -4.3E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.396 ΔH = -4.6E+4
Mg^{2+} + $(serine)^-$ ⇌ **$Mg(serine)^+$**	0.48954		1	Original data for β: $log_{10}(\beta)$ = 1.03, at I = 3.0 M.
Al^{3+} + $(serine)^-$ ⇌ **$Al(serine)^{2+}$**	6.34073		1	Original data for β: $log_{10}(\beta)$ = 5.7, at I = 0.1 M.
Al^{3+} + $(OH)^-$ + $(serine)^-$ ⇌ **$Al(OH)(serine)^+$**	15.51130		1	ALL ⇌ Al(OH)L + H $log_{10}(\beta)$ = -5.04 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 5.7 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L $log_{10}(\beta)$ = 14.44342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.51130
2 Al^{3+} + $(OH)^-$ + $(serine)^-$ ⇌ **$Al_2(OH)(serine)^{4+}$**	18.00057		1	Al(OH)L + Al ⇌ $Al_2(OH)L$ $log_{10}(\beta)$ = 3.13 I = 0.1 M Al + OH + L ⇌ Al(OH)L $log_{10}(\beta)$ = 14.44342 I = 0.1 M 2 Al + OH + L ⇌ $Al_2(OH)L$ $log_{10}(\beta)$ = 17.57342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.00057
Ca^{2+} + $(serine)^-$ ⇌ **$Ca(serine)^+$**	1.43		1	
$Mn(II)^{2+}$ + $(serine)^-$ ⇌ **$Mn(II)(serine)^+$**	2.92715	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 2.50, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Mn(II)^{2+}$ + 2 $(serine)^-$ ⇌ **$Mn(II)(serine)_2$ *(aq)***	4.62073	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.98, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Fe(II)^{2+}$ + $(serine)^-$ ⇌ **$Fe(II)(serine)^+$**	4.07715	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.65, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Fe(II)^{2+}$ + 2 $(serine)^-$ ⇌ **$Fe(II)(serine)_2$ *(aq)***	7.05073	-8E+3	1	Original data for β: $log_{10}(\beta)$ = 6.41, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Fe(II)^{2+}$ + 3 $(serine)^-$ ⇌ **$Fe(II)(serine)_3^-$**	9.48931		1	Original data for β: $log_{10}(\beta)$ = 10.3, at I = 3.0 M.
$Fe(III)^{3+}$ + $(serine)^-$ ⇌ **$Fe(III)(serine)^{2+}$**	9.80948		1	Original data for β: $log_{10}(\beta)$ = 9.2, at I = 1.0 M and 20°C.
$Co(II)^{2+}$ + $(serine)^-$ ⇌ **$Co(II)(serine)^+$**	4.77715	-1.1E+4	1	Original data for β: $log_{10}(\beta)$ = 4.35, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Co(II)^{2+}$ + 2 $(serine)^-$ ⇌ **$Co(II)(serine)_2$ *(aq)***	8.44073	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 7.8, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Co(II)^{2+}$ + 3 $(serine)^-$ ⇌ **$Co(II)(serine)_3^-$**	10.73931		1	Original data for β: $log_{10}(\beta)$ = 11.55, at I = 3.0 M.
Ni^{2+} + $(serine)^-$ ⇌ **$Ni(serine)^+$**	5.82715	-1.5E+4	1	Original data for β: $log_{10}(\beta)$ = 5.40, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 $(serine)^-$ ⇌ **$Ni(serine)_2$ *(aq)***	10.51073	-3.4E+4	1	Original data for β: $log_{10}(\beta)$ = 9.87, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 $(serine)^-$ ⇌ **$Ni(serine)_3^-$**	13.64073	-5.56E+4	1	Original data for β: $log_{10}(\beta)$ = 13.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + $(serine)^-$ ⇌ **$Cu(II)(serine)^+$**	8.32715	-2.3E+4	1	Original data for β: $log_{10}(\beta)$ = 7.90, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(serine)^-$ ⇌ **$Cu(II)(serine)_2$ *(aq)***	15.14073	-4.89E+4	1	Original data for β: $log_{10}(\beta)$ = 14.50, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(II)^{2+}$ + $(OH)^-$ + 2 $(serine)^-$ ⇌ **$Cu(II)(OH)(serine)_2^-$**	18.77415	-1.3671E+5	1	$Cu(II)L_2$ ⇌ $Cu(II)(OH)L_2$ + H $log_{10}(\beta)$ = -10.15 I = 0.1 M ΔH = -3.2E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + 2 L ⇌ $Cu(II)L_2$ $log_{10}(\beta)$ = 14.5 I = 0.1 M ΔH = -4.89E+4 H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cu(II) + OH + 2 L ⇌ $Cu(II)(OH)L_2$ $log_{10}(\beta)$ = 18.13342 I = 0.1 M ΔH = -1.3671E+5 I = 0 M: $log_{10}(\beta)$ = 18.77415
$Cu(II)^{2+}$ + 2 $(OH)^-$ + 2 $(serine)^-$ ⇌ **$Cu(II)(OH)_2(serine)_2^{2-}$**	21.19399	-2.0952E+5	1	$Cu(II)(OH)L_2$ ⇌ $Cu(II)(OH)_2L_2$ + H $log_{10}(\beta)$ = -11.15 I = 0.1 M ΔH = -1.7E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + OH + 2 L ⇌ $Cu(II)(OH)L_2$ $log_{10}(\beta)$ = 18.13342 I = 0.1 M ΔH = -1.3671E+5 H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cu(II) + 2 OH + 2 L ⇌ $Cu(II)(OH)_2L_2$ $log_{10}(\beta)$ = 20.76684 I = 0.1 M ΔH = -2.0952E+05 I = 0 M: $log_{10}(\beta)$ = 21.19399
Zn^{2+} + $(serine)^-$ ⇌ **$Zn(serine)^+$**	5.02715	-9.6E+3	1	Original data for β: $log_{10}(\beta)$ = 4.60, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 $(serine)^-$ ⇌ **$Zn(serine)_2$ *(aq)***	9.07073	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 8.43, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 3 $(serine)^-$ ⇌ **$Zn(serine)_3^-$**	11.08931		1	Original data for β: $log_{10}(\beta)$ = 11.9, at I = 3.0 M.
Ga^{3+} + $(serine)^-$ ⇌ **$Ga(serine)^{2+}$**	8.18931		1	Original data for β: $log_{10}(\beta)$ = 9.0, at I = 3.0 M.
Ga^{3+} + H^+ + $(serine)^-$ ⇌ **$GaH(serine)^{3+}$**	11.12977		1	GaL + H ⇌ GaHL $log_{10}(\beta)$ = 2.4 I = 3.0 M Ga + L ⇌ GaL $log_{10}(\beta)$ = 9.0 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 11.4 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 11.12977
Cd^{2+} + $(serine)^-$ ⇌ **$Cd(serine)^+$**	4.19715		1	Original data for β: $log_{10}(\beta)$ = 3.77, at I = 0.1 M.
Cd^{2+} + 2 $(serine)^-$ ⇌ **$Cd(serine)_2$ *(aq)***	7.67073		1	Original data for β: $log_{10}(\beta)$ = 7.03, at I = 0.1 M.
Cd^{2+} + 3 $(serine)^-$ ⇌ **$Cd(serine)_3^-$**	9.97073		1	Original data for β: $log_{10}(\beta)$ = 9.33, at I = 0.1 M.
Nd^{3+} + H^+ + $(serine)^-$ ⇌ **$NdH(serine)^{3+}$**	10.19900		1	Nd + HL ⇌ NdHL $log_{10}(\beta)$ = 0.99 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 8.99542 I = 0.1 M Nd + H + L ⇌ NdHL $log_{10}(\beta)$ = 9.98542 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 10.19900
$Pb(II)^{2+}$ + $(serine)^-$ ⇌ **$Pb(II)(serine)^+$**	4.60954		1	Original data for β: $log_{10}(\beta)$ = 5.15, at I = 3.0 M.
$Pb(II)^{2+}$ + 2 $(serine)^-$ ⇌ **$Pb(II)(serine)_2$ *(aq)***	7.52931		1	Original data for β: $log_{10}(\beta)$ = 8.34, at I = 3.0 M.
$Pb(II)^{2+}$ + 3 $(serine)^-$ ⇌ **$Pb(II)(serine)_3^-$**	9.18931		1	Original data for β: $log_{10}(\beta)$ = 10.0, at I = 3.0 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$(U(VI)O_2)^{2+}$ + $(serine)^-$ ⇌ **$(UO_2)H(serine)^{2+}$**	10.07900		1	$(U(VI)O_2)$ + HL ⇌ $(U(VI)O_2)HL$ $\log_{10}(\beta)$ = 0.87 I = 0.5 M H + L ⇌ HL $\log_{10}(\beta)$ = 8.94061 I = 0.5 M $(U(VI)O_2)$ + H + L ⇌ $(U(VI)O_2)HL$ $\log_{10}(\beta)$ = 9.81061 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 10.07900

2.2.37. Proline

The ligand in its neutral form is L-Pyrrolidine-2-carboxylic acid (L-proline; $C_5H_9NO_2$). The ligand L as it is present in the database is the anion $C_5H_8NO_2^-$. Its molecular weight is 114.124. Its structural formula is shown on the right.



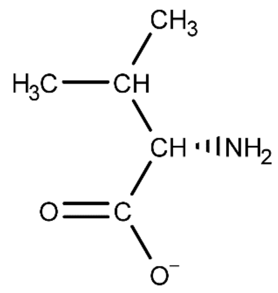
Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(proline)^-$ ⇌ **H(proline) *(aq)***	10.640	-4.330E+4	1	
2 H^+ + $(proline)^-$ ⇌ **$H_2(proline)^+$**	12.592	-4.45E+4	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 1.952 ΔH = -1.2E+3 H + L ⇌ HL $\log_{10}(\beta)$ = 10.640 ΔH = -4.330E+4 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 12.592 ΔH = -4.45+4
$Mn(II)^{2+}$ + $(proline)^-$ ⇌ **$Mn(II)(proline)^+$**	3.76715		1	Original data for β: $\log_{10}(\beta)$ = 3.34, at I = 0.1 M.
$Mn(II)^{2+}$ + 2 $(proline)^-$ ⇌ **$Mn(II)(proline)_2$ *(aq)***	6.24362		1	Original data for β: $\log_{10}(\beta)$ = 5.53, at I = 0.15 M and 37°C.
$Mn(II)^{2+}$ + 3 $(proline)^-$ ⇌ **$Mn(II)(proline)_3^-$**	7.41362		1	Original data for β: $\log_{10}(\beta)$ = 6.7, at I = 0.15 M and 37°C.
$Mn(II)^{2+}$ + H^+ + $(proline)^-$ ⇌ **$Mn(II)H(proline)^{2+}$**	12.52927		1	Mn(II)L + H ⇌ Mn(II)HL $\log_{10}(\beta)$ = 9.0 I = 0.15 M (Original data for β at T = 37°C) Mn(II) + L ⇌ Mn(II)L $\log_{10}(\beta)$ = 3.29140 I = 0.15 M Mn(II) + H + L ⇌ Mn(II)HL $\log_{10}(\beta)$ = 12.29140 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 12.52927
$Mn(II)^{2+}$ + H^+ + 2 $(proline)^-$ ⇌ **$Mn(II)H(proline)_2^+$**	15.44362		1	$Mn(II)L_2$ + H ⇌ $Mn(II)HL_2$ $\log_{10}(\beta)$ = 9.2 I = 0.15 M (Original data for β at T = 37°C) Mn(II) + 2 L ⇌ $Mn(II)L_2$ $\log_{10}(\beta)$ = 5.53 I = 0.15 M Mn(II) + H + 2 L ⇌ $Mn(II)HL_2$ $\log_{10}(\beta)$ = 14.73 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 15.44362
$Fe(II)^{2+}$ + $(proline)^-$ ⇌ **$Fe(II)(proline)^+$**	4.47632		1	Original data for β: $\log_{10}(\beta)$ = 4.07, at I = 1.0 M and 20°C.

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Fe(III)$^{3+}$ + (proline)$^{-}$ ⇌ **Fe(III)(proline)$^{2+}$**	10.60948		1	Original data for β: log$_{10}$(β) = 10.0, at I = 1.0 M and 20°C.
Co(II)$^{2+}$ + (proline)$^{-}$ ⇌ **Co(II)(proline)$^{+}$**	5.25715		1	Original data for β: log$_{10}$(β) = 4.83, at I = 0.1 M.
Co(II)$^{2+}$ + 2 (proline)$^{-}$ ⇌ **Co(II)(proline)$_2$ *(aq)***	9.47073		1	Original data for β: log$_{10}$(β) = 8.83, at I = 0.1 M.
Ni^{2+} + (proline)$^{-}$ ⇌ **Ni(proline)$^{+}$**	6.36715	-2.3E+4	1	Original data for β: log$_{10}$(β) = 5.94, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 (proline)$^{-}$ ⇌ **Ni(proline)$_2$ *(aq)***	11.51073	-4.93E+4	1	Original data for β: log$_{10}$(β) = 10.87, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 (proline)$^{-}$ ⇌ **Ni(proline)$_3^{-}$**	14.49073		1	Original data for β: log$_{10}$(β) = 13.85, at I = 0.1 M.
Cu(II)$^{2+}$ + (proline)$^{-}$ ⇌ **Cu(II)(proline)$^{+}$**	9.25715	-2.9E+4	1	Original data for β: log$_{10}$(β) = 8.83, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (proline)$^{-}$ ⇌ **Cu(II)(proline)$_2$ *(aq)***	17.01073	-5.98E+4	1	Original data for β: log$_{10}$(β) = 16.37, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + H^{+} + (proline)$^{-}$ ⇌ **Cu(II)H(proline)$^{2+}$**	11.61927		1	Cu(II)L + H ⇌ Cu(II)HL log$_{10}$(β) = 2.6 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + L ⇌ Cu(II)L log$_{10}$(β) = 8.78140 I = 0.15 M Cu(II) + H + L ⇌ Cu (II)HL log$_{10}$(β) = 11.38140 I = 0.15 M I = 0 M: log$_{10}$(β) = 11.61927
Cu(II)$^{2+}$ + H^{+} + 2 (proline)$^{-}$ ⇌ **Cu(II)H(proline)$_2^{+}$**	21.82435		1	Cu(II)L$_2$ + H ⇌ Cu(II)HL$_2$ log$_{10}$(β) = 4.1 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + 2 L ⇌ Cu (II)L$_2$ log$_{10}$(β) = 17.01073 I = 0.15 M Cu(II) + H + 2 L ⇌ Cu(II)HL$_2$ log$_{10}$(β) = 21.11073 I = 0.15 M I = 0 M: log$_{10}$(β) = 21.82435
Zn^{2+} + (proline)$^{-}$ ⇌ **Zn(proline)$^{+}$**	5.69715		1	Original data for β: log$_{10}$(β) = 5.27, at I = 0.1 M.
Zn^{2+} + 2 (proline)$^{-}$ ⇌ **Zn(proline)$_2$ *(aq)***	10.40362		1	Original data for β: log$_{10}$(β) = 9.69, at I = 0.15 M and 37°C.
Zn^{2+} + 3 (proline)$^{-}$ ⇌ **Zn(proline)$_3^{-}$**	12.01362		1	Original data for β: log$_{10}$(β) = 11.3, at I = 0.15 M and 37°C.
Zn^{2+} + (OH)$^{-}$ + (proline)$^{-}$ ⇌ **Zn(OH)(proline) *(aq)***	11.34415		1	ZnL ⇌ Zn(OH)L + H log$_{10}$(β) = -8.35 I = 0.15 M (Original data for β at T = 37°C) Zn + L ⇌ ZnL log$_{10}$(β) = 5.22140 I = 0.15 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.75913 I = 0.15 M Zn + OH + L ⇌ Zn(OH)L log$_{10}$(β) = 10.63053 I = 0.15 M I = 0 M: log$_{10}$(β) = 11.34415
Zn^{2+} + (OH)$^{-}$ + 2 (proline)$^{-}$ ⇌ **Zn(OH)(proline)$_2^{-}$**	14.43275		1	ZnL$_2$ ⇌ Zn(OH)L$_2$ + H log$_{10}$(β) = -9.73 I = 0.15 M (Original data for β at T = 37°C) Zn + 2 L ⇌ ZnL$_2$ log$_{10}$(β) = 9.69 I = 0.15 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.75913 I = 0.15 M Zn + OH + 2 L ⇌ Zn(OH)L$_2$ log$_{10}$(β) = 13.71913 I = 0.15 M I = 0 M: log$_{10}$(β) = 14.43275
Ga^{3+} + (proline)$^{-}$ ⇌ **Ga(proline)$^{2+}$**	9.38931		1	Original data for β: log$_{10}$(β) = 10.20, at I = 3.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ga^{3+} + H^{+} + $(proline)^{-}$ ⇌ **$GaH(proline)^{3+}$**	12.44000		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 1.80 I = 3.0 M <u>H + L ⇌ HL $log_{10}(\beta)$ = 10.91023 I = 3.0 M</u> Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 12.71023 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 12.44000
Pd^{2+} + H^{+} + $(proline)^{-}$ ⇌ **$PdH(proline)^{2+}$**	14.84000		1	Pd + HL ⇌ PdHL $log_{10}(\beta)$ = 4.2 I = 1.0 M (Original data for β at T = 20°C) <u>H + L ⇌ HL $log_{10}(\beta)$ = 10.43684 I = 1.0 M</u> Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 14.63684 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 14.84000
Pd^{2+} + 2 H^{+} + 2 $(proline)^{-}$ ⇌ **$PdH_2(proline)_2{}^{2+}$**	28.78000		1	Pd + 2 HL ⇌ PdH_2L_2 $log_{10}(\beta)$ = 7.5 I = 1.0 M (Original data for β at T = 20°C) <u>2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 20.87368 I = 1.0 M</u> Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 28.37368 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 28.78000
Cd^{2+} + $(proline)^{-}$ ⇌ **$Cd(proline)^{+}$**	4.76883		1	Original data for β: $log_{10}(\beta)$ = 4.27, at I = 0.7 M.
Cd^{2+} + 2 $(proline)^{-}$ ⇌ **$Cd(proline)_2$ *(aq)***	8.68824		1	Original data for β: $log_{10}(\beta)$ = 7.94, at I = 0.7 M.

2.2.38. Valine

The ligand in its neutral form is L-2-Amino-3-methylbutanoic acid (Valine; $C_5H_{11}NO_2$). The ligand L as it is present in the database is the anion $C_5H_{10}NO_2^-$. Its molecular weight is 116.14. Its structural formula is shown on the right.



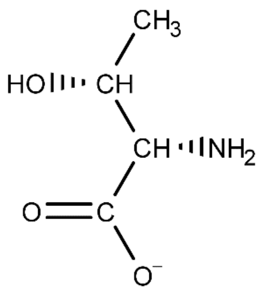
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + $(valine)^{-}$ ⇌ **H(valine) *(aq)***	9.719	-4.472E+4	1	
2 H^{+} + $(valine)^{-}$ ⇌ **$H_2(valine)^{+}$**	12.005	-4.543E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.286 ΔH = -7.1E+2 <u>H + L ⇌ HL $log_{10}(\beta)$ = 9.719 ΔH = -4.472E+4</u> 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 12.005 ΔH = -4.543E+4
$Mn(II)^{2+}$ + $(valine)^{-}$ ⇌ **$Mn(II)(valine)^{+}$**	2.79575		1	Original data for β: $log_{10}(\beta)$ = 2.32, at I = 0.15 M and 37°C.

Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Mn(II)^{2+}$ + 2 $(valine)^-$ ⇌ **$Mn(II)(valine)_2$ *(aq)***	4.51362		1	Original data for β: $log_{10}(β)$ = 3.8, at I = 0.15 M and 37°C.
$Fe(II)^{2+}$ + $(valine)^-$ ⇌ **$Fe(II)(valine)^+$**	3.79632		1	Original data for β: $log_{10}(β)$ = 3.39, at I = 1 M and 20°C.
$Co(II)^{2+}$ + $(valine)^-$ ⇌ **$Co(II)(valine)^+$**	4.71575		1	Original data for β: $log_{10}(β)$ = 4.24, at I = 0.15 M and 37°C.
$Co(II)^{2+}$ + 2 $(valine)^-$ ⇌ **$Co(II)(valine)_2$ *(aq)***	8.27362		1	Original data for β: $log_{10}(β)$ = 7.56, at I = 0.15 M and 37°C.
Ni^{2+} + $(valine)^-$ ⇌ **$Ni(valine)^+$**	5.72715	-1.7E+4	1	Original data for β: $log_{10}(β)$ = 5.3, at I = 0.1 M. Original data for ΔH at I = 1.0 M.
Ni^{2+} + 2 $(valine)^-$ ⇌ **$Ni(valine)_2$ *(aq)***	10.29073	-3.6E+4	1	Original data for β: $log_{10}(β)$ = 9.65, at I = 0.1 M. Original data for ΔH at I = 1.0 M.
Ni^{2+} + 3 $(valine)^-$ ⇌ **$Ni(valine)_3^-$**	12.84073	-5.4E+4	1	Original data for β: $log_{10}(β)$ = 12.2, at I = 0.1 M. Original data for ΔH at I = 1.0 M.
$Cu(II)^{2+}$ + $(valine)^-$ ⇌ **$Cu(II)(valine)^+$**	8.52715	-2.3E+4	1	Original data for β: $log_{10}(β)$ = 8.10, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(valine)^-$ ⇌ **$Cu(II)(valine)_2$ *(aq)***	15.54073	-4.81E+4	1	Original data for β: $log_{10}(β)$ = 14.9, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + H^+ + $(valine)^-$ ⇌ **$Cu(II)H(valine)^{2+}$**	10.71900		1	Cu(II) + HL ⇌ Cu(II)HL $log_{10}(β)$ = 1.0 I = 0.15 M (Original data for β at T = 37°C) H + L ⇌ HL $log_{10}(β)$ = 9.48113 I = 0.15 M Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(β)$ = 10.48113 I = 0.15 M I = 0 M: $log_{10}(β)$ = 10.71900
$Cu(II)^{2+}$ + H^+ + 2 $(valine)^-$ ⇌ **$Cu(II)H(valine)_2^+$**	19.32073		1	$Cu(II)L_2$ + H ⇌ $Cu(II)HL_2$ $log_{10}(β)$ = 3.78 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + 2 L ⇌ $Cu(II)L_2$ $log_{10}(β)$ = 14.82711 I = 0.15 M Cu(II) + H + 2 L ⇌ $Cu(II)HL_2$ $log_{10}(β)$ = 18.60711 I = 0.15 M I = 0 M: $log_{10}(β)$ = 19.32073
Zn^{2+} + $(valine)^-$ ⇌ **$Zn(valine)^+$**	4.94715		1	Original data for β: $log_{10}(β)$ = 4.52, at I = 0.1 M.
Zn^{2+} + 2 $(valine)^-$ ⇌ **$Zn(valine)_2$ *(aq)***	9.24073		1	Original data for β: $log_{10}(β)$ = 8.6, at I = 0.1 M.
Zn^{2+} + 3 $(valine)^-$ ⇌ **$Zn(valine)_3^-$**	11.31362		1	Original data for β: $log_{10}(β)$ = 10.66, at I = 0.15 M and 37°C.
Zn^{2+} + $(OH)^-$ + $(valine)^-$ ⇌ **Zn(OH)(valine) *(aq)***	10.34415		1	ZnL ⇌ Zn(OH)L + H $log_{10}(β)$ = -8.6 I = 0.15 M (Original data for β at T = 37°C) Zn + L ⇌ ZnL $log_{10}(β)$ = 4.47140 I = 0.15 M H + OH ⇌ H_2O $log_{10}(β)$ = 13.75913 I = 0.15 M Zn + OH + 2 L ⇌ $Zn(OH)L_2$ $log_{10}(β)$ = 9.63053 I = 0.15 M I = 0 M: $log_{10}(β)$ = 10.34415
Ga^{3+} + $(valine)^-$ ⇌ **$Ga(valine)^{2+}$**	9.66073		1	Original data for β: $log_{10}(β)$ = 9.02, at I = 0.1 M and 20°C.
Pd^{2+} + H^+ + $(valine)^-$ ⇌ **$PdH(valine)^{2+}$**	14.61900		1	Pd + HL ⇌ PdHL $log_{10}(β)$ = 4.9 I = 1.0 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(β)$ = 9.51584 I = 1.0 M Pd + H + L ⇌ PdHL $log_{10}(β)$ = 14.41584 I = 1.0 M I = 0 M: $log_{10}(β)$ = 14.61900

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Pd^{2+} + 2 H^{+} + 2 $(valine)^{-}$ ⇌ **$PdH_2(valine)_2^{2+}$**	27.93800		1	Pd + 2 HL ⇌ PdH_2L_2 $log_{10}(\beta)$ = 8.5 I = 1.0 M (Original data for β at T = 20°C) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 19.03168 I = 1.0 M Pd + 2 H + 2 L ⇌ PdH_2L_2 $log_{10}(\beta)$ = 27.53168 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 27.93800
Cd^{2+} + $(valine)^{-}$ ⇌ **$Cd(valine)^{+}$**	4.14715		1	Original data for β: $log_{10}(\beta)$ = 3.72, at I = 0.1 M.
Cd^{2+} + 2 $(valine)^{-}$ ⇌ **$Cd(valine)_2$ *(aq)***	7.45073		1	Original data for β: $log_{10}(\beta)$ = 6.81, at I = 0.1 M.
Cd^{2+} + 3 $(valine)^{-}$ ⇌ **$Cd(valine)_3^{-}$**	9.47073		1	Original data for β: $log_{10}(\beta)$ = 8.83, at I = 0.1 M.

2.2.39. Threonine

The ligand in its neutral form is L-2-Amino-3-hydroxybutanoic acid (Threonine; $C_4H_9NO_3$). The ligand L as it is present in the database is the anion $C_4H_8NO_3^-$. Its molecular weight is 118.112. Its structural formula is shown on the right.



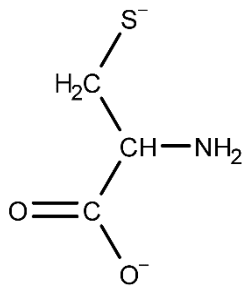
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + $(threonine)^{-}$ ⇌ **H(threonine) *(aq)***	9.100	-4.1E+4	1	
2 H^{+} + $(threonine)^{-}$ ⇌ **$H_2(threonine)^{+}$**	11.188	-4.6E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.088 ΔH = -5.0E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.100 ΔH = -4.1E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.188 ΔH = -4.6E+4
Al^{3+} + $(threonine)^{-}$ ⇌ **$Al(threonine)^{2+}$**	6.14073		1	Original data for β: $log_{10}(\beta)$ = 5.5, at I = 0.1 M.
Al^{3+} + $(OH)^{-}$ + $(threonine)^{-}$ ⇌ **$Al(OH)(threonine)^{+}$**	15.78130		1	AlL ⇌ Al(OH)L + H $log_{10}(\beta)$ = -4.57 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 5.5 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L $log_{10}(\beta)$ = 14.71342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.78130
$Mn(II)^{2+}$ + $(threonine)^{-}$ ⇌ **$Mn(II)(threonine)^{+}$**	2.91715	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 5.5, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Mn(II)^{2+}$ + 2 $(threonine)^{-}$ ⇌ **$Mn(II)(threonine)_2$ *(aq)***	4.60073	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.96, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Fe(II)$^{2+}$ + (threonine)$^{-}$ ⇌ **Fe(II)(threonine)$^{+}$**	4.06715	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.64, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Fe(II)$^{2+}$ + 2 (threonine)$^{-}$ ⇌ **Fe(II)(threonine)$_2$ *(aq)***	7.21073	-8E+3	1	Original data for β: $log_{10}(\beta)$ = 6.57, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Fe(III)$^{3+}$ + (threonine)$^{-}$ ⇌ **Fe(III)(threonine)$^{2+}$**	9.20948		1	Original data for β: $log_{10}(\beta)$ = 8.6, at I = 1.0 M and 20°C.
Co(II)$^{2+}$ + (threonine)$^{-}$ ⇌ **Co(II)(threonine)$^{+}$**	4.78715	-7.9E+3	1	Original data for β: $log_{10}(\beta)$ = 4.36, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Co(II)$^{2+}$ + 2 (threonine)$^{-}$ ⇌ **Co(II)(threonine)$_2$ *(aq)***	8.57073	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 7.93, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Co(II)$^{2+}$ + (OH)$^{-}$ + 2 (threonine)$^{-}$ ⇌ **Co(II)(OH)(threonine)$_2^{-}$**	12.65415		1	Co(II)L$_2$ ⇌ Co(II)(OH)L$_2$ + H $log_{10}(\beta)$ = -9.70 I = 0.1 M Co(II) + 2 L ⇌ Co(II)L$_2$ $log_{10}(\beta)$ = 7.93 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Co(II) + OH + 2 L ⇌ Co(II)(OH)L$_2$ $log_{10}(\beta)$ = 12.01342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 12.65415
Ni^{2+} + (threonine)$^{-}$ ⇌ **Ni(threonine)$^{+}$**	5.88715	-1.4E+4	1	Original data for β: $log_{10}(\beta)$ = 5.46, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 (threonine)$^{-}$ ⇌ **Ni(threonine)$_2$ *(aq)***	10.63073	-3.4E+4	1	Original data for β: $log_{10}(\beta)$ = 9.99, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 (threonine)$^{-}$ ⇌ **Ni(threonine)$_3^{-}$**	13.84073	-5.60E+4	1	Original data for β: $log_{10}(\beta)$ = 13.2, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + (threonine)$^{-}$ ⇌ **Cu(II)(threonine)$^{+}$**	8.43	-2.2E+4	1	
Cu(II)$^{2+}$ + 2 (threonine)$^{-}$ ⇌ **Cu(II)(threonine)$_2$ *(aq)***	15.36	-4.76E+4	1	
Cu(II)$^{2+}$ + (OH)$^{-}$ + (threonine)$^{-}$ ⇌ **Cu(II)(OH)(threonine) *(aq)***	16.237		1	Cu(II)L ⇌ Cu(II) (OH)L + H $log_{10}(\beta)$ = -6.19 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 7.95425 I = 0.15 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.75913 I = 0.15 M Cu(II) + OH + L ⇌ Cu(II) (OH)L $log_{10}(\beta)$ = 15.52338 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 16.237
Cu(II)$^{2+}$ + (OH)$^{-}$ + 2 (threonine)$^{-}$ ⇌ **Cu(II)(OH)(threonine)$_2^{-}$**	19.25342		1	Cu(II)L$_2$ ⇌ Cu(II)(OH)L$_2$ + H $log_{10}(\beta)$ = -9.89 I = 0.1 M Cu(II) + 2 L ⇌ Cu(II)L$_2$ $log_{10}(\beta)$ = 14.71927 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M C(II) + OH + 2 L ⇌ Cu(II)(OH)L$_2$ $log_{10}(\beta)$ = 18.61269 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.25342
Cu(II)$^{2+}$ + 2 (OH)$^{-}$ + 2 (threonine)$^{-}$ ⇌ **Cu(II)(OH)$_2$(threonine)$_2^{2-}$**	21.97326		1	Cu(II)(OH)L$_2$ ⇌ Cu(II)(OH)$_2$L$_2$ + H $log_{10}(\beta)$ = -10.85 I = 0.1 M Cu(II) + OH + 2 L ⇌ Cu(II)(OH)L$_2$ $log_{10}(\beta)$ = 18.61269 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M C(II) + OH + 2 L ⇌ Cu(II)(OH)L$_2$ $log_{10}(\beta)$ = 21.54611 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.97326
Zn^{2+} + (threonine)$^{-}$ ⇌ **Zn(threonine)$^{+}$**	5.05715	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 4.63, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 (threonine)$^{-}$ ⇌ **Zn(threonine)$_2$ *(aq)***	9.24073	-2.2E+4	1	Original data for β: $log_{10}(\beta)$ = 8.60, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Zn^{2+} + $(OH)^-$ + 2 $(threonine)^-$ ⇌ **$Zn(OH)(threonine)_2^-$**	13.55986		1	ZnL_2 ⇌ $Zn(OH)L_2$ + H $\log_{10}(\beta)$ = -9.44 I = 0.15 M (Original data for β at T = 37°C) Zn + 2 L ⇌ ZnL_2 $\log_{10}(\beta)$ = 8.52711 I = 0.15 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.75913 I = 0.15 M Zn + OH + 2 L ⇌ $Zn(OH)L_2$ $\log_{10}(\beta)$ = 12.84624 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 13.55986
Cd^{2+} + $(threonine)^-$ ⇌ **$Cd(threonine)^+$**	4.32715		1	Original data for β: $\log_{10}(\beta)$ = 3.9, at I = 0.1 M.
Cd^{2+} + 2 $(threonine)^-$ ⇌ **$Cd(threonine)_2$ *(aq)***	7.74073		1	Original data for β: $\log_{10}(\beta)$ = 7.1, at I = 0.1 M.
Nd^{3+} + H^+ + $(threonine)^-$ ⇌ **$NdH(threonine)^{3+}$**	9.98		1	Nd + HL ⇌ NdHL $\log_{10}(\beta)$ = 0.88 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 8.88642 I = 0.1 M Nd + H + L ⇌ NdHL $\log_{10}(\beta)$ = 9.76642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 9.98
$Pb(II)^{2+}$ + $(threonine)^-$ ⇌ **$Pb(II)(threonine)^+$**	4.90575		1	Original data for β: $\log_{10}(\beta)$ = 4.43, at I = 0.15 M and 37°C.
$Pb(II)^{2+}$ + 2 $(threonine)^-$ ⇌ **$Pb(II)(threonine)_2$ *(aq)***	7.91362		1	Original data for β: $\log_{10}(\beta)$ = 7.20, at I = 0.15 M and 37°C.

2.2.40. Cysteine

The ligand in its neutral form is L-2-Amino-3-mercaptopropanoic acid (cysteine; $C_3H_7NO_2S$). The ligand L as it is present in the database is the anion $C_3H_5NO_2S^{2-}$. Its molecular weight is 116.14. Its structural formula is shown on the right.



Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(cysteine)^{2-}$ ⇌ **$H(cysteine)^-$**	10.74	-3.5E+4	1	Original data for ΔH at I = 0.1 M.
2 H^+ + $(cysteine)^{2-}$ ⇌ **$H_2(cysteine)$ *(aq)***	19.10	-7.0E+4	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 8.36 ΔH = -3.5E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 10.74 ΔH = -3.5E+4 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 19.10 ΔH = -7.0E+4

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 H^+ + $(cysteine)^{2-}$ ⇌ **$H_3(cysteine)^+$**	20.8	-7.2E+4	1	H_2L + H ⇌ H_3L $\log_{10}(\beta)$ = 1.7 ΔH = -2.0E+3 (Original data for ΔH at I = 0.1 M) 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 19.10 ΔH = -7.0E+4 3 H + L ⇌ H_3L $\log_{10}(\beta)$ = 20.8 ΔH = -7.2E+4
Mg^{2+} + $(cysteine)^{2-}$ ⇌ **Mg(cysteine) *(aq)***	3.60430		1	Original data for β: $\log_{10}(\beta)$ = 2.75, at I = 0.1 M and 20°C.
Ca^{2+} + $(cysteine)^{2-}$ ⇌ **Ca(cysteine) *(aq)***	3.35430		1	Original data for β: $\log_{10}(\beta)$ = 2.50, at I = 0.1 M and 20°C.
$Mn(II)^{2+}$ + $(cysteine)^{2-}$ ⇌ **Mn(II)(cysteine) *(aq)***	5.60430		1	Original data for β: $\log_{10}(\beta)$ = 4.75, at I = 0.1 M.
$Fe(II)^{2+}$ + $(cysteine)^{2-}$ ⇌ **Fe(II)(cysteine) *(aq)***	7.45430		1	Original data for β: $\log_{10}(\beta)$ = 6.60, at I = 0.1 M and 20°C.
$Co(II)^{2+}$ + $(cysteine)^{2-}$ ⇌ **Co(II)(cysteine) *(aq)***	8.99430		1	Original data for β: $\log_{10}(\beta)$ = 8.14, at I = 0.1 M.
$Co(II)^{2+}$ + 2 $(cysteine)^{2-}$ ⇌ **$Co(II)(cysteine)_2^{2-}$**	15.33430		1	Original data for β: $\log_{10}(\beta)$ = 14.48, at I = 0.1 M.
2 $Co(II)^{2+}$ + 3 $(cysteine)^{2-}$ ⇌ **$Co(II)_2(cysteine)_3^{2-}$**	28.00860		1	Original data for β: $\log_{10}(\beta)$ = 26.3, at I = 0.1 M.
3 $Co(II)^{2+}$ + 4 $(cysteine)^{2-}$ ⇌ **$Co(II)_3(cysteine)_4^{2-}$**	40.56290		1	Original data for β: $\log_{10}(\beta)$ = 38.0, at I = 0.1 M.
Ni^{2+} + $(cysteine)^{2-}$ ⇌ **Ni(cysteine) *(aq)***	10.64430	-2.5E+4	1	Original data for β: $\log_{10}(\beta)$ = 19.9, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + H^+ + $(cysteine)^{2-}$ ⇌ **$NiH(cysteine)^+$**	15.49430		1	NiL + H ⇌ NiHL $\log_{10}(\beta)$ = 4.85 I = 0.1 M (Original data for β at T = 20°C) Ni + L ⇌ NiL $\log_{10}(\beta)$ = 9.79 I = 0.1 M Ni + H + L ⇌ NiHL $\log_{10}(\beta)$ = 14.64 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 15.49430
Ni^{2+} + 2 $(cysteine)^{2-}$ ⇌ **$Ni(cysteine)_2^{2-}$**	20.75430	-5.8E+4	1	Original data for β: $\log_{10}(\beta)$ = 19.9, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
2 Ni^{2+} + 3 $(cysteine)^{2-}$ ⇌ **$Ni_2(cysteine)_3^{2-}$**	34.70860		1	Original data for β: $\log_{10}(\beta)$ = 33.0, at I = 0.1 M and 20°C.
3 Ni^{2+} + 4 $(cysteine)^{2-}$ ⇌ **$Ni_3(cysteine)_4^{2-}$**	48.26290		1	Original data for β: $\log_{10}(\beta)$ = 45.7, at I = 0.1 M and 20°C.
Zn^{2+} + $(cysteine)^{2-}$ ⇌ **Zn(cysteine) *(aq)***	9.96430		1	Original data for β: $\log_{10}(\beta)$ = 9.11, at I = 0.1 M.
Zn^{2+} + H^+ + $(cysteine)^{2-}$ ⇌ **$ZnH(cysteine)^+$**	15.76715		1	Zn + HL ⇌ ZnHL $\log_{10}(\beta)$ = 4.60 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.31285 I = 0.1 M Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 14.91285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 15.76715
Zn^{2+} + 2 $(cysteine)^{2-}$ ⇌ **$Zn(cysteine)_2^{2-}$**	18.97430		1	Original data for β: $\log_{10}(\beta)$ = 18.12, at I = 0.1 M.
Zn^{2+} + H^+ + 2 $(cysteine)^{2-}$ ⇌ **$ZnH(cysteine)_2^-$**	25.70145		1	ZnL_2 + H ⇌ $ZnHL_2$ $\log_{10}(\beta)$ = 6.30 I = 0.1 M Zn + 2 L ⇌ ZnL_2 $\log_{10}(\beta)$ = 18.12 I = 0.1 M Zn + H + 2 L ⇌ $ZnHL_2$ $\log_{10}(\beta)$ = 24.42 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 25.70145
Zn^{2+} + 2 H^+ + 2 $(cysteine)^{2-}$ ⇌ **$ZnH_2(cysteine)_2$ *(aq)***	31.41503		1	$ZnHL_2$ + H ⇌ ZnH_2L_2 $\log_{10}(\beta)$ = 5.5 I = 0.1 M Zn + H + 2 L ⇌ $ZnHL_2$ $\log_{10}(\beta)$ = 24.42 I = 0.1 M Zn + 2 H + 2 L ⇌ $ZnHL_2$ $\log_{10}(\beta)$ = 29.92 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 31.41503
3 Zn^{2+} + 4 $(cysteine)^{2-}$ ⇌ **$Zn_3(cysteine)_4^{2-}$**	44.66290		1	Zn_3HL_4 ⇌ Zn_3L_4 + H $\log_{10}(\beta)$ = -6.90 I = 0.1 M 3 Zn + H + 4 L ⇌ Zn_3HL_4 $\log_{10}(\beta)$ = 49.0 I = 0.1 M 3 Zn + 4 L ⇌ Zn_3L_4 $\log_{10}(\beta)$ = 42.1 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 44.66290
3 Zn^{2+} + H^+ + 4 $(cysteine)^{2-}$ ⇌ **$Zn_3H(cysteine)_4^-$**	51.99005		1	Original data for β: $\log_{10}(\beta)$ = 49.0, at I = 0.1 M.

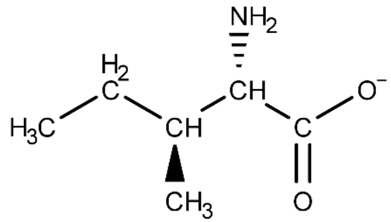
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 Zn^{2+} + $(OH)^-$ + 4 $(cysteine)^{2-}$ ⇌ **$Zn_3(OH)(cysteine)_4^{3-}$**	51.91628		1	Zn_3L_4 ⇌ $Zn_3(OH)L_4$ + H $log_{10}(\beta)$ = -6.03 I = 0.15 M (Original data for β at T = 37°C) 3 Zn + 4 L ⇌ Zn_3L_4 $log_{10}(\beta)$ = 41.80841 I = 0.15 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.75913 I = 0.15 M 3 Zn + OH + 4 L ⇌ $Zn_3(OH)L_4$ $log_{10}(\beta)$ = 49.53754 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 51.91628
Ga^{3+} + $(cysteine)^{2-}$ ⇌ **$Ga(cysteine)^+$**	14.47863		1	Original data for β: $log_{10}(\beta)$ = 16.1, at I = 3.0 M.
Ga^{3+} + H^+ + $(cysteine)^{2-}$ ⇌ **$GaH(cysteine)^{2+}$**	17.64886		1	GaL + H ⇌ GaHL $log_{10}(\beta)$ = 2.9 I = 3.0 M Ga + L ⇌ GaL $log_{10}(\beta)$ = 16.1 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 19.0 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 17.64886
Ga^{3+} + 2 H^+ + $(cysteine)^{2-}$ ⇌ **$GaH_2(cysteine)^{3+}$**	20.88931		1	GaHL + H ⇌ GaH_2L $log_{10}(\beta)$ = 2.7 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 19.0 I = 3.0 M Ga + 2 H + L ⇌ GaH_2L $log_{10}(\beta)$ = 21.7 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 20.88931
Cd^{2+} + $(cysteine)^{2-}$ ⇌ **Cd(cysteine) *(aq)***	11.05150		1	Original data for β: $log_{10}(\beta)$ = 10.1, at I = 0.15 M and 37°C.
Cd^{2+} + H^+ + $(cysteine)^{2-}$ ⇌ **$CdH(cysteine)^+$**	16.56575		1	Cd + HL ⇌ CdHL $log_{10}(\beta)$ = 5.35 I = 0.15 M (Original data for β at T = 37°C) H + L ⇌ HL $log_{10}(\beta)$ = 10.26425 I = 0.15 M Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 15.61425 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 16.56575
Cd^{2+} + 2 $(cysteine)^{2-}$ ⇌ **$Cd(cysteine)_2^{2-}$**	18.51909		1	Original data for β: $log_{10}(\beta)$ = 19.6, at I = 3.0 M.
Cd^{2+} + H^+ + 2 $(cysteine)^{2-}$ ⇌ **$CdH(cysteine)_2^-$**	26.89484		1	CdL_2 + H ⇌ $CdHL_2$ $log_{10}(\beta)$ = 7.9 I = 0.15 M (Original data for β at T = 37°C) Cd + 2 L ⇌ CdL_2 $log_{10}(\beta)$ = 17.56759 I = 0.15 M Cd + H + 2 L ⇌ $CdHL_2$ $log_{10}(\beta)$ = 25.46759 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 26.89484
Cd^{2+} + 2 H^+ + 2 $(cysteine)^{2-}$ ⇌ **$CdH_2(cysteine)_2^-$**	33.09271		1	$CdHL_2$ + H ⇌ CdH_2L_2 $log_{10}(\beta)$ = 5.96 I = 0.15 M (Original data for β at T = 37°C) Cd + H + 2 L ⇌ $CdHL_2$ $log_{10}(\beta)$ = 25.46759 I = 0.15 M Cd + 2 H + 2 L ⇌ CdH_2L_2 $log_{10}(\beta)$ = 31.42759 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 33.09271
Cd^{2+} + 3 $(cysteine)^{2-}$ ⇌ **$Cd(cysteine)_3^{4-}$**	20.1		1	Original data for β: $log_{10}(\beta)$ = 20.1, at I = 0.15 M and 37°C.
Cd^{2+} + H^+ + 3 $(cysteine)^{2-}$ ⇌ **$CdH(cysteine)_3^{3-}$**	30.25150		1	CdL_3 + H ⇌ $CdHL_3$ $log_{10}(\beta)$ = 9.2 I = 0.15 M (Original data for β at T = 37°C) Cd + 3 L ⇌ CdL_3 $log_{10}(\beta)$ = 20.1 I = 0.15 M Cd + H + 3 L ⇌ $CdHL_3$ $log_{10}(\beta)$ = 29.3 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 30.25150
In^{3+} + $(cysteine)^{2-}$ ⇌ **$In(cysteine)^+$**	15.40145		1	Original data for β: $log_{10}(\beta)$ = 14.12, at I = 0.1 M and 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
In^{3+} + H^{+} + $(cysteine)^{2-}$ ⇌ **$InH(cysteine)^{2+}$**	19.52788		1	InL + H ⇌ InHL $log_{10}(\beta)$ = 4.34 I = 0.1 M (Original data for β at T = 20°C) In + L ⇌ InL $log_{10}(\beta)$ = 14.12 I = 0.1 M In + H + L ⇌ InHL $log_{10}(\beta)$ = 18.46 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 19.52788
In^{3+} + 2 $(cysteine)^{2-}$ ⇌ **$In(cysteine)_2^{-}$**	28.96860		1	Original data for β: $log_{10}(\beta)$ = 27.26, at I = 0.1 M and 20°C.
In^{3+} + H^{+} + 2 $(cysteine)^{2-}$ ⇌ **$InH(cysteine)_2$ *(aq)***	33.70218		1	InL_2 + H ⇌ $InHL_2$ $log_{10}(\beta)$ = 4.52 I = 0.1 M (Original data for β at T = 20°C) In + 2 L ⇌ InL_2 $log_{10}(\beta)$ = 27.26 I = 0.1 M In + H + 2 L ⇌ $InHL_2$ $log_{10}(\beta)$ = 31.78 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 33.70218
In^{3+} + 2 H^{+} + 2 $(cysteine)^{2-}$ ⇌ **$InH_2(cysteine)_2^{+}$**	37.66218		1	$InHL_2$ + H ⇌ InH_2L_2 $log_{10}(\beta)$ = 3.96 I = 0.1 M (Original data for β at T = 20°C) In + H + 2 L ⇌ $InHL_2$ $log_{10}(\beta)$ = 31.78 I = 0.1 M In + H + 2 L ⇌ $InHL_2$ $log_{10}(\beta)$ = 35.74 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 37.66218
In^{3+} + 3 $(cysteine)^{2-}$ ⇌ **$In(cysteine)_3^{3-}$**	33.48145		1	Original data for β: $log_{10}(\beta)$ = 32.2, at I = 0.1 M and 20°C.
$Hg(II)^{2+}$ + $(cysteine)^{2-}$ ⇌ **Hg(II)(cysteine) *(aq)***	15.25430		1	Original data for β: $log_{10}(\beta)$ = 14.4, at I = 0.1 M.
$Pb(II)^{2+}$ + $(cysteine)^{2-}$ ⇌ **Pb(II)(cysteine) *(aq)***	13.05430	-4.1E+4	1	Original data for β: $log_{10}(\beta)$ = 19.9, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + H^{+} + $(cysteine)^{2-}$ ⇌ **$Pb(II)H(cysteine)^{+}$**	17.11632	-5.5E+4	1	Pb(II) + HL ⇌ Pb(II)HL $log_{10}(\beta)$ = 5.97 I = 1.0 M ΔH = -2.0E+4 (Original data for ΔH at I = 3.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.33368 I = 1.0 M ΔH = -3.5E+4 Pb(II) + H + L ⇌ Pb(II)HL $log_{10}(\beta)$ = 16.30368 I = 1.0 M ΔH = -5.5E+4 I = 0 M: $log_{10}(\beta)$ = 17.11632
$Pb(II)^{2+}$ + 2 $(cysteine)^{2-}$ ⇌ **$Pb(II)(cysteine)_2^{2-}$**	16.71264		1	Original data for β: $log_{10}(\beta)$ = 15.9, at I = 1.0 M.
$Pb(II)^{2+}$ + H^{+} + 2 $(cysteine)^{2-}$ ⇌ **$Pb(II)H(cysteine)_2^{-}$**	25.77863	-1.12E+5	1	Original data for β: $log_{10}(\beta)$ = 27.4, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + $(OH)^{-}$ + 2 $(cysteine)^{2-}$ ⇌ **$Pb(II)(OH)(cysteine)_2^{3-}$**	20.22032		1	$Pb(II)L_2$ ⇌ $Pb(II)(OH)L_2$ + H $log_{10}(\beta)$ = -11.3 I = 3.0 M Pb(II) + 2 L ⇌ $Pb(II)L_2$ $log_{10}(\beta)$ = 17.79355 I = 3.0 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 14.26723 I = 3.0 M Pb(II) + OH + 2 L ⇌ $Pb(II)(OH)L_2$ $log_{10}(\beta)$ = 20.76078 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 20.22032
Bi^{3+} + H^{+} + $(cysteine)^{2-}$ ⇌ **$BiH(cysteine)^{2+}$**	23.82516		1	Bi + HL ⇌ BiHL $log_{10}(\beta)$ = 12.28 I = 0.5 M H + L ⇌ HL $log_{10}(\beta)$ = 10.20322 I = 0.5 M Bi + H + L ⇌ BiHL $log_{10}(\beta)$ = 22.48322 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 23.82516

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Bi^{3+} + 2 H^+ + 2 $(cysteine)^{2-}$ ⇌ **$BiH_2(cysteine)_2^+$**	43.58193		1	Bi + 2 HL ⇌ BiH_2L_2 $log_{10}(\beta)$ = 20.76 I = 0.5 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 20.40644 I = 0.5 M Bi + H + L ⇌ BiHL $log_{10}(\beta)$ = 41.16644 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 43.58193

2.2.41. Isoleucine

The ligand in its neutral form is L-2-Amino-3-methylpentanoic acid (isoleucine; $C_6H_{13}NO_2$). The ligand L as it is present in the database is the anion $C_6H_{12}NO_2^-$. Its molecular weight is 130.167. Its structural formula is shown on the right.

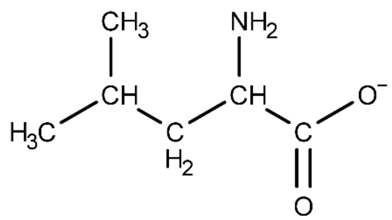


Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(isoleucine)^-$ ⇌ **H(isoleucine) *(aq)***	9.758	-4.47E+4	1	
2 H^+ + $(isoleucine)^-$ ⇌ **$H_2(isoleucine)^+$**	12.076	-4.57E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.318 ΔH = -1E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.758 ΔH = -4.47E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 12.076 ΔH = -4.57E+4
$Co(II)^{2+}$ + $(isoleucine)^-$ ⇌ **$Co(II)(isoleucine)^+$**	5.01715	-1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 4.59, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Co(II)^{2+}$ + 2 $(isoleucine)^-$ ⇌ **$Co(II)(isoleucine)_2$ *(aq)***	9.57073	-2.2E+4	1	Original data for β: $log_{10}(\beta)$ = 8.93, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + $(isoleucine)^-$ ⇌ **$Ni(isoleucine)^+$**	5.82715		1	Original data for β: $log_{10}(\beta)$ = 5.4, at I = 0.1 M.
Ni^{2+} + 2 $(isoleucine)^-$ ⇌ **$Ni(isoleucine)_2$ *(aq)***	10.34073		1	Original data for β: $log_{10}(\beta)$ = 9.7, at I = 0.1 M.
Ni^{2+} + 3 $(isoleucine)^-$ ⇌ **$Ni(isoleucine)_3^-$**	13.34073		1	Original data for β: $log_{10}(\beta)$ = 12.7, at I = 0.1 M.
$Cu(II)^{2+}$ + $(isoleucine)^-$ ⇌ **$Cu(II)(isoleucine)^+$**	8.56715	-2.6E+4	1	Original data for β: $log_{10}(\beta)$ = 8.14, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(isoleucine)^-$ ⇌ **$Cu(II)(isoleucine)_2$ *(aq)***	15.64073	-4.43E+4	1	Original data for β: $log_{10}(\beta)$ = 15.0, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + $(OH)^-$ + $(isoleucine)^-$ ⇌ **Cu(II)(OH)(isoleucine) *(aq)***	15.05415		1	Cu(II)L ⇌ Cu(II)(OH)L + H $log_{10}(\beta)$ = -7.51 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + L ⇌ Cu(II)L $log_{10}(\beta)$ = 8.09140 I = 0.15 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.75913 I = 0.15 M Cu(II) + OH + L ⇌ Cu(II)(OH)L $log_{10}(\beta)$ = 14.34053 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 15.05415

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Zn^{2+} + (isoleucine)$^-$ ⇌ **Zn(isoleucine)$^+$**	5.02678		1	Original data for β: $\log_{10}(\beta)$ = 4.49, at I = 0.5 M.
Zn^{2+} + 2 (isoleucine)$^-$ ⇌ **Zn(isoleucine)$_2$ *(aq)***	9.29516		1	Original data for β: $\log_{10}(\beta)$ = 8.49, at I = 0.5 M.
Zn^{2+} + 3 (isoleucine)$^-$ ⇌ **Zn(isoleucine)$_3^-$**	11.70516		1	Original data for β: $\log_{10}(\beta)$ = 10.9, at I = 0.5 M.
Zn^{2+} + (OH)$^-$ + (isoleucine)$^-$ ⇌ **Zn(OH)(isoleucine) *(aq)***	11.12378		1	ZnL ⇌ Zn(OH)L + H $\log_{10}(\beta)$ = -7.90 I = 0.15 M (Original data for β at T = 37°C) Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 4.55103 I = 0.15 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.75913 I = 0.15 M Zn + OH + 2 L ⇌ Zn(OH)L_2 $\log_{10}(\beta)$ = 10.41016 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 11.12378
Ga^{3+} + (isoleucine)$^-$ ⇌ **Ga(isoleucine)$^{2+}$**	8.78931		1	Original data for β: $\log_{10}(\beta)$ = 9.60, at I = 3.0 M.
Ga^{3+} + H^+ + (isoleucine)$^-$ ⇌ **GaH(isoleucine)$^{3+}$**	11.79800		1	Ga + HL ⇌ GaHL $\log_{10}(\beta)$ = 2.04 I = 3.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.02823 I = 3.0 M Ga + H + L ⇌ GaHL $\log_{10}(\beta)$ = 12.06823 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 11.79800
Cd^{2+} + (isoleucine)$^-$ ⇌ **Cd(isoleucine)$^+$**	4.13883		1	Original data for β: $\log_{10}(\beta)$ = 3.64, at I = 0.7 M.
Cd^{2+} + 2 (isoleucine)$^-$ ⇌ **Cd(isoleucine)$_2$ *(aq)***	7.57824		1	Original data for β: $\log_{10}(\beta)$ = 6.83, at I = 0.7 M.

2.2.42. Leucine

The ligand in its neutral form is L-2-Amino-4-methylpentanoic acid (leucine; $C_6H_{13}NO_2$). The ligand L as it is present in the database is the anion $C_6H_{12}NO_2^-$. Its molecular weight is 130.167. Its structural formula is shown on the right.



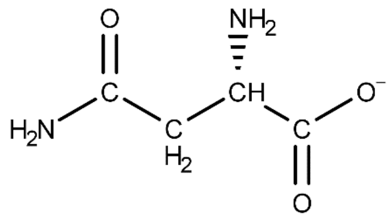
Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + (leucine)$^-$ ⇌ **H(leucine) *(aq)***	9.744	-4.539E+4	1	
2 H^+ + (leucine)$^-$ ⇌ **H_2(leucine)$^+$**	12.072	-4.699E+4	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 2.328 ΔH = -1.6E+3 H + L ⇌ HL $\log_{10}(\beta)$ = 9.744 ΔH = -4.539E+4 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 12.072 ΔH = -4.699E+4
Mn(II)$^{2+}$ + (leucine)$^-$ ⇌ **Mn(II)(leucine)$^+$**	2.72715		1	Original data for β: $\log_{10}(\beta)$ = 2.3, at I = 0.1 M.
Fe(II)$^{2+}$ + (leucine)$^-$ ⇌ **Fe(II)(leucine)$^+$**	3.82632		1	Original data for β: $\log_{10}(\beta)$ = 3.42, at I = 1.0 M and 20°C.
Ni^{2+} + (leucine)$^-$ ⇌ **Ni(leucine)$^+$**	5.75715		1	Original data for β: $\log_{10}(\beta)$ = 5.33, at I = 0.1 M.
Ni^{2+} + 2 (leucine)$^-$ ⇌ **Ni(leucine)$_2$ *(aq)***	10.35073		1	Original data for β: $\log_{10}(\beta)$ = 9.71, at I = 0.1 M and 20°C.

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Cu(II)$^{2+}$ + (leucine)$^{-}$ ⇌ **Cu(II)(leucine)$^{+}$**	8.56715	-2.3E+4	1	Original data for β: log$_{10}$(β) = 8.14, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (leucine)$^{-}$ ⇌ **Cu(II)(leucine)$_2$** ***(aq)***	15.54073	-7.11E+4	1	Original data for β: log$_{10}$(β) = 14.9, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + H^{+} + (leucine)$^{-}$ ⇌ **Cu(II)H(leucine)$^{2+}$**	11.84400		1	Cu(II) + HL ⇌ Cu(II)HL log$_{10}$(β) = 2.1 I = 0.15 M (Original data for β at T = 37°C) H + L ⇌ HL log$_{10}$(β) = 9.50613 I = 0.15 M Cu(II) + H + L ⇌ Cu(II)HL log$_{10}$(β) = 11.60613 I = 0.15 M I = 0 M: log$_{10}$(β) = 11.84400
Cu(II)$^{2+}$ + H^{+} + 2 (leucine)$^{-}$ ⇌ **Cu(II)H(leucine)$_2^{+}$**	20.14073		1	Cu(II)L$_2$ + H ⇌ Cu(II)HL$_2$ log$_{10}$(β) = 4.6 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + 2 L ⇌ Cu(II)L$_2$ log$_{10}$(β) = 14.82711 I = 0.15 M Cu(II) + H + 2 L ⇌ Cu(II)HL$_2$ log$_{10}$(β) = 19.42711 I = 0.15 M I = 0 M: log$_{10}$(β) = 20.14073
Zn^{2+} + (leucine)$^{-}$ ⇌ **Zn(leucine)$^{+}$**	4.98715		1	Original data for β: log$_{10}$(β) = 4.56, at I = 0.1 M.
Zn^{2+} + 2 (leucine)$^{-}$ ⇌ **Zn(leucine)$_2$** ***(aq)***	9.38073		1	Original data for β: log$_{10}$(β) = 8.74, at I = 0.1 M.
Zn^{2+} + (OH)$^{-}$ + (leucine)$^{-}$ ⇌ **Zn(OH)(leucine)** ***(aq)***	10.34415		1	ZnL ⇌ Zn(OH)L + H log$_{10}$(β) = -8.64 I = 0.15 M (Original data for β at T = 37°C) Zn + L ⇌ ZnL log$_{10}$(β) = 4.51140 I = 0.15 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.75913 I = 0.15 M Zn + OH + 2 L ⇌ Zn(OH)L$_2$ log$_{10}$(β) = 9.63053 I = 0.15 M I = 0 M: log$_{10}$(β) = 10.34415
Zn^{2+} + 2 H^{+} + (leucine)$^{-}$ ⇌ **ZnH(leucine)$_2^{+}$**	15.68073		1	ZnL$_2$ + H ⇌ ZnHL$_2$ log$_{10}$(β) = 6.3 I = 0.15 M (Original data for β at T = 37°C) Zn + 2 L ⇌ ZnL$_2$ log$_{10}$(β) = 8.66711 I = 0.15 M Zn + H + 2 L ⇌ ZnHL$_2$ log$_{10}$(β) = 14.96711 I = 0.15 M I = 0 M: log$_{10}$(β) = 15.68073
Pd^{2+} + H^{+} + (leucine)$^{-}$ ⇌ **PdH(leucine)$^{2+}$**	14.64400		1	Pd + HL ⇌ PdHL log10(β) = 4.9 I = 1.0 M (Original data for β at T = 20°C) H + L ⇌ HL log10(β) = 9.54084 I = 1.0 M Pd + H + L ⇌ PdHL log10(β) = 14.44084 I = 1.0 M I = 0 M: log10(β) = 14.64400
Pd^{2+} + 2 H^{+} + 2 (leucine)$^{-}$ ⇌ **PdH$_2$(leucine)$_2^{2+}$**	27.98800		1	Pd + 2 HL ⇌ PdH$_2$L$_2$ log$_{10}$(β) = 8.5 I = 1.0 M (Original data for β at T = 20°C) 2 H + 2 L ⇌ H$_2$L$_2$ log$_{10}$(β) = 19.08168 I = 1.0 M Pd + H + L ⇌ PdHL log$_{10}$(β) = 27.58168 I = 1.0 M I = 0 M: log$_{10}$(β) = 27.98800
Cd^{2+} + (leucine)$^{-}$ ⇌ **Cd(leucine)$^{+}$**	4.24632		1	Original data for β: log$_{10}$(β) = 3.84, at I = 1.0 M.
Cd^{2+} + 2 (leucine)$^{-}$ ⇌ **Cd(leucine)$_2$** ***(aq)***	7.14948		1	Original data for β: log$_{10}$(β) = 6.54, at I = 1.0 M.

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + 3 (leucine)$^{-}$ ⇌ **Cd(leucine)$_3^{-}$**	9.20948		1	Original data for β: log$_{10}$(β) = 8.60, at I = 1.0 M.

2.2.43. Asparagine

The ligand in its neutral form is L-2-Aminobutanedioic acid 4-amide (asparagine; $C_4H_8N_2O_3$). The ligand L as it is present in the database is the anion $C_4H_7N_2O_3^-$. Its molecular weight is 131.111. Its structural formula is shown on the right.

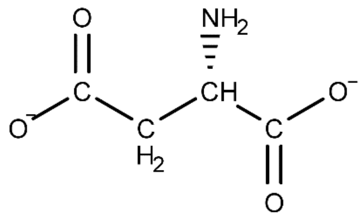


Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + (asparagine)$^{-}$ ⇌ **H(asparagine) *(aq)***	8.94358	-4.0E+4	1	Original data for β: log$_{10}$(β) = 8.73, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
2 H^{+} + (asparagine)$^{-}$ ⇌ **H$_2$(asparagine)$^{+}$**	11.10358	-4.3E+4	1	HL + H ⇌ H$_2$L log$_{10}$(β) = 2.16 I = 0.1 M ΔH = -3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 8.73 I = 0.1 M ΔH = -4.0E+4 2 H + L ⇌ H$_2$L log$_{10}$(β) = 10.89 I = 0.1 M ΔH = -4.3E+4 I = 0 M: log$_{10}$(β) = 11.10358
Al^{3+} + (asparagine)$^{-}$ ⇌ **Al(asparagine)$^{2+}$**	6.14073		1	Original data for β: log$_{10}$(β) = 5.5, at I = 0.1 M.
Al^{3+} + (OH)$^{-}$ + (asparagine)$^{-}$ ⇌ **Al(OH)(asparagine)$^{+}$**	15.52130		1	AlL ⇌ Al(OH)L + H log$_{10}$(β) = -4.83 I = 0.1 M Al + L ⇌ AlL log$_{10}$(β) = 5.5 I = 0.1 M H + OH ⇌ H$_2$O log$_{10}$(β) = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L log$_{10}$(β) = 14.45342 I = 0.1 M I = 0 M: log$_{10}$(β) = 15.52130
Mn(II)$^{2+}$ + (asparagine)$^{-}$ ⇌ **Mn(II)(asparagine)$^{+}$**	2.55954	-7.1E+3	1	Original data for β: log$_{10}$(β) = 3.10, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Mn(II)$^{2+}$ + 2 (asparagine)$^{-}$ ⇌ **Mn(II)(asparagine)$_2$ *(aq)***	4.40931	-1.3E+4	1	Original data for β: log$_{10}$(β) = 5.22, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Fe(II)$^{2+}$ + (asparagine)$^{-}$ ⇌ **Fe(II)(asparagine)$^{+}$**	3.82954		1	Original data for β: log$_{10}$(β) = 4.37, at I = 3.0 M.
Fe(II)$^{2+}$ + 2 (asparagine)$^{-}$ ⇌ **Fe(II)(asparagine)$_2$ *(aq)***	6.75931		1	Original data for β: log$_{10}$(β) = 7.57, at I = 3.0 M.
Fe(II)$^{2+}$ + 3 (asparagine)$^{-}$ ⇌ **Fe(II)(asparagine)$_3^{-}$**	9.44931		1	Original data for β: log$_{10}$(β) = 10.26, at I = 3.0 M.
Fe(III)$^{3+}$ + (asparagine)$^{-}$ ⇌ **Fe(III)(asparagine)$^{2+}$**	9.20948		1	Original data for β: log$_{10}$(β) = 8.6, at I = 1.0 M and 20°C.
Co(II)$^{2+}$ + (asparagine)$^{-}$ ⇌ **Co(II)(asparagine)$^{+}$**	4.95715	-1.2E+4	1	Original data for β: log$_{10}$(β) = 4.53, at I = 0.1 M. Original data for ΔH at I = 3.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Co(II)$^{2+}$ + 2 (asparagine)$^{-}$ ⇌ **Co(II)(asparagine)$_2$ *(aq)***	8.71073	-2.6E+4	1	Original data for β: $log_{10}(\beta)$ = 8.07, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Co(II)$^{2+}$ + 3 (asparagine)$^{-}$ ⇌ **Co(II)(asparagine)$_3^-$**	10.60073	-3.5E+4	1	Original data for β: $log_{10}(\beta)$ = 9.96, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + (asparagine)$^{-}$ ⇌ **Ni(asparagine)$^+$**	6.10715	-1.7E+4	1	Original data for β: $log_{10}(\beta)$ = 5.68, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 2 (asparagine)$^{-}$ ⇌ **Ni(asparagine)$_2$ *(aq)***	10.92073	-4.35E+4	1	Original data for β: $log_{10}(\beta)$ = 10.28, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 3 (asparagine)$^{-}$ ⇌ **Ni(asparagine)$_3^-$**	13.73931	-6.35E+4	1	Original data for β: $log_{10}(\beta)$ = 14.55, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Cu(II)$^{2+}$ + (asparagine)$^{-}$ ⇌ **Cu(II)(asparagine)$^+$**	8.26715	-2.4E+4	1	Original data for β: $log_{10}(\beta)$ = 7.84, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (asparagine)$^{-}$ ⇌ **Cu(II)(asparagine)$_2$ *(aq)***	15.04073	-5.06E+4	1	Original data for β: $log_{10}(\beta)$ = 14.4, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + (OH)$^{-}$ + 2 (asparagine)$^{-}$ ⇌ **Cu(II)(OH)(asparagine)$_2^-$**	18.37415		1	Cu(II)L_2 ⇌ Cu(II)(OH)L_2 + H $log_{10}(\beta)$ = -10.45 I = 0.1 M Cu(II) + 2 L ⇌ Cu(II)L_2 $log_{10}(\beta)$ = 14.4 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Cu(II) + OH + 2 L ⇌ Cu(II)(OH)L_2 $log_{10}(\beta)$ = 17.73342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.37415
Zn^{2+} + (asparagine)$^{-}$ ⇌ **Zn(asparagine)$^+$**	4.52954	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 5.07, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Zn^{2+} + 2 (asparagine)$^{-}$ ⇌ **Zn(asparagine)$_2$ *(aq)***	9.26073	-2.3E+4	1	Original data for β: $log_{10}(\beta)$ = 8.62, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Zn^{2+} + 3 (asparagine)$^{-}$ ⇌ **Zn(asparagine)$_3^-$**	11.48931	-2.8E+4	1	Original data for β: $log_{10}(\beta)$ = 12.30, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Ga^{3+} + (asparagine)$^{-}$ ⇌ **Ga(asparagine)$^{2+}$**	11.81073		1	Original data for β: $log_{10}(\beta)$ = 11.17, at I = 0.1 M and 20°C.
Pd^{2+} + H^+ + (asparagine)$^{-}$ ⇌ **PdH(asparagine)$^{2+}$**	11.75358		1	Pd + HL ⇌ PdHL $log_{10}(\beta)$ = 2.81 I = 3.0 M H + L ⇌ HL $log_{10}(\beta)$ = 9.21381 I = 3.0 M Pd + H + L ⇌ PdHL $log_{10}(\beta)$ = 12.02381 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 11.75358
Pd^{2+} + (asparagine)$^{-}$ ⇌ **PdH_{-1}(asparagine) *(aq)*** + H^+	8.55954		1	Original data for β: $log_{10}(\beta)$ = 9.1, at I = 3.0 M.
Cd^{2+} + (asparagine)$^{-}$ ⇌ **Cd(asparagine)$^+$**	3.52954		1	Original data for β: $log_{10}(\beta)$ = 4.07, at I = 3.0 M.
Cd^{2+} + 2 (asparagine)$^{-}$ ⇌ **Cd(asparagine)$_2$ *(aq)***	7.69073		1	Original data for β: $log_{10}(\beta)$ = 7.05, at I = 0.1 M.
Cd^{2+} + 3 (asparagine)$^{-}$ ⇌ **Cd(asparagine)$_3^-$**	8.79931		1	Original data for β: $log_{10}(\beta)$ = 9.61, at I = 3.0 M.
Pb(II)$^{2+}$ + (asparagine)$^{-}$ ⇌ **Pb(II)(asparagine)$^+$**	4.36954		1	Original data for β: $log_{10}(\beta)$ = 4.91, at I = 3.0 M.
Pb(II)$^{2+}$ + 2 (asparagine)$^{-}$ ⇌ **Pb(II)(asparagine)$_2$ *(aq)***	7.00931		1	Original data for β: $log_{10}(\beta)$ = 7.82, at I = 3.0 M.
Pb(II)$^{2+}$ + 3 (asparagine)$^{-}$ ⇌ **Pb(II)(asparagine)$_3^-$**	7.98931		1	Original data for β: $log_{10}(\beta)$ = 8.8, at I = 3.0 M.

2.2.44. Aspartate

The ligand in its neutral form is L-Aminobutanedioic acid (aspartic acid; $C_4H_7NO_4$). The ligand L as it is present in the database is the anion $C_4H_5NO_4{}^{2-}$. Its molecular weight is 132.095. Its structural formula is shown on the right.



Equilibrium reaction	Log₁₀(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + (aspartate)$^{2-}$ ⇌ **H(aspartate)$^-$**	10.002	-3.8E+4	1	
2 H^+ + (aspartate)$^{2-}$ ⇌ **H_2(aspartate) *(aq)***	13.902	-4.21E+4	1	HL + H ⇌ H_2L log₁₀(β) = 3.900 ΔH = -4.1E+3 H + L ⇌ HL log₁₀(β) = 10.002 ΔH = -3.8E+4 2 H + L ⇌ H_2L log₁₀(β) = 13.902 ΔH = -4.21E+4
3 H^+ + (aspartate)$^{2-}$ ⇌ **H_3(aspartate)$^+$**	15.892	-4.96E+4	1	H_2L + H ⇌ H_3L log₁₀(β) = 1.990 ΔH = -7.5E+3 H + L ⇌ HL log₁₀(β) = 13.902 ΔH = -4.21E+4 2 H + L ⇌ H_2L log₁₀(β) = 15.892 ΔH = -4.96E
Be^{2+} + 2 $(OH)^-$ + (aspartate)$^{2-}$ ⇌ **Be$(OH)_2$(aspartate)$^{2-}$**	22.32516		1	Original data for β: log₁₀(β) = 21.52, at I = 0.5 M.
Na^+ + (aspartate)$^{2-}$ ⇌ **Na(aspartate)$^-$**	0.42		1	
Mg^{2+} + (aspartate)$^{2-}$ ⇌ **Mg(aspartate) *(aq)***	3.25430		1	Original data for β: log₁₀(β) = 2.4, at I = 0.1 M.
Al^{3+} + (aspartate)$^{2-}$ ⇌ **Al(aspartate)$^+$**	9.15145		1	Original data for β: log₁₀(β) = 7.87, at I = 0.1 M.
Al^{3+} + H^+ + (aspartate)$^{2-}$ ⇌ **AlH(aspartate)$^{2+}$**	12.78273		1	Al + HL ⇌ AlHL log₁₀(β) = 2.14 I = 0.1 M H + L ⇌ HL log₁₀(β) = 9.57485 I = 0.1 M Al + H + L ⇌ AlHL log₁₀(β) = 11.71485 I = 0.1 M I = 0 M: log₁₀(β) = 12.78273
Al^{3+} + $(OH)^-$ + (aspartate)$^{2-}$ ⇌ **Al(OH)(aspartate) *(aq)***	18.57845		1	AlL ⇌ Al(OH)L + H log₁₀(β) = -4.57 I = 0.1 M Al + L ⇌ AlL log₁₀(β) = 7.87 I = 0.1 M H + OH ⇌ H_2O log₁₀(β) = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L log₁₀(β) = 17.08342 I = 0.1 M I = 0 M: log₁₀(β) = 18.57845
Al^{3+} + 2 $(OH)^-$ + (aspartate)$^{2-}$ ⇌ **Al$(OH)_2$(aspartate)$^-$**	26.74187		1	Al(OH)L ⇌ Al$(OH)_2$L + H log₁₀(β) = -5.62 I = 0.1 M Al + OH + L ⇌ Al(OH)L log₁₀(β) = 17.08342 I = 0.1 M H + OH ⇌ H_2O log₁₀(β) = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L log₁₀(β) = 25.24684 I = 0.1 M I = 0 M: log₁₀(β) = 26.74187
Ca^{2+} + (aspartate)$^{2-}$ ⇌ **Ca(aspartate) *(aq)***	2.5		1	
Ca^{2+} + H^+ + (aspartate)$^{2-}$ ⇌ **CaH(aspartate)$^+$**	11.402		1	
Mn(II)$^{2+}$ + (aspartate)$^{2-}$ ⇌ **Mn(II)(aspartate) *(aq)***	4.55430		1	Original data for β: log₁₀(β) = 3.7, at I = 0.1 M.
Fe(II)$^{2+}$ + (aspartate)$^{2-}$ ⇌ **Fe(II)(aspartate) *(aq)***	5.19430		1	Original data for β: log₁₀(β) = 4.34, at I = 1.0 M and 20°C.

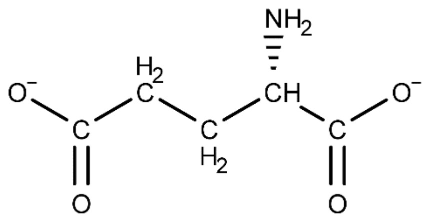
Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Fe(III)$^{3+}$ + (aspartate)$^{2-}$ ⇌ **Fe(III)(aspartate)$^{+}$**	12.61896		1	Original data for β: log$_{10}$(β) = 11.4, at I = 1.0 M and 20°C.
Co(II)$^{2+}$ + (aspartate)$^{2-}$ ⇌ **Co(II)(aspartate) *(aq)***	6.80430		1	Original data for β: log$_{10}$(β) = 5.95, at I = 0.1 M.
Co(II)$^{2+}$ + 2 (aspartate)$^{2-}$ ⇌ **Co(II)(aspartate)$_2^{2-}$**	11.08430		1	Original data for β: log$_{10}$(β) = 10.23, at I = 0.1 M.
Ni^{2+} + (aspartate)$^{2-}$ ⇌ **Ni(aspartate) *(aq)***	8.01430	-1.2E+4	1	Original data for β: log$_{10}$(β) = 7.16, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 (aspartate)$^{2-}$ ⇌ **Ni(aspartate)$_2^{2-}$**	13.27430	-3.3E+4	1	Original data for β: log$_{10}$(β) = 12.42, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + H^{+} + (aspartate)$^{2-}$ ⇌ **NiH(aspartate)$^{+}$**	11.94915		1	Ni + HL ⇌ NiHL log$_{10}$(β) = 1.52 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 9.57485 I = 0.1 M Ni + H + L ⇌ NiHL log$_{10}$(β) = 11.09485 I = 0.1 M I = 0 M: log$_{10}$(β) = 11.94915
Cu(II)$^{2+}$ + (aspartate)$^{2-}$ ⇌ **Cu(II)(aspartate) *(aq)***	9.74430	-2.5E+4	1	Original data for β: log$_{10}$(β) = 8.89, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (aspartate)$^{2-}$ ⇌ **Cu(II)(aspartate)$_2^{2-}$**	16.74430	-5.18E+4	1	Original data for β: log$_{10}$(β) = 15.89, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + H^{+} + (aspartate)$^{2-}$ ⇌ **Cu(II)H(aspartate)$^{+}$**	13.34915	-3.5E+4	1	Cu(II) + HL ⇌ Cu(II)HL log$_{10}$(β) = 2.92 I = 0.1 M ΔH = 3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL log$_{10}$(β) = 9.57485 I = 0.1 M ΔH = -3.8E+4 Cu(II) + H + L ⇌ Cu(II)HL log$_{10}$(β) = 12.49485 I = 0.1 M ΔH - -3.5E+4 I = 0 M: log$_{10}$(β) = 13.34915
Zn^{2+} + (aspartate)$^{2-}$ ⇌ **Zn(aspartate) *(aq)***	6.72430	-8E+3	1	Original data for β: log$_{10}$(β) = 5.87, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 (aspartate)$^{2-}$ ⇌ **Zn(aspartate)$_2^{2-}$**	11.00355		1	Original data for β: log$_{10}$(β) = 9.93, at I = 0.5 M.
Zn^{2+} + H^{+} + (aspartate)$^{2-}$ ⇌ **ZnH(aspartate)$^{+}$**	12.02775		1	Zn + HL ⇌ ZnHL log$_{10}$(β) = 1.55 I = 0.15 M (Original data for β at T = 37°C) H + L ⇌ HL log$_{10}$(β) = 9.52625 I = 0.15 M Zn + H + L ⇌ ZnHL log$_{10}$(β) = 11.07625 I = 0.15 M I = 0 M: log$_{10}$(β) = 12.02775
Sr^{2+} + (aspartate)$^{2-}$ ⇌ **Sr(aspartate) *(aq)***	2.35430		1	Original data for β: log$_{10}$(β) = 1.5, at I = 0.1 M.
Cd^{2+} + (aspartate)$^{2-}$ ⇌ **Cd(aspartate) *(aq)***	5.20430		1	Original data for β: log$_{10}$(β) = 4.35, at I = 0.1 M.
Cd^{2+} + 2 (aspartate)$^{2-}$ ⇌ **Cd(aspartate)$_2^{2-}$**	8.40430		1	Original data for β: log$_{10}$(β) = 7.55, at I = 0.1 M.
In^{3+} + (aspartate)$^{2-}$ ⇌ **In(aspartate)$^{+}$**	10.84145		1	Original data for β: log$_{10}$(β) = 9.56, at I = 0.1 M.
In^{3+} + 2 (aspartate)$^{2-}$ ⇌ **In(aspartate)$_2^{-}$**	18.40860		1	Original data for β: log$_{10}$(β) = 16.7, at I = 0.1 M.
In^{3+} + H^{+} + 2 (aspartate)$^{2-}$ ⇌ **InH(aspartate)$_2$ *(aq)***	23.37218		1	InL$_2$ + H ⇌ InHL$_2$ log$_{10}$(β) = 4.75 I = 0.1 M In + 2 L ⇌ InL$_2$ log$_{10}$(β) = 16.7 I = 0.1 M In + H + L ⇌ InHL log$_{10}$(β) = 21.45 I = 0.1 M I = 0 M: log$_{10}$(β) = 23.37218
Ba^{2+} + (aspartate)$^{2-}$ ⇌ **Ba(aspartate) *(aq)***	1.95430		1	Original data for β: log$_{10}$(β) = 1.1, at I = 0.1 M.
La^{3+} + (aspartate)$^{2-}$ ⇌ **La(aspartate)$^{+}$**	6.12145		1	Original data for β: log$_{10}$(β) = 4.84, at I = 0.1 M and 30°C.
La^{3+} + 2 (aspartate)$^{2-}$ ⇌ **La(aspartate)$_2^{-}$**	9.96860		1	Original data for β: log$_{10}$(β) = 8.26, at I = 0.1 M and 30°C.
Ce^{3+} + (aspartate)$^{2-}$ ⇌ **Ce(aspartate)$^{+}$**	6.41145		1	Original data for β: log$_{10}$(β) = 5.13, at I = 0.1 M and 30°C.
Ce^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Ce(aspartate)$_2^{-}$**	10.48860		1	Original data for β: log$_{10}$(β) = 8.78, at I = 0.1 M and 30°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ce^{3+} + 3 (aspartate)$^{2-}$ ⇌ **Ce(aspartate)$_3^{3-}$**	12.81145		1	Original data for β: $log_{10}(\beta)$ = 11.53, at I = 0.1 M and 30°C.
Pr^{3+} + (aspartate)$^{2-}$ ⇌ **Pr(aspartate)$^+$**	6.48145		1	Original data for β: $log_{10}(\beta)$ = 5.20, at I = 0.1 M.
Pr^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Pr(aspartate)$_2^-$**	10.50860		1	Original data for β: $log_{10}(\beta)$ = 8.8, at I = 0.1 M.
Pr^{3+} + 3 (aspartate)$^{2-}$ ⇌ **Pr(aspartate)$_3^{3-}$**	13.07145		1	Original data for β: $log_{10}(\beta)$ = 11.79, at I = 0.1 M and 30°C.
Nd^{3+} + (aspartate)$^{2-}$ ⇌ **Nd(aspartate)$^+$**	6.64145		1	Original data for β: $log_{10}(\beta)$ = 5.36, at I = 0.1 M.
Nd^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Nd(aspartate)$_2^-$**	11.00860		1	Original data for β: $log_{10}(\beta)$ = 9.3, at I = 0.1 M.
Nd^{3+} + 3 (aspartate)$^{2-}$ ⇌ **Nd(aspartate)$_3^{3-}$**	13.82145		1	Original data for β: $log_{10}(\beta)$ = 12.54, at I = 0.1 M and 30°C.
Sm^{3+} + (aspartate)$^{2-}$ ⇌ **Sm(aspartate)$^+$**	6.83145		1	Original data for β: $log_{10}(\beta)$ = 5.55, at I = 0.1 M.
Sm^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Sm(aspartate)$_2^-$**	11.40860		1	Original data for β: $log_{10}(\beta)$ = 9.7, at I = 0.1 M.
Eu^{3+} + (aspartate)$^{2-}$ ⇌ **Eu(aspartate)$^+$**	6.90145		1	Original data for β: $log_{10}(\beta)$ = 5.62, at I = 0.1 M.
Eu^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Eu(aspartate)$_2^-$**	11.50860		1	Original data for β: $log_{10}(\beta)$ = 9.8, at I = 0.1 M.
Gd^{3+} + (aspartate)$^{2-}$ ⇌ **Gd(aspartate)$^+$**	7.02145		1	Original data for β: $log_{10}(\beta)$ = 5.74, at I = 0.1 M.
Gd^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Gd(aspartate)$_2^-$**	12.20860		1	Original data for β: $log_{10}(\beta)$ = 10.5, at I = 0.1 M.
Tb^{3+} + (aspartate)$^{2-}$ ⇌ **Tb(aspartate)$^+$**	7.08145		1	Original data for β: $log_{10}(\beta)$ = 5.80, at I = 0.1 M.
Tb^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Tb(aspartate)$_2^-$**	12.00860		1	Original data for β: $log_{10}(\beta)$ = 10.3, at I = 0.1 M.
Dy^{3+} + (aspartate)$^{2-}$ ⇌ **Dy(aspartate)$^+$**	7.13145		1	Original data for β: $log_{10}(\beta)$ = 5.85, at I = 0.1 M.
Dy^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Dy(aspartate)$_2^-$**	12.50860		1	Original data for β: $log_{10}(\beta)$ = 10.8, at I = 0.1 M.
Ho^{3+} + (aspartate)$^{2-}$ ⇌ **Ho(aspartate)$^+$**	7.19145		1	Original data for β: $log_{10}(\beta)$ = 5.91, at I = 0.1 M.
Ho^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Ho(aspartate)$_2^-$**	12.50860		1	Original data for β: $log_{10}(\beta)$ = 10.8, at I = 0.1 M.
Er^{3+} + (aspartate)$^{2-}$ ⇌ **Er(aspartate)$^+$**	7.36145		1	Original data for β: $log_{10}(\beta)$ = 6.08, at I = 0.1 M.
Er^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Er(aspartate)$_2^-$**	12.60860		1	Original data for β: $log_{10}(\beta)$ = 10.9, at I = 0.1 M.
Tm^{3+} + (aspartate)$^{2-}$ ⇌ **Tm(aspartate)$^+$**	7.38145		1	Original data for β: $log_{10}(\beta)$ = 6.10, at I = 0.1 M.
Tm^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Tm(aspartate)$_2^-$**	12.80860		1	Original data for β: $log_{10}(\beta)$ = 11.1, at I = 0.1 M.
Yb^{3+} + (aspartate)$^{2-}$ ⇌ **Yb(aspartate)$^+$**	7.46145		1	Original data for β: $log_{10}(\beta)$ = 6.18, at I = 0.1 M.
Yb^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Yb(aspartate)$^-$**	13.20860		1	Original data for β: $log_{10}(\beta)$ = 11.5, at I = 0.1 M.
Lu^{3+} + (aspartate)$^{2-}$ ⇌ **Lu(aspartate)$^+$**	7.53145		1	Original data for β: $log_{10}(\beta)$ = 6.25, at I = 0.1 M.
Lu^{3+} + 2 (aspartate)$^{2-}$ ⇌ **Lu(aspartate)$^-$**	13.30860		1	Original data for β: $log_{10}(\beta)$ = 11.6, at I = 0.1 M.
Pb(II)$^{2+}$ + (aspartate)$^{2-}$ ⇌ **Pb(II)(aspartate) *(aq)***	6.93430		1	Original data for β: $log_{10}(\beta)$ = 6.08, at I = 0.1 M.
Pb(II)$^{2+}$ + 2 (aspartate)$^{2-}$ ⇌ **Pb(II)(aspartate)$_2^{2-}$**	9.36430		1	Original data for β: $log_{10}(\beta)$ = 8.51, at I = 0.1 M.
Pb(II)$^{2+}$ + H^+ + (aspartate)$^{2-}$ ⇌ **Pb(II)H(aspartate)$^+$**	12.19832		1	Pb(II) + HL ⇌ Pb(II)HL $log_{10}(\beta)$ = 1.79 I = 1.0 M H + L ⇌ HL $log_{10}(\beta)$ = 9.59568 I = 1.0 M Pb(II) + H + L ⇌ Pb(II)HL $log_{10}(\beta)$ = 11.38568 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 12.19832
$(U(VI)O_2)^{2+}$ + (aspartate)$^{2-}$ ⇌ **$(U(VI)O_2)$(aspartate) *(aq)***	4.51765		1	Original data for β: $log_{10}(\beta)$ = 3.52, at I = 0.7 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$(U(VI)O_2)^{2+}$ + H^+ + $(aspartate)^{2-}$ ⇌ **$(U(VI)O_2)H(aspartate)^+$**	13.03915	-2.930E+4	1	$(U(VI)O_2)$ + HL ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 2.61 I = 0.1 M ΔH = 8.7E+3 (Original data for ΔH at I = 1.0 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.57485 I = 0.1 M ΔH = -3.8E+4 $(U(VI)O_2)$ + H + L ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 12.18485 I = 0.1 M ΔH = -2.930E+4 I = 0 M: $log_{10}(\beta)$ = 13.03915
$(U(VI)O_2)^{2+}$ + 2 H^+ + 2 $(aspartate)^{2-}$ ⇌ **$(U(VI)O_2)H_2(aspartate)_2$ *(aq)***	24.75348	-6.6E+4	1	$(U(VI)O_2)$ + 2 HL ⇌ $(U(VI)O_2)H_2L_2$ $log_{10}(\beta)$ = 4.14 I = 1.0 M ΔH = 1E+4 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 19.19136 I = 1.0 M ΔH = -7.6E+4 $(U(VI)O_2)$ + H + L ⇌ $(U(VI)O_2)HL$ $log_{10}(\beta)$ = 23.33136 I = 1.0 M ΔH = -6.6E+4 I = 0 M: $log_{10}(\beta)$ = 24.75348

2.2.45. Glutamate

The ligand in its neutral form is L-2-Aminopentanedioic acid (glutamic acid; $C_5H_9NO_4$). The ligand L as it is present in the database is the anion $C_5H_7NO_4^{\ 2-}$. Its molecular weight is 145.114. Its structural formula is shown on the right. Do not mix up this one with glutamine (next section).



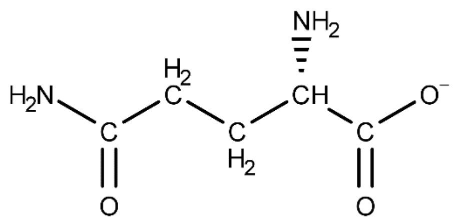
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(glutamate)^{2-}$ ⇌ **$H(glutamate)^-$**	9.960	-4.0E+4	1	
2 H^+ + $(glutamate)^{2-}$ ⇌ **$H_2(glutamate)$ *(aq)***	14.26	-4.3E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 4.30 ΔH = -3E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.96 ΔH = -4.0E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 14.26 ΔH = -4.3E+4
3 H^+ + $(glutamate)^{2-}$ ⇌ **$H_3(glutamate)^+$**	16.42	-4.6E+4	1	H_2L + H ⇌ H_3L $log_{10}(\beta)$ = 2.160 ΔH = -3E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 14.26 ΔH = -4.3E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 16.42 ΔH = -4.6E+4
Mg^{2+} + $(glutamate)^{2-}$ ⇌ **$Mg(glutamate)$ *(aq)***	2.75430		1	Original data for β: $log_{10}(\beta)$ = 1.9, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Al^{3+} + $(glutamate)^{2-}$ ⇌ **Al(glutamate)$^{+}$**	8.57145		1	Original data for β: $\log_{10}(\beta)$ = 7.29, at I = 0.1 M.
Al^{3+} + H^{+} + $(glutamate)^{2-}$ ⇌ **AlH(glutamate)$^{2+}$**	11.98073		1	Al + HL ⇌ AlHL $\log_{10}(\beta)$ = 1.38 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.53285 I = 0.1 M Al + H + L ⇌ AlHL $\log_{10}(\beta)$ = 10.91285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 11.98073
Al^{3+} + $(OH)^{-}$ + $(glutamate)^{2-}$ ⇌ **Al(OH)(glutamate) *(aq)***	17.82845		1	AlL ⇌ Al(OH)L + H $\log_{10}(\beta)$ = -4.74 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 7.29 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L $\log_{10}(\beta)$ = 16.33342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 17.82845
2 Al^{3+} + $(glutamate)^{2-}$ ⇌ **Al_2(glutamate)$^{4+}$**	10.13073		1	Al + AlL ⇌ Al_2L $\log_{10}(\beta)$ = 2.2 I = 0.1 M Al + L ⇌ AlL $\log_{10}(\beta)$ = 7.29 I = 0.1 M 2 Al + L ⇌ Al_2L $\log_{10}(\beta)$ = 9.49 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 10.13073
Ca^{2+} + $(glutamate)^{2-}$ ⇌ **Ca(glutamate) *(aq)***	2.06		1	
Ca^{2+} + H^{+} + $(glutamate)^{2-}$ ⇌ **CaH(glutamate)$^{+}$**	11.13		1	
$Fe(II)^{2+}$ + $(glutamate)^{2-}$ ⇌ **Fe(II)(glutamate) *(aq)***	4.33264		1	Original data for β: $\log_{10}(\beta)$ = 3.52, at I = 1.0 M and 20 °C.
$Fe(III)^{3+}$ + $(glutamate)^{2-}$ ⇌ **Fe(III)(glutamate)$^{+}$**	13.31896		1	Original data for β: $\log_{10}(\beta)$ = 12.1, at I = 1.0 M and 20 °C.
$Co(II)^{2+}$ + $(glutamate)^{2-}$ ⇌ **Co(II)(glutamate) *(aq)***	5.41430		1	Original data for β: $\log_{10}(\beta)$ = 4.56, at I = 0.1 M.
$Co(II)^{2+}$ + 2 $(glutamate)^{2-}$ ⇌ **Co(II)(glutamate)$_2^{2-}$**	8.71430		1	Original data for β: $\log_{10}(\beta)$ = 7.86, at I = 0.1 M.
Ni^{2+} + $(glutamate)^{2-}$ ⇌ **Ni(glutamate) *(aq)***	6.46430		1	Original data for β: $\log_{10}(\beta)$ = 5.61, at I = 0.1 M.
Ni^{2+} + 2 $(glutamate)^{2-}$ ⇌ **Ni(glutamate)$_2^{2-}$**	10.67430	-3.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 9.82, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 $(glutamate)^{2-}$ ⇌ **Ni(glutamate)$_3^{4-}$**	12.0		1	Original data for β: $\log_{10}(\beta)$ = 12.0, at I = 0.15 M and 37 °C.
Ni^{2+} + H^{+} + $(glutamate)^{2-}$ ⇌ **NiH(glutamate)$^{+}$**	11.57575		1	Ni + HL ⇌ NiHL $\log_{10}(\beta)$ = 1.14 I = 0.15 M (Original data for β at T = 37°C) H + L ⇌ HL $\log_{10}(\beta)$ = 9.48425 I = 0.15 M Ni + H + L ⇌ NiHL $\log_{10}(\beta)$ = 10.62425 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 11.57575
$Cu(II)^{2+}$ + $(glutamate)^{2-}$ ⇌ **Cu(II)(glutamate) *(aq)***	9.17430	-2.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.32, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(glutamate)^{2-}$ ⇌ **Cu(II)(glutamate)$_2^{2-}$**	15.77430	-4.81E+4	1	Original data for β: $\log_{10}(\beta)$ = 14.92, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + H^{+} + $(glutamate)^{2-}$ ⇌ **Cu(II)H(glutamate)$^{+}$**	13.27715	-2.8E+4	1	Cu(II) + HL ⇌ Cu(II)HL $\log_{10}(\beta)$ = 2.89 I = 0.1 M ΔH = 1.2E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 9.53285 I = 0.1 M ΔH = -4.0E+4 Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 12.42285 I = 0.1 M ΔH = -2.8E+4 I = 0 M: $\log_{10}(\beta)$ = 13.27715
Zn^{2+} + $(glutamate)^{2-}$ ⇌ **Zn(glutamate) *(aq)***	5.56355		1	Original data for β: $\log_{10}(\beta)$ = 4.49, at I = 0.5 M.
Zn^{2+} + 2 $(glutamate)^{2-}$ ⇌ **Zn(glutamate)$_2^{2-}$**	9.32355		1	Original data for β: $\log_{10}(\beta)$ = 8.25, at I = 0.5 M.
Ga^{3+} + $(glutamate)^{2-}$ ⇌ **Ga(glutamate)$^{+}$**	12.43145		1	Original data for β: $\log_{10}(\beta)$ = 11.30, at I = 3.0 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ga^{3+} + H^{+} + $(glutamate)^{2-}$ ⇌ **$GaH(glutamate)^{2+}$**	12.03932		1	Ga + HL ⇌ GaHL $\log_{10}(\beta)$ = 2.89 I = 3.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.50046 I = 3.0 M Ga + H + L ⇌ GaHL $\log_{10}(\beta)$ = 13.39046 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 12.03932
Ga^{3+} + 2 H^{+} + $(glutamate)^{2-}$ ⇌ **$GaH_2(glutamate)^{3+}$**	16.80000		1	Ga + H_2L ⇌ GaH_2L $\log_{10}(\beta)$ = 2.54 I = 3.0 M 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 15.07069 I = 3.0 M Ga + 2 H + L ⇌ GaH_2L $\log_{10}(\beta)$ = 17.61069 I = 3.0 M I = 0 M: $\log_{10}(\beta)$ = 16.80000
Sr^{2+} + $(glutamate)^{2-}$ ⇌ **Sr(glutamate) *(aq)***	2.22430		1	Original data for β: $\log_{10}(\beta)$ = 1.37, at I = 0.1 M.
Ag^{+} + $(glutamate)^{2-}$ ⇌ **$Ag(glutamate)^{-}$**	4.21715		1	Original data for β: $\log_{10}(\beta)$ = 3.79, at I = 0.1 M.
2 Ag^{+} + $(glutamate)^{2-}$ ⇌ **Ag_2(glutamate) *(aq)***	3.40073		1	Original data for β: $\log_{10}(\beta)$ = 2.76, at I = 0.1 M.
Cd^{2+} + $(glutamate)^{2-}$ ⇌ **Cd(glutamate) *(aq)***	4.65430		1	Original data for β: $\log_{10}(\beta)$ = 3.8, at I = 0.1 M.
Cd^{2+} + 2 $(glutamate)^{2-}$ ⇌ **$Cd(glutamate)_2^{2-}$**	7.58430		1	Original data for β: $\log_{10}(\beta)$ = 6.73, at I = 0.1 M.
Ba^{2+} + $(glutamate)^{2-}$ ⇌ **Ba(glutamate) *(aq)***	2.13430		1	Original data for β: $\log_{10}(\beta)$ = 1.28, at I = 0.1 M.
$Pb(II)^{2+}$ + $(glutamate)^{2-}$ ⇌ **Pb(II)(glutamate) *(aq)***	5.57355		1	Original data for β: $\log_{10}(\beta)$ = 4.5, at I = 0.5 M.
$Pb(II)^{2+}$ + 2 $(glutamate)^{2-}$ ⇌ **$Pb(II)(glutamate)_2^{2-}$**	7.61264		1	Original data for β: $\log_{10}(\beta)$ = 6.80, at I = 1.0 M.
$Pb(II)^{2+}$ + H^{+} + $(glutamate)^{2-}$ ⇌ **$Pb(II)H(glutamate)^{+}$**	12.33632		1	Pb(II) + HL ⇌ Pb(II)HL $\log_{10}(\beta)$ = 1.97 I = 1.0 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.55368 I = 1.0 M Pb(II) + H + L ⇌ Pb(II)HL $\log_{10}(\beta)$ = 11.52368 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 12. 33632
$(U(VI)O_2)^{2+}$ + H^{+} + $(glutamate)^{2-}$ ⇌ **$(U(VI)O_2)H(glutamate)^{+}$**	13.04715		1	(U(VI)O2) + HL ⇌ (U(VI)O2)HL $\log_{10}(\beta)$ = 2.66 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 9.53285 I = 0.1 M (U(VI)O2) + H + L ⇌ (U(VI)O2)HL $\log_{10}(\beta)$ = 12.19285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 13.04715

2.2.46. Glutamine

The ligand in its neutral form is L-2-Aminopentanedioic acid 5-amide (glutamine; $C_5H_{10}N_2O_3$). The ligand L as it is present in the database is the anion $C_5H_9N_2O_3^{-}$. Its molecular weight is 145.138. Its structural formula is shown on the right.
Do not mix up this one with glutamic acid / glutamate (previous section).

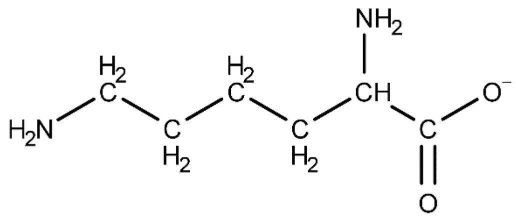


Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^{+} + $(glutamine)^{-}$ ⇌ **H(glutamine) *(aq)***	9.21358	-4.0E+4	1	Original data for β: $\log_{10}(\beta)$ = 9.00, at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + (glutamine)$^-$ ⇌ **H_2(glutamine)$^+$**	11.40358	-4.2E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.19 I = 0.1 M ΔH = -2E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.00 I = 0.1 M ΔH = -4.0E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.19 I = 0.1 M ΔH = -4.2E+4 I = 0 M: $log_{10}(\beta)$ = 11.40358
Al^{3+} + (glutamine)$^-$ ⇌ **Al(glutamine)$^{2+}$**	6.24073		1	Original data for β: $log_{10}(\beta)$ = 5.6, at I = 0.1 M.
Al^{3+} + $(OH)^-$ + (glutamine)$^-$ ⇌ **Al(OH)(glutamine)$^+$**	16.33130		1	AlL ⇌ Al(OH)L + H $log_{10}(\beta)$ = -4.28 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 5.6 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.78342 I = 0.1 M Al + OH + L ⇌ Al(OH)L $log_{10}(\beta)$ = 15.26342 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.33130
Mn(II)$^{2+}$ + (glutamine)$^-$ ⇌ **Mn(II)(glutamine)$^+$**	2.31954		1	Original data for β: $log_{10}(\beta)$ = 2.86, at I = 3.0 M.
Mn(II)$^{2+}$ + 2 (glutamine)$^-$ ⇌ **Mn(II)(glutamine)$_2$ *(aq)***	3.78931		1	Original data for β: $log_{10}(\beta)$ = 4.6, at I = 3.0 M.
Fe(II)$^{2+}$ + (glutamine)$^-$ ⇌ **Fe(II)(glutamine)$^+$**	3.88954		1	Original data for β: $log_{10}(\beta)$ = 4.43, at I = 3.0 M.
Fe(II)$^{2+}$ + 2 (glutamine)$^-$ ⇌ **Fe(II)(glutamine)$_2$ *(aq)***	6.44931		1	Original data for β: $log_{10}(\beta)$ = 7.26, at I = 3.0 M.
Fe(II)$^{2+}$ + 3 (glutamine)$^-$ ⇌ **Fe(II)(glutamine)$_3^-$**	9.58931		1	Original data for β: $log_{10}(\beta)$ = 10.40, at I = 3.0 M.
Co(II)$^{2+}$ + (glutamine)$^-$ ⇌ **Co(II)(glutamine)$^+$**	4.47715		1	Original data for β: $log_{10}(\beta)$ = 4.05, at I = 0.1 M.
Co(II)$^{2+}$ + 2 (glutamine)$^-$ ⇌ **Co(II)(glutamine)$_2$ *(aq)***	7.92073		1	Original data for β: $log_{10}(\beta)$ = 7.28, at I = 0.1 M.
Co(II)$^{2+}$ + 3 (glutamine)$^-$ ⇌ **Co(II)(glutamine)$_3^-$**	10.59931		1	Original data for β: $log_{10}(\beta)$ = 11.41, at I = 3.0 M.
Ni^{2+} + (glutamine)$^-$ ⇌ **Ni(glutamine)$^+$**	5.58715	-1.3E+4	1	Original data for β: $log_{10}(\beta)$ = 5.16, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 2 (glutamine)$^-$ ⇌ **Ni(glutamine)$_2$ *(aq)***	10.06073	-3.5E+4	1	Original data for β: $log_{10}(\beta)$ = 9.42, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 3 (glutamine)$^-$ ⇌ **Ni(glutamine)$_3^-$**	12.98931	-5.48E+4	1	Original data for β: $log_{10}(\beta)$ = 13.8, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Cu(II)$^{2+}$ + (glutamine)$^-$ ⇌ **Cu(II)(glutamine)$^+$**	8.12715	-2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 7.70, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (glutamine)$^-$ ⇌ **Cu(II)(glutamine)$_2$ *(aq)***	14.74073	-4.6E+4	1	Original data for β: $log_{10}(\beta)$ = 14.1, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + (glutamine)$^-$ ⇌ **Zn(glutamine)$^+$**	4.28954		1	Original data for β: $log_{10}(\beta)$ = 4.83, at I = 3.0 M.
Zn^{2+} + 2 (glutamine)$^-$ ⇌ **Zn(glutamine)$_2$ *(aq)***	8.35931		1	Original data for β: $log_{10}(\beta)$ = 9.17, at I = 3.0 M.
Zn^{2+} + 3 (glutamine)$^-$ ⇌ **Zn(glutamine)$_3^-$**	10.98931		1	Original data for β: $log_{10}(\beta)$ = 11.8, at I = 3.0 M.
Cd^{2+} + (glutamine)$^-$ ⇌ **Cd(glutamine)$^+$**	4.11883		1	Original data for β: $log_{10}(\beta)$ = 3.62, at I = 0.7 M.
Cd^{2+} + 2 (glutamine)$^-$ ⇌ **Cd(glutamine)$_2$ *(aq)***	7.40824		1	Original data for β: $log_{10}(\beta)$ = 6.66, at I = 0.7 M.
Cd^{2+} + 3 (glutamine)$^-$ ⇌ **Cd(glutamine)$_3^-$**	9.18931		1	Original data for β: $log_{10}(\beta)$ = 10.00, at I = 3.0 M.
Pb(II)$^{2+}$ + (glutamine)$^-$ ⇌ **Pb(II)(glutamine)$^+$**	4.15954		1	Original data for β: $log_{10}(\beta)$ = 4.70, at I = 3.0 M.
Pb(II)$^{2+}$ + 2 (glutamine)$^-$ ⇌ **Pb(II)(glutamine)$_2$ *(aq)***	7.58931		1	Original data for β: $log_{10}(\beta)$ = 8.4, at I = 3.0 M.
Pb(II)$^{2+}$ + 3 (glutamine)$^-$ ⇌ **Pb(II)(glutamine)$_3^-$**	9.28931		1	Original data for β: $log_{10}(\beta)$ = 10.1, at I = 3.0 M.

2.2.47. Lysine

The ligand in its neutral form is L-2,6-Diaminohexanoic acid (lysine; $C_6H_{14}N_2O_2$). The ligand L as it is present in the database is the anion $C_6H_{13}N_2O_2^-$. Its molecular weight is 145.182. Its structural formula is shown on the right.



Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(lysine)^-$ ⇌ **H(lysine)** ***(aq)***	10.82	-5.39E+4	1	Original data for ΔH at I = 0.1 M.
2 H^+ + $(lysine)^-$ ⇌ **H_2(lysine)$^+$**	19.89	-1.007E+5	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 9.07 ΔH = -4.68E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 10.82 ΔH = -5.39E+4 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 19.89 ΔH = -1.007E+5
3 H^+ + $(lysine)^-$ ⇌ **H_3(lysine)$^{2+}$**	21.66	-1.017E+5	1	H_2L + H ⇌ H_3L $\log_{10}(\beta)$ = 1.77 ΔH = -1E+3 (Original data for ΔH at I = 0.1 M) 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 19.89 ΔH = -1.007E+5 3 H + L ⇌ H_3L $\log_{10}(\beta)$ = 21.66 ΔH = -1.017E+5
Na^+ + $(lysine)^-$ ⇌ **Na(lysine)** ***(aq)***	-0.3		1	
Ca^{2+} + $(lysine)^-$ ⇌ **Ca(lysine)$^+$**	1.40		1	
Ca^{2+} + H^+ + $(lysine)^-$ ⇌ **CaH(lysine)$^{2+}$**	11.67		1	Ca + HL ⇌ CaHL $\log_{10}(\beta)$ = 0.85 H + L ⇌ HL $\log_{10}(\beta)$ = 10.82 Ca + H + L ⇌ CaHL $\log_{10}(\beta)$ = 11.67
Co(II)$^{2+}$ + H^+ + $(lysine)^-$ ⇌ **Co(II)H(lysine)$^{2+}$**	14.68000		1	Co(II) + HL ⇌ Co(II)HL $\log_{10}(\beta)$ = 3.86 I = 0.1 M H + L ⇌ HL $\log_{10}(\beta)$ = 10.60642 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $\log_{10}(\beta)$ = 14.46642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 14.68000
Co(II)$^{2+}$ + 2 $(lysine)^-$ ⇌ **Co(II)(lysine)$_2$** ***(aq)***	8.99357		1	Co(II)HL_2 ⇌ Co(II)L_2 + H $\log_{10}(\beta)$ = -10.04 I = 0.1 M Co(II) + H + 2 L ⇌ Co(II)HL_2 $\log_{10}(\beta)$ = 18.39284 I = 0.1 M Co(II) + H + 2 L ⇌ Co(II)HL_2 $\log_{10}(\beta)$ = 8.35284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 8.99357
Co(II)$^{2+}$ + H^+ + 2 $(lysine)^-$ ⇌ **Co(II)H(lysine)$_2^+$**	19.03357		1	Co(II)H_2L_2 ⇌ Co(II)HL_2 + H $\log_{10}(\beta)$ = -9.89 I = 0.1 M Co(II) + 2 H + 2 L ⇌ Co(II)H_2L_2 $\log_{10}(\beta)$ = 28.28284 I = 0.1 M Co(II) + H + 2 L ⇌ Co(II)HL_2 $\log_{10}(\beta)$ = 18.39284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.03357

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+}$ + 2 H^+ + 2 $(lysine)^-$ ⇌ **$Co(II)H_2(lysine)_2^{2+}$**	28.70999		1	Co(II) + 2 HL ⇌ $Co(II)H_2L_2$ $log_{10}(\beta)$ = 7.07 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 21.21284 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 28.28284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 28.70999
$Co(II)^{2+}$ + 2 H^+ + 3 $(lysine)^-$ ⇌ **$Co(II)H_2(lysine)_3^{+}$**	32.20356		1	$Co(II)H_3L_3$ ⇌ $Co(II)H_2L_3$ + H $log_{10}(\beta)$ = -9.9 I = 0.1 M Co(II) + 3 H + 3 L ⇌ $Co(II)H_3L_3$ $log_{10}(\beta)$ = 41.24926 I = 0.1 M Co(II) + 2 H + 3 L ⇌ $Co(II)H_2L_3$ $log_{10}(\beta)$ = 31.34926 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.20356
$Co(II)^{2+}$ + 3 H^+ + 3 $(lysine)^-$ ⇌ **$Co(II)H_3(lysine)_3^{2+}$**	41.88999		1	Co(II) + 3 HL ⇌ $Co(II)H_3L_3$ $log_{10}(\beta)$ = 9.43 I = 0.1 M 3 H + 3 L ⇌ 3 HL $log_{10}(\beta)$ = 31.81926 I = 0.1 M Co(II) + 3 H + 3 L ⇌ $Co(II)H_3L_3$ $log_{10}(\beta)$ = 41.24926 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 41.88999
Ni^{2+} + $(lysine)^-$ ⇌ **$Ni(lysine)^{+}$**	6.08357		1	NiHL ⇌ NiL + H $log_{10}(\beta)$ = -9.85 I = 0.1 M Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 15.50642 I = 0.1 M Ni + L ⇌ NiL $log_{10}(\beta)$ = 5.65642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 6.08357
Ni^{2+} + H^+ + $(lysine)^-$ ⇌ **$NiH(lysine)^{2+}$**	15.72000	-7.19E+4	1	Ni + HL ⇌ NiHL $log_{10}(\beta)$ = 4.90 I = 0.1 M ΔH = -1.8E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.60642 I = 0.1 M ΔH = -5.39E+4 Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 15.50642 I = 0.1 M ΔH = -7.19E+4 I = 0 M: $log_{10}(\beta)$ = 15.72000
Ni^{2+} + 2 $(lysine)^-$ ⇌ **$Ni(lysine)_2$ *(aq)***	11.05357		1	$NiHL_2$ ⇌ NiL_2 + H $log_{10}(\beta)$ = -10.1 I = 0.1 M Ni + H + 2 L ⇌ $NiHL_2$ $log_{10}(\beta)$ = 20.51284 I = 0.1 M Ni + 2 L ⇌ NiL_2 $log_{10}(\beta)$ = 10.41284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 11.05357
Ni^{2+} + H^+ + 2 $(lysine)^-$ ⇌ **$NiH(lysine)_2^{+}$**	21.15357	-1.049E+05	1	NiH_2L_2 ⇌ $NiHL_2$ + H $log_{10}(\beta)$ = -9.9 I = 0.1 M ΔH = -4.64E+4 (Original data for ΔH at I = 0.1 M) Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 30.41284 I = 0.1 M ΔH = -1.513E+05 Ni + H + 2 L ⇌ $NiHL_2$ $log_{10}(\beta)$ = 20.51284 I = 0.1 M ΔH = -1.049E+5 I = 0 M: $log_{10}(\beta)$ = 21.15357
Ni^{2+} + 2 H^+ + 2 $(lysine)^-$ ⇌ **$NiH_2(lysine)_2^{2+}$**	30.83999	-1.513E+5	1	Ni + 2 HL ⇌ NiH_2L_2 $log_{10}(\beta)$ = 9.20 I = 0.1 M ΔH = -4.35E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 21.21284 I = 0.1 M ΔH = -1.078E+5 Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 30.41284 I = 0.1 M ΔH = -1.513E+05 I = 0 M: $log_{10}(\beta)$ = 30.83999
Ni^{2+} + 3 $(lysine)^-$ ⇌ **$Ni(lysine)_3^{-}$**	13.15999		1	$NiHL_3$ ⇌ NiL_3 + H $log_{10}(\beta)$ = -10.9 I = 0.1 M Ni + H + 3 L ⇌ $NiHL_3$ $log_{10}(\beta)$ = 23.41926 I = 0.1 M Ni + 3 L ⇌ NiL_3 $log_{10}(\beta)$ = 12.51926 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.15999

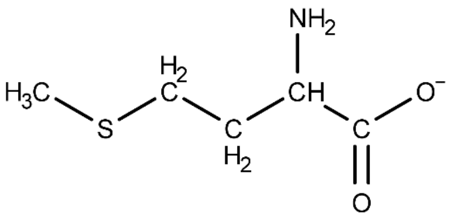
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ni^{2+} + H^+ + 3 $(lysine)^-$ ⇌ **$NiH(lysine)_3$ *(aq)***	24.27356		1	NiH_2L_3 ⇌ $NiHL_3$ + H $log_{10}(\beta)$ = -10.4 I = 0.1 M Ni + 2 H + 3 L ⇌ NiH_2L_3 $log_{10}(\beta)$ = 33.81926 I = 0.1 M Ni + H + 3 L ⇌ $NiHL_3$ $log_{10}(\beta)$ = 23.41926 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 24.27356
Ni^{2+} + 2 H^+ + 3 $(lysine)^-$ ⇌ **$NiH_2(lysine)_3^+$**	34.67356		1	NiH_3L_3 ⇌ NiH_2L_3 + H log10(β) = -10.0 I = 0.1 M Ni + 3 H + 3 L ⇌ NiH_3L_3 log10(β) = 43.81926 I = 0.1 M Ni + 2 H + 3 L ⇌ NiH_2L_3 log10(β) = 33.81926 I = 0.1 M I = 0 M: log10(β) = 34.67356
Ni^{2+} + 3 H^+ + 3 $(lysine)^-$ ⇌ **$NiH_3(lysine)_3^{2+}$**	44.45999	-2.165E+5	1	Ni + 3 HL ⇌ NiH_3L_3 $log_{10}(\beta)$ = 12.0 I = 0.1 M ΔH = -5.48E+4 (Original data for ΔH at I = 0.1 M) 3 H + 3 L ⇌ H_3L_3 $log_{10}(\beta)$ = 31.81926 I = 0.1 M ΔH = -1.078E+5 Ni + 3 H + 3 L ⇌ NiH_3L_3 $log_{10}(\beta)$ = 43.81926 I = 0.1 M ΔH = -2.165E+05 I = 0 M: $log_{10}(\beta)$ = 44.45999
$Cu(II)^{2+}$ + H^+ + $(lysine)^-$ ⇌ **$Cu(II)H(lysine)^{2+}$**	18.47000	-7.89E+4	1	Cu(II) + HL ⇌ Cu(II)HL $log_{10}(\beta)$ = 7.65 I = 0.1 M ΔH = -2.5E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.60642 I = 0.1 M ΔH = -5.39E+4 Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 18.25642 I = 0.1 M ΔH = -7.89E+4 I = 0 M: $log_{10}(\beta)$ = 18.47000
$Cu(II)^{2+}$ + $(lysine)^-$ ⇌ **$Cu(II)(lysine)_2$ *(aq)***	15.55357	-5.22E+4	1	$Cu(II)HL_2$ ⇌ $Cu(II)L_2$ + H $log_{10}(\beta)$ = -10.44 I = 0.1 M ΔH = 5.39E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + H + 2 L ⇌ $Cu(II)HL_2$ $log_{10}(\beta)$ = 25.35284 I = 0.1 M ΔH = -1.061E+5 Cu(II) + 2 L ⇌ $Cu(II)L_2$ $log_{10}(\beta)$ = 14.91284 I = 0.1 M ΔH = -5.22E+4 I = 0 M: $log_{10}(\beta)$ = 15.55357
$Cu(II)^{2+}$ + H^+ + 2 $(lysine)^-$ ⇌ **$Cu(II)H(lysine)_2^+$**	25.99357	-1.061E+5	1	$Cu(II)H_2L_2$ ⇌ $Cu(II)HL_2$ + H $log_{10}(\beta)$ = -9.94 I = 0.1 M ΔH = 5.31+4 (Original data for ΔH at I = 0.1 M) Cu(II) + 2 H + 2 L ⇌ $Cu(II)H_2L_2$ $log_{10}(\beta)$ = 35.29284 I = 0.1 M ΔH = -1.592E+5 Cu(II) + H + 2 L ⇌ $Cu(II)HL_2$ $log_{10}(\beta)$ = 25.35284 I = 0.1 M ΔH = -1.061E+5 I = 0 M: $log_{10}(\beta)$ = 25.99357

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(II)^{2+} + 2\ H^+ + 2\ (lysine)^- \rightleftharpoons$ **$Cu(II)H_2(lysine)_2^{2+}$**	35.71999	-1.592E+5	1	$Cu(II) + 2\ HL \rightleftharpoons Cu(II)H_2L_2$ $\log_{10}(\beta)$ = 14.08 I = 0.1 M ΔH = -5.14E+4 (Original data for ΔH at I = 0.1 M) $2\ H + 2\ L \rightleftharpoons H_2L_2$ $\log_{10}(\beta)$ = 21.21284 I = 0.1 M ΔH = -1.078E+5 $Cu(II) + 2\ H + 2\ L \rightleftharpoons Cu(II)H_2L_2$ $\log_{10}(\beta)$ = 35.29284 I = 0.1 M ΔH = -1.592E+5 I = 0 M: $\log_{10}(\beta)$ = 35.71999
$Zn^{2+} + (lysine)^- \rightleftharpoons$ **$Zn(lysine)^+$**	6.74357		1	$ZnHL \rightleftharpoons ZnL + H$ $\log_{10}(\beta)$ = -8.40 I = 0.1 M $Zn + H + L \rightleftharpoons ZnHL$ $\log_{10}(\beta)$ = 14.71642 I = 0.1 M $Zn + L \rightleftharpoons ZnL$ $\log_{10}(\beta)$ = 6.31642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ 6.74357
$Zn^{2+} + H^+ + (lysine)^- \rightleftharpoons$ **$ZnH(lysine)^{2+}$**	14.93000		1	$Zn + HL \rightleftharpoons ZnHL$ $\log_{10}(\beta)$ = 4.11 I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 10.60642 I = 0.1 M $Zn + H + L \rightleftharpoons ZnHL$ $\log_{10}(\beta)$ = 14.71642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 14.93000
$Zn^{2+} + H^+ + 2\ (lysine)^- \rightleftharpoons$ **$ZnH(lysine)_2^+$**	20.73357		1	$ZnH_2L_2 \rightleftharpoons ZnHL_2 + H$ $\log_{10}(\beta)$ = -9.11 I = 0.1 M $Zn + 2\ H + 2\ L \rightleftharpoons ZnH_2L_2$ $\log_{10}(\beta)$ = 29.20284 I = 0.1 M $Zn + H + 2\ L \rightleftharpoons ZnHL_2$ $\log_{10}(\beta)$ = 20.09284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.73357
$Zn^{2+} + 2\ H^+ + 2\ (lysine)^- \rightleftharpoons$ **$ZnH_2(lysine)_2^{2+}$**	29.62999		1	$Zn + 2\ HL \rightleftharpoons ZnH_2L_2$ $\log_{10}(\beta)$ = 7.99 I = 0.1 M $2\ H + 2\ L \rightleftharpoons H_2L_2$ $\log_{10}(\beta)$ = 21.21284 I = 0.1 M $Zn + 2\ H + 2\ L \rightleftharpoons ZnH_2L_2$ $\log_{10}(\beta)$ = 29.20284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 29.62999
$Ga^{3+} + (lysine)^- \rightleftharpoons$ **$Ga(lysine)^{2+}$**	17.64073		1	Original data for β: $\log_{10}(\beta)$ = 17.00, at I = 0.1 M.
$Ga^{3+} + H^+ + (lysine)^- \rightleftharpoons$ **$GaH(lysine)^{3+}$**	19.42000		1	$Ga + HL \rightleftharpoons GaHL$ $\log_{10}(\beta)$ = 8.60 I = 0.1 M $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 10.60642 I = 0.1 M $Ga + H + L \rightleftharpoons GaHL$ $\log_{10}(\beta)$ = 19.20642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.42000
$Ga^{3+} + 2\ H^+ + (lysine)^- \rightleftharpoons$ **$GaH_2(lysine)^{4+}$**	20.84927		1	$Ga + H_2L \rightleftharpoons GaH_2L$ $\log_{10}(\beta)$ = 1.60 I = 0.1 M $2\ H + L \rightleftharpoons H_2L$ $\log_{10}(\beta)$ = 19.67642 I = 0.1 M $Ga + H + L \rightleftharpoons GaHL$ $\log_{10}(\beta)$ = 21.27642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 20.84927
$Cd^{2+} + H^+ + (lysine)^- \rightleftharpoons$ **$CdH(lysine)^{2+}$**	13.88000		1	$Cd + HL \rightleftharpoons CdHL$ $\log_{10}(\beta)$ = 3.06 I = 0.15 M (Original data for β at T = 37°C) $H + L \rightleftharpoons HL$ $\log_{10}(\beta)$ = 10.58213 I = 0.15 M $Cd + H + L \rightleftharpoons CdHL$ $\log_{10}(\beta)$ = 13.64213 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 13.88000

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cd^{2+} + 2 $(lysine)^{-}$ ⇌ **$Cd(lysine)_2$ *(aq)***	8.43788		1	$CdHL_2$ ⇌ CdL_2 + H $log_{10}(\beta)$ = -9.78 I = 0.15 M (Original data for β at T = 37°C) $Cd + 2 H + 2 L$ ⇌ CdH_2L_2 $log_{10}(\beta)$ = 17.50426 I = 0.15 M $Cd + H + 2 L$ ⇌ $CdHL_2$ $log_{10}(\beta)$ = 7.72426 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 8.43788
Cd^{2+} + H^+ + 2 $(lysine)^{-}$ ⇌ **$CdH(lysine)_2^{+}$**	18.21788		1	CdH_2L_2 ⇌ $CdHL_2$ + H $log_{10}(\beta)$ = -9.43 I = 0.15 M (Original data for β at T = 37°C) $Cd + 2 H + 2 L$ ⇌ CdH_2L_2 $log_{10}(\beta)$ = 26.93426 I = 0.15 M $Cd + H + 2 L$ ⇌ $CdHL_2$ $log_{10}(\beta)$ = 17.50426 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 18.21788
Cd^{2+} + 2 H^+ + 2 $(lysine)^{-}$ ⇌ **$CdH_2(lysine)_2^{2+}$**	27.41001		1	$Cd + 2 HL$ ⇌ CdH_2L_2 $log_{10}(\beta)$ = 5.77 I = 0.15 M (Original data for β at T = 37°C) $2 H + 2 L$ ⇌ H_2L_2 $log_{10}(\beta)$ = 21.16426 I = 0.15 M $Cd + 2 H + 2 L$ ⇌ CdH_2L_2 $log_{10}(\beta)$ = 26.93426 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 27.41001

2.2.48. Methionine

The ligand in its neutral form is L-2-Amino-4-(methylthio)butanoic acid (methionine; $C_5H_{11}NO_2S$). The ligand L as it is present in the database is the anion $C_5H_{10}NO_2S^-$. Its molecular weight is 148.2. Its structural formula is shown on the right.



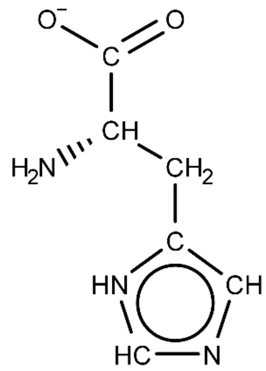
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(methionine)^{-}$ ⇌ **H(methionine) *(aq)***	9.29358	-4.30E+4	1	Original data for β: $log_{10}(\beta)$ = 9.08, at I = 0.1 M.
2 H^+ + $(methionine)^{-}$ ⇌ **$H_2(methionine)^{+}$**	11.47358	-4.5E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.18 I = 0.1 M ΔH = -2E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.08 I = 0.1 M ΔH = -4.30E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.26 I = 0.1 M ΔH = -4.5E+4 I = 0 M: $log_{10}(\beta)$ = 11.47358
Be^{2+} + 2 $(OH)^{-}$ + $(methionine)^{-}$ ⇌ **$Be(methionine)(OH)_2^{-}$**	21.45516		1	Original data for β: $log_{10}(\beta)$ = 20.65, at I = 0.5 M.
$Mn(II)^{2+}$ + $(methionine)^{-}$ ⇌ **$Mn(II)(methionine)^{+}$**	3.19715		1	Original data for β: $log_{10}(\beta)$ = 2.77, at I = 0.1 M.

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Mn(II)$^{2+}$ + 2 (methionine)$^{-}$ ⇌ **Mn(II)(methionine)$_2$ *(aq)***	5.21073		1	Original data for β: log$_{10}$(β) = 4.57, at I = 0.1 M.
Fe(II)$^{2+}$ + (methionine)$^{-}$ ⇌ **Fe(II)(methionine)$^{+}$**	3.64632		1	Original data for β: log$_{10}$(β) = 3.24, at I = 1.0 M and 20°C.
Fe(III)$^{3+}$ + (methionine)$^{-}$ ⇌ **Fe(III)(methionine)$^{2+}$**	9.70948		1	Original data for β: log$_{10}$(β) = 9.1, at I = 1.0 M and 20°C.
Co(II)$^{2+}$ + (methionine)$^{-}$ ⇌ **Co(II)(methionine)$^{+}$**	4.56715		1	Original data for β: log$_{10}$(β) = 4.14, at I = 0.1 M.
Co(II)$^{2+}$ + 2 (methionine)$^{-}$ ⇌ **Co(II)(methionine)$_2$ *(aq)***	8.23073		1	Original data for β: log$_{10}$(β) = 7.59, at I = 0.1 M.
Ni^{2+} + (methionine)$^{-}$ ⇌ **Ni(methionine)$^{+}$**	5.69715	-1.3E+4	1	Original data for β: log$_{10}$(β) = 5.27, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 (methionine)$^{-}$ ⇌ **Ni(methionine)$_2$ *(aq)***	10.44073	-3.5E+4	1	Original data for β: log$_{10}$(β) = 9.80, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 3 (methionine)$^{-}$ ⇌ **Ni(methionine)$_3^{-}$**	12.24073		1	Original data for β: log$_{10}$(β) = 11.6, at I = 0.1 M.
Cu(II)$^{2+}$ + (methionine)$^{-}$ ⇌ **Cu(II)(methionine)$^{+}$**	8.27715		1	Original data for β: log$_{10}$(β) = 7.85, at I = 0.1 M.
Cu(II)$^{2+}$ + 2 (methionine)$^{-}$ ⇌ **Cu(II)(methionine)$_2$ *(aq)***	15.14073		1	Original data for β: log$_{10}$(β) = 14.5, at I = 0.1 M.
Zn^{2+} + (methionine)$^{-}$ ⇌ **Zn(methionine)$^{+}$**	4.80715		1	Original data for β: log$_{10}$(β) = 4.38, at I = 0.1 M.
Zn^{2+} + 2 (methionine)$^{-}$ ⇌ **Zn(methionine)$_2$ *(aq)***	9.04073		1	Original data for β: log$_{10}$(β) = 8.40 at I = 0.1 M.
Ga^{3+} + (methionine)$^{-}$ ⇌ **Ga(methionine)$^{2+}$**	8.08931		1	Original data for β: log$_{10}$(β) = 8.9 at I = 3.0 M.
Ga^{3+} + H^{+} + (methionine)$^{-}$ ⇌ **GaH(methionine)$^{3+}$**	11.22977		1	GaL + H ⇌ GaHL log$_{10}$(β) = 2.6 I = 3.0 M Ga + L ⇌ GaL log$_{10}$(β) = 8.9 I = 3.0 M Ga + H + L ⇌ GaHL log$_{10}$(β) = 11.5 I = 3.0 M I = 0 M: log$_{10}$(β) = 11.22977
Ag^{+} + (methionine)$^{-}$ ⇌ **Ag(methionine) *(aq)***	5.45358		1	AgHL ⇌ AgL + H log$_{10}$(β) = -6.99 I = 0.1 M Ag + H + L ⇌ AgHL log$_{10}$(β) = 12.23 I = 0.1 M Ag + L ⇌ AgL log$_{10}$(β) = 5.24 I = 0.1 M I = 0 M: log$_{10}$(β) = 5.45358
Ag^{+} + H^{+} + (methionine)$^{-}$ ⇌ **AgH(methionine)$^{+}$**	12.44358		1	Ag + HL ⇌ AgHL log$_{10}$(β) = 3.15 I = 0.1 M H + L ⇌ HL log$_{10}$(β) = 9.08 I = 0.1 M Ag + H + L ⇌ AgHL log$_{10}$(β) = 12.23 I = 0.1 M I = 0 M: log$_{10}$(β) = 12.44358
Ag^{+} + 2 H^{+} + (methionine)$^{-}$ ⇌ **AgH$_2$(methionine)$^{2+}$**	14.07519		1	AgHL + H ⇌ AgH$_2$L log$_{10}$(β) = 1.9 I = 0.5 M Ag + H + L ⇌ AgHL log$_{10}$(β) = 12.17519 I = 0.5 M Ag + 2 H + L ⇌ AgH$_2$L log$_{10}$(β) = 14.07519 I = 0.5 M I = 0 M: log$_{10}$(β) = 14.07519
Ag^{+} + 2 (methionine)$^{-}$ ⇌ **Ag(methionine)$_2^{-}$**	8.61876		1	AgHL$_2$ ⇌ AgL$_2$ + H log$_{10}$(β) = -8.59 I = 0.5 M Ag + H + 2 L ⇌ AgHL$_2$ log$_{10}$(β) = 16.94037 I = 0.5 M Ag + 2 L ⇌ AgL$_2$ log$_{10}$(β) = 8.35037 I = 0.5 M I = 0 M: log$_{10}$(β) = 8.61876
Ag^{+} + H^{+} + 2 (methionine)$^{-}$ ⇌ **AgH(methionine)$_2$ *(aq)***	17.47715		1	AgH$_2$L$_2$ ⇌ AgHL$_2$ + H log$_{10}$(β) = -7.59 I = 0.5 M Ag + 2 H + 2 L ⇌ AgH$_2$L$_2$ log$_{10}$(β) = 24.53037 I = 0.5 M Ag + H + 2 L ⇌ AgHL$_2$ log$_{10}$(β) = 16.94037 I = 0.5 M I = 0 M: log$_{10}$(β) = 17.47715

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Ag^{+} + 2\ H^{+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$AgH_2(\text{methionine})_2^{+}$**	25.06715		1	$Ag + 2\ HL \rightleftharpoons AgH_2L_2$ $log_{10}(\beta) = 6.48$ I = 0.1 M $2\ H + 2\ L \rightleftharpoons 2\ HL$ $log_{10}(\beta) = 18.16$ I = 0.1 M $Ag + 2\ H + 2\ L \rightleftharpoons AgH_2L_2$ $log_{10}(\beta) = 24.64$ I = 0.1 M I = 0 M: $log_{10}(\beta) = 25.06715$
$Ag^{+} + 3\ H^{+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$AgH_3(\text{methionine})_2^{2+}$**	26.99876		1	$AgH_2L_2 + H \rightleftharpoons AgH_3L_2$ $log_{10}(\beta) = 2.20$ I = 0.5 M $Ag + 2\ H + 2\ L \rightleftharpoons AgH_2L_2$ $log_{10}(\beta) = 24.53037$ I = 0.5 M $Ag + 3\ H + 2\ L \rightleftharpoons AgH_3L_2$ $log_{10}(\beta) = 26.73037$ I = 0.5 M I = 0 M: $log_{10}(\beta) = 26.99876$
$Ag^{+} + 4\ H^{+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$AgH_4(\text{methionine})_2^{3+}$**	28.16198		1	$AgH_3L_2 + H \rightleftharpoons AgH_4L_2$ $log_{10}(\beta) = 1.7$ I = 0.5 M $Ag + 3\ H + 2\ L \rightleftharpoons AgH_3L_2$ $log_{10}(\beta) = 26.73037$ I = 0.5 M $Ag + 4\ H + 2\ L \rightleftharpoons AgH_4L_2$ $log_{10}(\beta) = 28.43037$ I = 0.5 M I = 0 M: $log_{10}(\beta) = 28.16198$
$2\ Ag^{+} + (\text{methionine})^{-} \rightleftharpoons$ **$Ag_2(\text{methionine})^{+}$**	7.72839		1	Original data for β: $log_{10}(\beta) = 7.46$ at I = 0.5 M.
$2\ Ag^{+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$Ag_2(\text{methionine})_2$ *(aq)***	6.56678		1	Original data for β: $log_{10}(\beta) = 6.03$ at I = 0.5 M.
$Cd^{2+} + (\text{methionine})^{-} \rightleftharpoons$ **$Cd(\text{methionine})^{+}$**	4.10715		1	Original data for β: $log_{10}(\beta) = 3.68$ at I = 0.1 M.
$Cd^{2+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$Cd(\text{methionine})_2$ *(aq)***	7.64073		1	Original data for β: $log_{10}(\beta) = 7.00$, at I = 0.1 M.
$Hg(II)^{2+} + (\text{methionine})^{-} \rightleftharpoons$ **$Hg(II)(\text{methionine})^{+}$**	6.94715		1	Original data for β: $log_{10}(\beta) = 6.52$, at I = 0.1 M.
$Hg(II)^{2+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$Hg(II)(\text{methionine})_2$ *(aq)***	12.09073		1	Original data for β: $log_{10}(\beta) = 11.45$, at I = 0.1 M.
$Pb(II)^{2+} + (\text{methionine})^{-} \rightleftharpoons$ **$Pb(II)(\text{methionine})^{+}$**	4.81715		1	Original data for β: $log_{10}(\beta) = 4.39$, at I = 0.1 M.
$Pb(II)^{2+} + 2\ (\text{methionine})^{-} \rightleftharpoons$ **$Pb(II)(\text{methionine})_2$ *(aq)***	9.26073		1	Original data for β: $log_{10}(\beta) = 8.62$, at I = 0.1 M.

2.2.49. Histidine

The ligand in its neutral form is L-2-Amino-3-(4-imidazolyl)propanoic acid (histidine; $C_6H_9N_3O_2$). The ligand L as it is present in the database is the anion $C_6H_8N_3O_2^{-}$. Its molecular weight is 154.149. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(histidine)^-$ ⇌ $H(histidine)$ *(aq)*	9.28	-4.39E+4	1	
2 H^+ + $(histidine)^-$ ⇌ $H_2(histidine)^+$	15.25	-7.29E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 5.97 ΔH = -2.9E+4 H + L ⇌ HL $log_{10}(\beta)$ = 9.28 ΔH = -4.39E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 15.25 ΔH = -7.29E+4
3 H^+ + $(histidine)^-$ ⇌ $H_3(histidine)^{2+}$	16.85	-7.70E+4	1	H_2L + H ⇌ H_3L $log_{10}(\beta)$ = 1.6 ΔH = -4.1E+3 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 15.25 ΔH = -7.29E+4 3 H + L ⇌ H_3L $log_{10}(\beta)$ = 16.85 ΔH = -7.70E+4
Be^{2+} + $(histidine)^-$ ⇌ $Be(histidine)^+$	6.70715		1	Original data for β: $log_{10}(\beta)$ = 6.28 at I = 0.1 M.
Be^{2+} + 2 $(histidine)^-$ ⇌ $Be(histidine)_2$ *(aq)*	11.62073		1	Original data for β: $log_{10}(\beta)$ = 10.98 at I = 0.1 M.
Na^+ + $(histidine)^-$ ⇌ $Na(histidine)$ *(aq)*	-0.5		1	
Al^{3+} + $(histidine)^-$ ⇌ $Al(histidine)^{2+}$	8.91516		1	Original data for β: $log_{10}(\beta)$ = 8.11 at I = 0.1 M.
Al^{3+} + $(OH)^-$ + $(histidine)^-$ ⇌ $Al(OH)(histidine)^+$	18.82055		1	AlL ⇌ Al(OH)L + H $log_{10}(\beta)$ = -4.36 I = 0.1 M Al + L ⇌ AlL $log_{10}(\beta)$ = 8.11 I = 0.1 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.72861 I = 0.1 M Al + OH + L ⇌ Al(OH)L $log_{10}(\beta)$ = 17.47861 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.82055
Ca^{2+} + $(histidine)^-$ ⇌ $Ca(histidine)^+$	1.63715	-4E+3	1	Original data for β: $log_{10}(\beta)$ = 6.28 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ca^{2+} + H^+ + $(histidine)^-$ ⇌ $CaH(histidine)^{2+}$	9.94000	-3.99E+4	1	Ca + HL ⇌ CaHL $log_{10}(\beta)$ = 0.66 I = 0.1 M ΔH = 4E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 9.06642 I = 0.1 M ΔH = -4.39E+4 Ca + H + L ⇌ CaHL $log_{10}(\beta)$ = 9.72642 I = 0.1 M ΔH = -3.99E+4 I = 0 M: $log_{10}(\beta)$ = 9.94000
$Mn(II)^{2+}$ + $(histidine)^-$ ⇌ $Mn(II)(histidine)^+$	3.74715	-1.1E+4	1	Original data for β: $log_{10}(\beta)$ = 3.32 at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Mn(II)^{2+}$ + 2 $(histidine)^-$ ⇌ $Mn(II)(histidine)_2$ *(aq)*	6.93073	-2.1E+4	1	Original data for β: $log_{10}(\beta)$ = 6.29 at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Fe(II)^{2+}$ + $(histidine)^-$ ⇌ $Fe(II)(histidine)^+$	5.33954	-1.8E+4	1	Original data for β: $log_{10}(\beta)$ = 5.88 at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Fe(II)^{2+}$ + 2 $(histidine)^-$ ⇌ $Fe(II)(histidine)_2$ *(aq)*	9.61931	-3.8E+4	1	Original data for β: $log_{10}(\beta)$ = 10.43 at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Fe(III)^{3+}$ + H^+ + $(histidine)^-$ ⇌ $Fe(III)H(histidine)^{3+}$	13.98000		1	Fe(III) + HL ⇌ Fe(III)HL $log_{10}(\beta)$ = 4.7 I = 0.1 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 9.06642 I = 0.1 M Fe(III) + H + L ⇌ Fe(III)HL $log_{10}(\beta)$ = 13.76642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 13.98000
$Co(II)^{2+}$ + $(histidine)^-$ ⇌ $Co(II)(histidine)^+$	7.29715	-2.3E+4	1	Original data for β: $log_{10}(\beta)$ = 6.87 at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Co(II)^{2+}$ + 2 $(histidine)^-$ ⇌ $Co(II)(histidine)_2$ *(aq)*	13.02073	-4.93E+4	1	Original data for β: $log_{10}(\beta)$ = 12.38 at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+}$ + H^+ + $(histidine)^-$ ⇌ **$Co(II)H(histidine)^{2+}$**	11.70358		1	Co(II)L + H ⇌ Co(II)HL $\log_{10}(\beta)$ = 4.62 I = 0.1 M Co(II) + L ⇌ Co(II)L $\log_{10}(\beta)$ = 6.87 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $\log_{10}(\beta)$ = 11.49 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 11.70358
$Co(II)^{2+}$ + H^+ + 2 $(histidine)^-$ ⇌ **$Co(II)H(histidine)_2^+$**	19.01073		1	$Co(II)L_2$ + H ⇌ $Co(II)HL_2$ $\log_{10}(\beta)$ = 5.99 I = 0.1 M Co(II) + 2 L ⇌ $Co(II)L_2$ $\log_{10}(\beta)$ = 12.38 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $\log_{10}(\beta)$ = 18.37 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 19.01073
$Co(II)^{2+}$ + $(OH)^-$ + $(histidine)^-$ ⇌ **$Co(II)(OH)(histidine)_2^-$**	15.30934		1	$Co(II)L_2$ ⇌ $Co(II)(OH)L_2$ + H $\log_{10}(\beta)$ = -11.44 I = 0.5 M Co(II) + 2 L ⇌ $Co(II)L_2$ $\log_{10}(\beta)$ = 12.21557 I = 0.5 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.72861 I = 0.5 M Co(II) + OH + 2 L ⇌ $Co(II)(OH)L_2$ $\log_{10}(\beta)$ = 14.50418 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 15.30934
Ni^{2+} + $(histidine)^-$ ⇌ **$Ni(histidine)^+$**	9.08715	-3.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.66 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + 2 $(histidine)^-$ ⇌ **$Ni(histidine)_2$ *(aq)***	16.16073	-6.90E+4	1	Original data for β: $\log_{10}(\beta)$ = 15.52 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + H^+ + $(histidine)^-$ ⇌ **$NiH(histidine)^{2+}$**	12.49358		1	NiL + H ⇌ NiHL $\log_{10}(\beta)$ = 3.62 I = 0.1 M Ni + L ⇌ NiL $\log_{10}(\beta)$ = 8.66 I = 0.1 M Ni + H + L ⇌ NiHL $\log_{10}(\beta)$ = 12.28 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 12.49358
Ni^{2+} + H^+ + 2 $(histidine)^-$ ⇌ **$NiH(histidine)_2^+$**	21.19073		1	NiL_2 + H ⇌ $NiHL_2$ $\log_{10}(\beta)$ = 5.03 I = 0.1 M Ni + 2 L ⇌ NiL_2 $\log_{10}(\beta)$ = 15.52 I = 0.1 M Ni + H + L ⇌ NiHL $\log_{10}(\beta)$ = 20.55 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 21.19073
Ni^{2+} + $(OH)^-$ + 2 $(histidine)^-$ ⇌ **$Ni(OH)(histidine)_2^-$**	19.79934		1	NiL_2 ⇌ $Ni(OH)L_2$ + H $\log_{10}(\beta)$ = -10.09 I = 0.5 M Ni + 2 L ⇌ NiL_2 $\log_{10}(\beta)$ = 15.35557 I = 0.5 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.72861 I = 0.5 M Ni + OH + 2 L ⇌ $Ni(OH)L_2$ $\log_{10}(\beta)$ = 18.99418 I = 0.5 M I = 0 M: $\log_{10}(\beta)$ = 19.79934
$Cu(I)^+$ + H^+ + $(histidine)^-$ ⇌ **$Cu(I)H(histidine)^+$**	12.30000		1	$Cu(I)H_2L$ ⇌ Cu(I)HL + H $\log_{10}(\beta)$ = -6.60 I = 0.1 M (Original data for β at T = 20°C) Cu(I) + 2 H + L ⇌ $Cu(I)H_2L$ $\log_{10}(\beta)$ = 18.68642 I = 0.1 M Cu(I) + H + L ⇌ Cu(I)HL $\log_{10}(\beta)$ = 12.08642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 12.30000
$Cu(I)^+$ + 2 H^+ + $(histidine)^-$ ⇌ **$Cu(I)H_2(histidine)^{2+}$**	18.68642		1	Cu(I) + H_2L ⇌ $Cu(I)H_2L$ $\log_{10}(\beta)$ = 3.65 I = 0.1 M (Original data for β at T = 20°C) 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 15.03642 I = 0.1 M Cu(I) + 2 H + L ⇌ $Cu(I)H_2L$ $\log_{10}(\beta)$ = 18.68642 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 18.68642

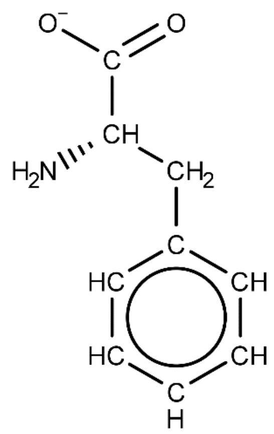
Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(I)^{+}$ + 4 H^{+} + 2 $(histidine)^{-}$ ⇌ **$Cu(I)H_4(histidine)_2^{3+}$**	36.75926		1	Cu(I) + 2 H_2L ⇌ $Cu(I)H_4L_2$ $\log_{10}(\beta)$ = 6.90 I = 0.1 M (Original data for β at T = 20°C) 4 H + 2 L ⇌ 2 H_2L $\log_{10}(\beta)$ = 30.07284 I = 0.1 M Cu(I) + 4 H + 2 L ⇌ $Cu(I)H_4L_2$ $\log_{10}(\beta)$ = 36.97284 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 36.75926
$Cu(II)^{2+}$ + $(histidine)^{-}$ ⇌ **$Cu(II)(histidine)^{+}$**	10.58715	-4.60E+4	1	Original data for β: $\log_{10}(\beta)$ = 10.16 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(histidine)^{-}$ ⇌ **$Cu(II)(histidine)_2$ *(aq)***	18.71073	-8.53E+4	1	Original data for β: $\log_{10}(\beta)$ = 18.07 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + H^{+} + $(histidine)^{-}$ ⇌ **$Cu(II)H(histidine)^{2+}$**	14.41358	-5.9E+4	1	Cu(II)L + H ⇌ Cu(II)HL $\log_{10}(\beta)$ = 4.04 I = 0.1 M ΔH = -1.3E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 10.16 I = 0.1 M ΔH = -4.6E+4 Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 14.20 I = 0.1 M ΔH = -5.9E+4 I = 0 M: $\log_{10}(\beta)$ = 14.41358
$Cu(II)^{2+}$ + H^{+} + 2 $(histidine)^{-}$ ⇌ **$Cu(II)H(histidine)_2^{+}$**	24.47073	-1.093E+5	1	$Cu(II)L_2$ + H ⇌ $Cu(II)HL_2$ $\log_{10}(\beta)$ = 5.76 I = 0.1 M ΔH = -2.4E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + 2 L ⇌ $Cu(II)L_2$ $\log_{10}(\beta)$ = 18.07 I = 0.1 M ΔH = -8.53E+4 Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 23.83 I = 0.1 M ΔH = -1.093E+5 I = 0 M: $\log_{10}(\beta)$ = 24.47073
$Cu(II)^{2+}$ + 2 H^{+} + 2 $(histidine)^{-}$ ⇌ **$Cu(II)H_2(histidine)_2^{2+}$**	27.65715	-1.173E+5	1	$Cu(II)HL_2$ + H ⇌ $Cu(II)H_2L_2$ $\log_{10}(\beta)$ = 3.4 I = 0.1 M ΔH = -8E+3 (Original data for ΔH at I = 0.1 M) Cu(II) + H + 2 L ⇌ $Cu(II)HL_2$ $\log_{10}(\beta)$ = 23.83 I = 0.1 M ΔH = -1.093E+5 Cu(II) + 2 H + L ⇌ $Cu(II)H_2L$ $\log_{10}(\beta)$ = 27.23 I = 0.1 M ΔH = -1.173E+5 I = 0 M: $\log_{10}(\beta)$ = 27.65715
$Cu(II)^{2+}$ + $(OH)^{-}$ + $(histidine)^{-}$ ⇌ **Cu(II)(OH)(histidine) *(aq)***	16.58415		1	Cu(II)L ⇌ Cu(II)(OH)L + H $\log_{10}(\beta)$ = -8.0 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 10.16 I = 0.1 M H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M Cu(II) + OH + L ⇌ Cu(II)(OH)L $\log_{10}(\beta)$ = 15.94342 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 16.58415
$Cu(II)^{2+}$ + $(OH)^{-}$ + 2 $(histidine)^{-}$ ⇌ **$Cu(II)(OH)(histidine)_2^{-}$**	21.09415	-9.511E+4	1	$Cu(II)L_2$ ⇌ $Cu(II)(OH)L_2$ + H $\log_{10}(\beta)$ = -11.4 I = 0.1 M ΔH = 4.6E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + 2 L ⇌ $Cu(II)L_2$ $\log_{10}(\beta)$ = 18.07 I = 0.1 M ΔH = -8.53E+4 H + OH ⇌ H_2O $\log_{10}(\beta)$ = 13.78342 I = 0.1 M ΔH = -5.581E+4 Cu(II) + OH + L ⇌ Cu(II)(OH)L $\log_{10}(\beta)$ = 20.45342 I = 0.1 M ΔH = -9.511E+4 I = 0 M: $\log_{10}(\beta)$ = 21.09415

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 $Cu(II)^{2+}$ + 2 $(OH)^-$ + 2 $(histidine)^-$ ⇌ **$Cu(II)_2(OH)_2(histidine)_2$ *(aq)***	20.84829	-9.662E+4	1	2 Cu(II) + 2 L ⇌ $Cu(II)_2(OH)L_2$ + 2 H $log_{10}(\beta)$ = -8.0 I = 0.1 M ΔH = 1.5E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 OH ⇌ 2 H_2O $log_{10}(\beta)$ = 27.56684 I = 0.1 M ΔH = -1.1162E+05 2 Cu(II) + 2 OH + 2 L ⇌ $Cu(II)_2(OH)_2L_2$ $log_{10}(\beta)$ = 19.56684 I = 0.1 M ΔH = -9.662E+4 I = 0 M: $log_{10}(\beta)$ = 20.84829
Zn^{2+} + $(histidine)^-$ ⇌ **$Zn(histidine)^+$**	6.93715	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 6.51 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 $(histidine)^-$ ⇌ **$Zn(histidine)_2$ *(aq)***	12.68073	-4.72E+4	1	Original data for β: $log_{10}(\beta)$ = 12.04 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + H^+ + $(histidine)^-$ ⇌ **$ZnH(histidine)^{2+}$**	11.58358	-7.42E+4	1	ZnL + H ⇌ ZnHL $log_{10}(\beta)$ = 4.86 I = 0.1 M ΔH = -2.7E+4 (Original data for ΔH at I = 0.1 M) Zn + L ⇌ ZnL $log_{10}(\beta)$ = 6.51 I = 0.1 M ΔH = -4.72E+4 Zn + H + L ⇌ ZnHL $log_{10}(\beta)$ = 11.37 I = 0.1 M ΔH = -7.42E+4 I = 0 M: $log_{10}(\beta)$ = 11.58358
Zn^{2+} + H^+ + 2 $(histidine)^-$ ⇌ **$ZnH(histidine)_2^+$**	18.48073		1	ZnL_2 + H ⇌ $ZnHL_2$ $log_{10}(\beta)$ = 5.80 I = 0.1 M Zn + 2 L ⇌ ZnL_2 $log_{10}(\beta)$ = 12.04 I = 0.1 M Zn + H + 2 L ⇌ $ZnHL_2$ $log_{10}(\beta)$ = 17.84 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 18.48073
Zn^{2+} + 2 H^+ + 2 $(histidine)^-$ ⇌ **$ZnH_2(histidine)_2^{2+}$**	23.93715		1	$ZnHL_2$ + H ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 5.67 I = 0.1 M Zn + H + 2 L ⇌ $ZnHL_2$ $log_{10}(\beta)$ = 17.84 I = 0.1 M Zn + 2 H + 2 L ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 23.51 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 23.93715
Zn^{2+} + $(OH)^-$ + 2 $(histidine)^-$ ⇌ **$Zn(OH)(histidine)_2^-$**	16.45934		1	ZnL_2 ⇌ $Zn(OH)L_2$ + H $log_{10}(\beta)$ = -9.95 I = 0.5 M Zn + 2 L ⇌ ZnL_2 $log_{10}(\beta)$ = 11.87557 I = 0.5 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.72861 I = 0.5 M Zn + OH + 2 L ⇌ $Zn(OH)L_2$ $log_{10}(\beta)$ = 15.65418 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 16.45934
Ga^{3+} + $(histidine)^-$ ⇌ **$Ga(histidine)^{2+}$**	11.68931		1	Original data for β: $log_{10}(\beta)$ = 12.50 at I = 3.0 M.
Ga^{3+} + H^+ + $(histidine)^-$ ⇌ **$GaH(histidine)^{3+}$**	14.78000		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 5.50 I = 3.0 M H + L ⇌ HL $log_{10}(\beta)$ = 9.55023 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 15.05023 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 14.78000
Ga^{3+} + 2 H^+ + $(histidine)^-$ ⇌ **$GaH_2(histidine)^{4+}$**	17.56069		1	Ga + H_2L ⇌ GaH_2L $log_{10}(\beta)$ = 1.50 I = 3.0 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 15.52023 I = 3.0 M Ga + 2 H + L ⇌ GaH_2L $log_{10}(\beta)$ = 17.02023 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 17.56069
Ag^+ + H^+ + $(histidine)^-$ ⇌ **$AgH(histidine)^+$**	12.41000		1	Ag + HL ⇌ AgHL log10(β) = 3.13 I = 0.1 M H + L ⇌ HL log10(β) = 9.06642 I = 0.1 M Ag + H + L ⇌ AgHL log10(β) = 12.19642 I = 0.1 M I = 0 M: log10(β) = 12.41000

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ag^+ + 2 H^+ + 2 (histidine)$^-$ ⇌ **AgH_2(histidine)$_2^+$**	25.40999		1	Ag + 2 HL ⇌ AgH_2L_2 $log_{10}(\beta)$ = 6.85 I = 0.1 M 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 18.13284 I = 0.1 M Ag + 2 H + 2 L ⇌ AgH_2L_2 $log_{10}(\beta)$ = 24.98284 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 25.40999
2 Ag^+ + 2 (histidine)$^-$ ⇌ **Ag_2(histidine)$_2$ *(aq)***	16.15715		1	Original data for β: $log_{10}(\beta)$ = 15.73 at I = 0.1 M.
Cd^{2+} + (histidine)$^-$ ⇌ **Cd(histidine)$^+$**	6.08715	-2.0E+4	1	Original data for β: $log_{10}(\beta)$ = 5.66 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cd^{2+} + 2 (histidine)$^-$ ⇌ **Cd(histidine)$_2$ *(aq)***	10.58073	-4.1E+4	1	Original data for β: $log_{10}(\beta)$ = 9.94 at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cd^{2+} + H^+ + (histidine)$^-$ ⇌ **CdH(histidine)$^{2+}$**	11.37358	-5.7E+4	1	CdL + H ⇌ CdHL $log_{10}(\beta)$ = 5.50 I = 0.1 M ΔH = -3.7E+4 (Original data for ΔH at I = 0.1 M) Cd + L ⇌ CdL $log_{10}(\beta)$ = 5.66 I = 0.1 M ΔH = -2.0E+4 Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 11.16 I = 0.1 M ΔH = -5.7E+4 I = 0 M: $log_{10}(\beta)$ = 11.37358
Cd^{2+} + (OH)$^-$ + (histidine)$^-$ ⇌ **Cd(OH)(histidine) *(aq)***	8.98414		1	CdL ⇌ Cd(OH)L + H $log_{10}(\beta)$ = -11.10 I = 0.5 M Cd + L ⇌ CdL $log_{10}(\beta)$ = 5.55037 I = 0.5 M H + OH ⇌ H_2O $log_{10}(\beta)$ = 13.72861 I = 0.5 M Cd + OH + 2 L ⇌ Cd(OH)L_2 $log_{10}(\beta)$ = 8.17898 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 8.98414
Nd^{3+} + (histidine)$^-$ ⇌ **Nd(histidine)$^{2+}$**	3.00073		1	Original data for β: $log_{10}(\beta)$ = 2.36 at I = 0.1 M.
Nd^{3+} + H^+ + (histidine)$^-$ ⇌ **NdH(histidine)$^{3+}$**	9.54000		1	Nd + HL ⇌ NdHL $log_{10}(\beta)$ = 0.26 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 9.06642 I = 0.1 M Nd + H + L ⇌ NdHL $log_{10}(\beta)$ = 9.32642 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 9.54000
Pb(II)$^{2+}$ + (histidine)$^-$ ⇌ **Pb(II)(histidine)$^+$**	6.36715		1	Original data for β: $log_{10}(\beta)$ = 5.94 at I = 0.1 M.
Pb(II)$^{2+}$ + 2 (histidine)$^-$ ⇌ **Pb(II)(histidine)$_2$ *(aq)***	10.75073		1	Original data for β: $log_{10}(\beta)$ = 10.11 at I = 0.1 M.
Pb(II)$^{2+}$ + H^+ + 2 (histidine)$^-$ ⇌ **Pb(II)H(histidine)$_2^+$**	17.79073		1	Pb(II)L_2 + H ⇌ Pb(II)HL_2 $log_{10}(\beta)$ = 7.04 I = 0.1 M Pb(II) + 2 L ⇌ Pb(II)L_2 $log_{10}(\beta)$ = 10.11 I = 0.1 M Pb(II) + H + 2 L ⇌ Pb(II)HL_2 $log_{10}(\beta)$ = 17.15 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 17.79073
Pb(II)$^{2+}$ + 2 H^+ + 2 (histidine)$^-$ ⇌ **Pb(II)H_2(histidine)$_2^{2+}$**	23.79715		1	Pb(II)HL_2 + H ⇌ Pb(II)H_2L_2 $log_{10}(\beta)$ = 6.22 I = 0.1 M Pb(II) + H + 2 L ⇌ Pb(II)HL_2 $log_{10}(\beta)$ = 17.15 I = 0.1 M Pb(II) + 2 H + 2 L ⇌ Pb(II)H_2L_2 $log_{10}(\beta)$ = 23.37 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 23.79715

2.2.50. Phenylalanine

The ligand in its neutral form is L-2-Amino-3-phenylpropanoic acid (phenylalanine; $C_9H_{11}NO_2$). The ligand L as it is present in the database is the anion $C_9H_{10}NO_2^-$. Its molecular weight is 164.184. Its structural formula is shown on the right.

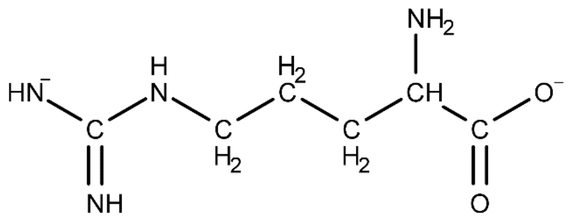


Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + (phenylalanine)$^-$ ⇌ **H(phenylalanine) *(aq)***	9.31	-4.47E+4	1	
2 H^+ + (phenylalanine)$^-$ ⇌ **H_2(phenylalanine)$^+$**	11.51	-4.67E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 2.20 ΔH = -2E+3 H + L ⇌ HL $log_{10}(\beta)$ = 9.31 ΔH = -4.47E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 11.51 ΔH = -4.67E+4
Mn(II)$^{2+}$ + (phenylalanine)$^-$ ⇌ **Mn(II)(phenylalanine)$^+$**	2.82715		1	Original data for β: $log_{10}(\beta)$ = 2.4, at I = 0.1 M.
Mn(II)$^{2+}$ + 2 (phenylalanine)$^-$ ⇌ **Mn(II)(phenylalanine)$_2$ *(aq)***	5.34073		1	Original data for β: $log_{10}(\beta)$ = 4.7, at I = 0.1 M.
Fe(II)$^{2+}$ + (phenylalanine)$^-$ ⇌ **Fe(II)(phenylalanine)$^+$**	3.19954		1	Original data for β: $log_{10}(\beta)$ = 3.74, at I = 3.0 M.
Fe(II)$^{2+}$ + 2 (phenylalanine)$^-$ ⇌ **Fe(II)(phenylalanine)$_2$ *(aq)***	6.37931		1	Original data for β: $log_{10}(\beta)$ = 7.19, at I = 3.0 M.
Fe(II)$^{2+}$ + 3 (phenylalanine)$^-$ ⇌ **Fe(II)(phenylalanine)$_3^-$**	9.88931		1	Original data for β: $log_{10}(\beta)$ = 10.7, at I = 3.0 M.
Fe(III)$^{3+}$ + (phenylalanine)$^-$ ⇌ **Fe(III)(phenylalanine)$^{2+}$**	9.57931		1	Original data for β: $log_{10}(\beta)$ = 10.39, at I = 3.0 M.
Fe(III)$^{3+}$ + 2 (phenylalanine)$^-$ ⇌ **Fe(III)(phenylalanine)$_2^+$**	17.75886		1	Original data for β: $log_{10}(\beta)$ = 19.11, at I = 3.0 M.
Fe(III)$^{3+}$ + 3 (phenylalanine)$^-$ ⇌ **Fe(III)(phenylalanine)$_3$ *(aq)***	24.37863		1	Original data for β: $log_{10}(\beta)$ = 26.0, at I = 3.0 M.
Co(II)$^{2+}$ + (phenylalanine)$^-$ ⇌ **Co(II)(phenylalanine)$^+$**	4.41715	-5.4E+3	1	Original data for β: $log_{10}(\beta)$ = 3.99, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+}$ + 2 $(phenylalanine)^-$ ⇌ **Co(II)(phenylalanine)$_2$ *(aq)***	8.14073	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 7.5, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Ni^{2+} + $(phenylalanine)^-$ ⇌ **Ni(phenylalanine)$^+$**	5.56	-1.3E+4	1	
Ni^{2+} + 2 $(phenylalanine)^-$ ⇌ **Ni(phenylalanine)$_2$ *(aq)***	10.22	-2.7E+4	1	
$Cu(II)^{2+}$ + $(phenylalanine)^-$ ⇌ **Cu(II)(phenylalanine)$^+$**	8.28	-2.2E+4	1	
$Cu(II)^{2+}$ + 2 $(phenylalanine)^-$ ⇌ **Cu(II)(phenylalanine)$_2$ *(aq)***	15.4	-4.89E+4	1	
Zn^{2+} + $(phenylalanine)^-$ ⇌ **Zn(phenylalanine)$^+$**	4.73715	-4.1E+3	1	Original data for β: $log_{10}(\beta)$ = 4.31, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 $(phenylalanine)^-$ ⇌ **Zn(phenylalanine)$_2$ *(aq)***	8.94073	-1.0E+4	1	Original data for β: $log_{10}(\beta)$ = 8.3, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Cd^{2+} + $(phenylalanine)^-$ ⇌ **Cd(phenylalanine)$^+$**	4.04715		1	Original data for β: $log_{10}(\beta)$ = 3.62, at I = 0.1 M.
Cd^{2+} + 2 $(phenylalanine)^-$ ⇌ **Cd(phenylalanine)$_2$ *(aq)***	7.46073		1	Original data for β: $log_{10}(\beta)$ = 6.82, at I = 0.1 M.
Cd^{2+} + 3 $(phenylalanine)^-$ ⇌ **Cd(phenylalanine)$_3^-$**	9.84073		1	Original data for β: $log_{10}(\beta)$ = 9.2, at I = 0.1 M.
$Pb(II)^{2+}$ + $(phenylalanine)^-$ ⇌ **Pb(II)(phenylalanine)$^+$**	4.08954		1	Original data for β: $log_{10}(\beta)$ = 4.63, at I = 3.0 M.
$Pb(II)^{2+}$ + 2 $(phenylalanine)^-$ ⇌ **Pb(II)(phenylalanine)$_2$ *(aq)***	7.53931		1	Original data for β: $log_{10}(\beta)$ = 8.35, at I = 3.0 M.

2.2.51. Arginine

The ligand in its neutral form is L-2-Amino-5-guanidopentanoic acid (arginine; $C_6H_{14}N_4O_2$). The ligand L as it is present in the database is the anion $C_6H_{12}N_4O_2^{\ 2-}$. Its molecular weight is 172.188. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(arginine)^{2-}$ ⇌ **H(arginine)$^-$**	12.52715		1	Original data for β: $log_{10}(\beta)$ = 12.1, at I = 0.1 M.
2 H^+ + $(arginine)^{2-}$ ⇌ **H_2(arginine) *(aq)***	21.51815		1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 8.991 H + L ⇌ HL $log_{10}(\beta)$ = 12.52715 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 21.51815

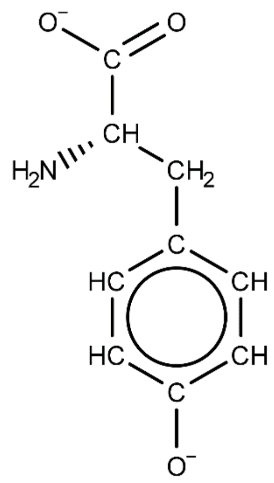
Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 H^+ + (arginine)$^{2-}$ ⇌ **H_3(arginine)$^+$**	23.34115		1	H_2L + H ⇌ H_3L $log_{10}(\beta)$ = 1.823 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 21.51815 3 H + L ⇌ H_3L $log_{10}(\beta)$ = 23.34115
Mg^{2+} + H^+ + (arginine)$^{2-}$ ⇌ **MgH(arginine)$^+$**	14.25430		1	Mg + HL ⇌ MgHL $log_{10}(\beta)$ = 1.30 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Mg + H + L ⇌ MgHL $log_{10}(\beta)$ = 13.4 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 14.25430
Fe(II)$^{2+}$ + H^+ + (arginine)$^{2-}$ ⇌ **Fe(II)H(arginine)$^+$**	15.81430		1	Fe(II) + HL ⇌ Fe(II)HL $log_{10}(\beta)$ = 2.86 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Fe(II) + H + L ⇌ Fe(II)HL $log_{10}(\beta)$ = 14.96 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 15.81430
Fe(III)$^{3+}$ + H^+ + (arginine)$^{2-}$ ⇌ **Fe(III)H(arginine)$^{2+}$**	21.83663		1	Fe(III) + HL ⇌ Fe(III)HL $log_{10}(\beta)$ = 8.7 I = 1.0 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 12.12083 I = 1.0 M Fe(III) + H + L ⇌ Fe(III)HL $log_{10}(\beta)$ = 20.82083 I = 1.0 M I = 0 M: $log_{10}(\beta)$ = 21.83663
Co(II)$^{2+}$ + H^+ + (arginine)$^{2-}$ ⇌ **Co(II)H(arginine)$^+$**	16.81430		1	Co(II) + HL ⇌ Co(II)HL $log_{10}(\beta)$ = 3.86 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 15.96 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.81430
Co(II)$^{2+}$ + 2 H^+ + 2 (arginine)$^{2-}$ ⇌ **Co(II)H_2(arginine)$_2$ *(aq)***	32.68503		1	Co(II) + 2 HL ⇌ Co(II)H_2L_2 $log_{10}(\beta)$ = 6.99 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Co(II) + 2 H + 2 L ⇌ Co(II)H_2L_2 $log_{10}(\beta)$ = 31.19 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.68503
Co(II)$^{2+}$ + 3 H^+ + 3 (arginine)$^{2-}$ ⇌ **Co(II)H_3(arginine)$_3^-$**	47.46218		1	Co(II) + 3 HL ⇌ Co(II)H_3L_3 $log_{10}(\beta)$ = 9.24 I = 0.1 M 3 H + 3 L ⇌ H_3L_3 $log_{10}(\beta)$ = 36.3 I = 0.1 M Co(II) + 2 H + 2 L ⇌ Co(II)H_2L_2 $log_{10}(\beta)$ = 45.54 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 47.46218
Ni^{2+} + H^+ + (arginine)$^{2-}$ ⇌ **NiH(arginine)$^+$**	17.88430		1	Ni + HL ⇌ NiHL $log_{10}(\beta)$ = 4.93 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 17.03 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 17.88430
Ni^{2+} + 2 H^+ + 2 (arginine)$^{2-}$ ⇌ **NiH_2(arginine)$_2$ *(aq)***	34.64503		1	Ni + 2 HL ⇌ NiH_2L_2 $log_{10}(\beta)$ = 8.95 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 33.15 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 34.64503
Ni^{2+} + 3 H^+ + 3 (arginine)$^{2-}$ ⇌ **NiH_3(arginine)$_3^-$**	50.34218		1	Ni + 3 HL ⇌ NiH_3L_3 $log_{10}(\beta)$ = 12.12 I = 0.1 M 3 H + 3 L ⇌ H_3L_3 $log_{10}(\beta)$ = 36.3 I = 0.1 M Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 48.42 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 50.34218

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Cu(II)^{2+}$ + H^+ + $(arginine)^{2-}$ ⇌ **$Cu(II)H(arginine)^+$**	20.45430		1	Cu(II) + HL ⇌ Cu(II)HL $log_{10}(\beta)$ = 7.50 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL $log_{10}(\beta)$ = 19.6 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 20.45430
$Cu(II)^{2+}$ + 2 H^+ + 2 $(arginine)^{2-}$ ⇌ **$Cu(II)H_2(arginine)_2$** ***(aq)***	39.49503		1	Cu(II) + 2 HL ⇌ $Cu(II)H_2L_2$ $log_{10}(\beta)$ = 13.8 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Cu(II) + 2 H + 2 L ⇌ $Cu(II)H_2L_2$ $log_{10}(\beta)$ = 38.0 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 39.49503
2 $Cu(II)^{2+}$ + 2 $(OH)^-$ + 2 $(arginine)^{2-}$ ⇌ **$Cu(II)_2(OH)_2(arginine)_2^{2-}$**	32.35338		1	2 Cu(II) + 2 L ⇌ $Cu(II)2(OH)_2L_2$ $log_{10}(\beta)$ = 3.17 I = 0.15 M (Original data for β at T = 37°C) 2 H + 2 OH ⇌ 2 H_2O $log_{10}(\beta)$ = 27.51826 I = 0.15 M Cu(II) + 2 H + 2 L ⇌ $Cu(II)H_2L_2$ $log_{10}(\beta)$ = 30.68826 I = 0.15 M I = 0 M: $log_{10}(\beta)$ = 32.35338
Zn^{2+} + H^+ + $(arginine)^{2-}$ ⇌ **$ZnH(arginine)^+$**	17.05430		1	Zn + HL ⇌ ZnHL $log_{10}(\beta)$ = 4.10 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Zn + H + L ⇌ ZnHL $log_{10}(\beta)$ = 16.2 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 17.05430
Zn^{2+} + 2 H^+ + 2 $(arginine)^{2-}$ ⇌ **$ZnH_2(arginine)_2$** ***(aq)***	33.72503		1	Zn + 2 HL ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 8.03 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Zn + 2 H + 2 L ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 32.23 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 33.72503
Ga^{3+} + $(arginine)^{2-}$ ⇌ **$Ga(arginine)^+$**	21.28145		1	Original data for β: $log_{10}(\beta)$ = 20.00, at I = 0.1 M.
Ga^{3+} + H^+ + $(arginine)^{2-}$ ⇌ **$GaH(arginine)^{2+}$**	21.76788		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 8.60 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 20.7 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.76788
Ga^{3+} + 2 H^+ + $(arginine)^{2-}$ ⇌ **$GaH_2(arginine)^{3+}$**	23.41815		1	Ga + H_2L ⇌ GaH_2L $log_{10}(\beta)$ = 1.90 I = 0.1 M 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 20.87742 I = 0.1 M Ga + 2 H + 2 L ⇌ GaH_2L_2 $log_{10}(\beta)$ = 22.77742 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 23.41815
Cd^{2+} + H^+ + $(arginine)^{2-}$ ⇌ **$CdH(arginine)^+$**	16.22430		1	Cd + HL ⇌ CdHL $log_{10}(\beta)$ = 3.27 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 15.37 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 16.22430
Cd^{2+} + 2 H^+ + 2 $(arginine)^{2-}$ ⇌ **$CdH_2(arginine)_2$** ***(aq)***	32.14503		1	Cd + 2 HL ⇌ CdH_2L_2 $log_{10}(\beta)$ = 6.45 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Cd + 2 H + 2 L ⇌ CdH_2L_2 $log_{10}(\beta)$ = 30.65 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.14503
$Hg(II)^{2+}$ + H^+ + $(arginine)^{2-}$ ⇌ **$Hg(II)H(arginine)^+$**	18.29430		1	Hg(II) + HL ⇌ Hg(II)HL $log_{10}(\beta)$ = 5.34 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 12.1 I = 0.1 M Hg(II) + H + L ⇌ Hg(II)HL $log_{10}(\beta)$ = 17.44 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 17.05430

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Hg(II)^{2+}$ + 2 H^+ + 2 $(arginine)^{2-}$ ⇌ **$Hg(II)H_2(arginine)_2$ *(aq)***	35.90503		1	Hg(II) + 2 HL ⇌ $Hg(II)H_2L_2$ $log_{10}(\beta)$ = 10.21 I = 0.1 M 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 24.2 I = 0.1 M Hg(II) + 2 H + 2 L ⇌ $Hg(II)H_2L_2$ $log_{10}(\beta)$ = 34.41 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 33.72503

2.2.52. Tyrosine

The ligand in its neutral form is L-2-Amino-3-(4-hydroxyphenyl)propanoic acid (tyrosine; $C_9H_{11}NO_3$). The ligand L as it is present in the database is the anion $C_9H_9NO_3{}^{2-}$. Its molecular weight is 179.175. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
H^+ + $(tyrosine)^{2-}$ ⇌ **$H(tyrosine)^-$**	10.47	-2.6E+4	1	Original data for ΔH at I = 0.1 M.
2 H^+ + $(tyrosine)^{2-}$ ⇌ **$H_2(tyrosine)$ *(aq)***	19.66	-6.6E+4	1	HL + H ⇌ H_2L $log_{10}(\beta)$ = 9.19 ΔH = -4.0E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.47 ΔH = -2.6E+4 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 19.66 ΔH = -6.6E+4
3 H^+ + $(tyrosine)^{2-}$ ⇌ **$H_3(tyrosine)^+$**	21.90000	-6.7E+4	1	H_2L + H ⇌ H_3L $log_{10}(\beta)$ = 2.24 I = 0.1 M ΔH = -1E+3 (Original data for ΔH at I = 0.1 M) 2 H + L ⇌ H_2L $log_{10}(\beta)$ = 19.01927 I = 0.1 M ΔH = -6.6E+4 3 H + L ⇌ H_3L $log_{10}(\beta)$ = 21.25927 I = 0.1 M ΔH = -6.7E+4 I = 0 M: $log_{10}(\beta)$ = 21.90000

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ca^{2+} + $(tyrosine)^{2-}$ ⇌ **Ca(tyrosine)** ***(aq)***	11.95		1	
$Mn(II)^{2+}$ + H^{+} + $(tyrosine)^{2-}$ ⇌ **$Mn(II)H(tyrosine)^{+}$**	14.03715	-2.8E+4	1	Mn(II) + HL ⇌ Mn(II)HL $log_{10}(\beta)$ = 3.14 I = 0.1 M ΔH = -2E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.04285 I = 0.1 M ΔH = -2.6E+4 Mn(II) + H + L ⇌ Mn(II)HL $log_{10}(\beta)$ = 13.18285 I = 0.1 M ΔH = -2.8E+4 I = 0 M: $log_{10}(\beta)$ = 14.03715
$Mn(II)^{2+}$ + 2 $(tyrosine)^{2-}$ ⇌ **$Mn(II)(tyrosine)_2^{2-}$**	7.74000	6E+3	1	$Mn(II)HL_2$ ⇌ $Mn(II)L_2$ + H $log_{10}(\beta)$ = -10.1 I = 0.1 M ΔH = 4E+4 (Original data for ΔH at I = 0.1 M) Mn(II) + H + 2 L ⇌ $Mn(II)HL_2$ $log_{10}(\beta)$ = 16.98570 I = 0.1 M ΔH = -3.4E+4 Mn(II) + 2 L ⇌ $Mn(II)L_2$ $log_{10}(\beta)$ = 6.88570 I = 0.1 M ΔH = 6E+3 I = 0 M: $log_{10}(\beta)$ = 7.74000
$Mn(II)^{2+}$ + H^{+} + 2 $(tyrosine)^{2-}$ ⇌ **$Mn(II)H(tyrosine)_2^{-}$**	18.26715	-3.4E+4	1	$Mn(II)H_2L_2$ ⇌ $Mn(II)HL_2$ + H $log_{10}(\beta)$ = -8.9 I = 0.1 M ΔH = 2.3E+4 (Original data for ΔH at I = 0.1 M) Mn(II) + 2 H + 2 L ⇌ $Mn(II)H_2L_2$ $log_{10}(\beta)$ = 25.88570 I = 0.1 M ΔH = -5.7E+4 Mn(II) + H + 2 L ⇌ $Mn(II)HL_2$ $log_{10}(\beta)$ = 16.98570 I = 0.1 M ΔH = -3.4E+4 I = 0 M: $log_{10}(\beta)$ = 18.26715
$Mn(II)^{2+}$ + 2 H^{+} + 2 $(tyrosine)^{2-}$ ⇌ **$Mn(II)H_2(tyrosine)_2$** ***(aq)***	27.38073	-5.E+4	1	Mn(II) + 2 HL ⇌ $Mn(II)H_2L_2$ $log_{10}(\beta)$ = 5.8 I = 0.1 M ΔH = -5E+3 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.2E+4 Mn(II) + 2 H + 2 L ⇌ $Mn(II)H_2L_2$ $log_{10}(\beta)$ = 25.88570 I = 0.1 M ΔH = -5.7E+4 I = 0 M: $log_{10}(\beta)$ = 27.38073
$Co(II)^{2+}$ + $(tyrosine)^{2-}$ ⇌ **Co(II)(tyrosine)** ***(aq)***	5.60715		1	Co(II) + HL ⇌ Co(II)L + H $log_{10}(\beta)$ = -9.29 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 14.04285 I = 0.1 M Co(II) + L ⇌ Co(II)L $log_{10}(\beta)$ = 4.75285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 5.60715
$Co(II)^{2+}$ + H^{+} + $(tyrosine)^{2-}$ ⇌ **$Co(II)H(tyrosine)^{+}$**	14.89715		1	Co(II) + HL ⇌ Co(II)HL $log_{10}(\beta)$ = 4.0 I = 0.1 M H + L ⇌ HL $log_{10}(\beta)$ = 10.04285 I = 0.1 M Co(II) + H + L ⇌ Co(II)HL $log_{10}(\beta)$ = 14.04285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 14.89715
$Co(II)^{2+}$ + 2 $(tyrosine)^{2-}$ ⇌ **$Co(II)(tyrosine)_2^{2-}$**	9.34000	4.8E+3	1	$Co(II)HL_2$ ⇌ $Co(II)L_2$ + H $log_{10}(\beta)$ = -9.9 I = 0.1 M ΔH = 4.18E+4 (Original data for ΔH at I = 0.1 M) Co(II) + H + 2 L ⇌ $Co(II)HL_2$ $log_{10}(\beta)$ = 18.38570 I = 0.1 M ΔH = -3.7E+4 Co(II) + 2 L ⇌ $Co(II)L_2$ $log_{10}(\beta)$ = 8.48570 I = 0.1 M ΔH = 4.8E+3 I = 0 M: $log_{10}(\beta)$ = 9.34000

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+} + H^{+} + 2\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)H(tyrosine)_2^{-}$**	19.66715	-3.7E+4	1	$Co(II)H_2L_2 \rightleftharpoons Co(II)HL_2 + H$ $log_{10}(\beta)$ = -9.2 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 0.1 M) $Co(II) + 2\ H + 2\ L \rightleftharpoons Co(II)H_2L_2$ $log_{10}(\beta)$ = 27.58570 I = 0.1 M ΔH = -6.2E+4 $Co(II) + H + 2\ L \rightleftharpoons Co(II)HL_2$ $log_{10}(\beta)$ = 18.38570 I = 0.1 M ΔH = -3.7E+4 I = 0 M: $log_{10}(\beta)$ = 19.66715
$Co(II)^{2+} + 2\ H^{+} + 2\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)H_2(tyrosine)_2$ *(aq)***	29.08073	-6.2E+4	1	$Co(II) + 2\ HL \rightleftharpoons Co(II)H_2L_2$ $log_{10}(\beta)$ = 7.5 I = 0.1 M ΔH = -1E+4 (Original data for ΔH at I = 0.1 M) $2\ H + 2\ L \rightleftharpoons H_2L_2$ $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.2E+4 $Co(II) + 2\ H + 2\ L \rightleftharpoons Co(II)H_2L_2$ $log_{10}(\beta)$ = 27.58570 I = 0.1 M ΔH = -6.2E+4 I = 0 M: $log_{10}(\beta)$ = 29.08073
$Co(II)^{2+} + 3\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)(tyrosine)_3^{4-}$**	11.02855		1	$Co(II)HL_3 \rightleftharpoons Co(II)L_3 + H$ $log_{10}(\beta)$ = -10.0 I = 0.1 M $Co(II) + H + 3\ L \rightleftharpoons Co(II)HL_3$ $log_{10}(\beta)$ = 21.02855 I = 0.1 M $Co(II) + 3\ L \rightleftharpoons Co(II)L_3$ $log_{10}(\beta)$ = 11.02855 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 11.02855
$Co(II)^{2+} + H^{+} + 3\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)H(tyrosine)_3^{3-}$**	21.88285		1	$Co(II)H_2L_3 \rightleftharpoons Co(II)HL_3 + H$ $log_{10}(\beta)$ = -9.9 I = 0.1 M $Co(II) + 2\ H + 3\ L \rightleftharpoons Co(II)H_2L_3$ $log_{10}(\beta)$ = 30.92855 I = 0.1 M $Co(II) + H + 3\ L \rightleftharpoons Co(II)HL_3$ $log_{10}(\beta)$ = 21.02855 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 21.88285
$Co(II)^{2+} + 2\ H^{+} + 3\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)H_2(tyrosine)_3^{2-}$**	32.42358		1	$Co(II)H_3L_3 \rightleftharpoons Co(II)H_2L_3 + H$ $log_{10}(\beta)$ = -9.6 I = 0.1 M $Co(II) + 3\ H + 3\ L \rightleftharpoons Co(II)H_3L_3$ $log_{10}(\beta)$ = 40.52855 I = 0.1 M $Co(II) + 2\ H + 3\ L \rightleftharpoons Co(II)H_2L_3$ $log_{10}(\beta)$ = 30.92855 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 32.42358
$Co(II)^{2+} + 3\ H^{+} + 3\ (tyrosine)^{2-} \rightleftharpoons$ **$Co(II)H_3(tyrosine)_3^{-}$**	42.45073		1	$Co(II) + 3\ HL \rightleftharpoons Co(II)H_3L_3$ $log_{10}(\beta)$ = 10.4 I = 0.1 M $3\ H + 3\ L \rightleftharpoons H_3L_3$ $log_{10}(\beta)$ = 30.12855 I = 0.1 M $Co(II) + 3\ H + 3\ L \rightleftharpoons Co(II)H_3L_3$ $log_{10}(\beta)$ = 40.52855 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 42.45073
$Ni^{2+} + (tyrosine)^{2-} \rightleftharpoons$ **Ni(tyrosine) *(aq)***	6.61715		1	Ni + HL ⇌ NiL + H $log_{10}(\beta)$ = -9.35 I = 0.1 M Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 15.11285 I = 0.1 M Ni + L ⇌ NiL $log_{10}(\beta)$ = 5.76285 I = 0.1 M I = 0 M: $log_{10}(\beta)$ = 6.61715
$Ni^{2+} + H^{+} + (tyrosine)^{2-} \rightleftharpoons$ **$NiH(tyrosine)^{+}$**	15.96715	-3.6E+4	1	Ni + HL ⇌ NiHL $log_{10}(\beta)$ = 5.07 I = 0.1 M ΔH = -1E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.04285 I = 0.1 M ΔH = -2.6E+4 Ni + H + L ⇌ NiHL $log_{10}(\beta)$ = 15.11285 I = 0.1 M ΔH = -3.6E+4 I = 0 M: $log_{10}(\beta)$ = 15.96715

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ni^{2+} + 2 $(tyrosine)^{2-}$ ⇌ **$Ni(tyrosine)_2^{2-}$**	11.09000	-2.9E+4	1	$NiHL_2$ ⇌ NiL_2 + H $log_{10}(\beta)$ = -9.85 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 0.1 M) Ni + H + 2 L ⇌ $NiHL_2$ $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.4E+4 Ni + 2 L ⇌ NiL_2 $log_{10}(\beta)$ = 10.23570 I = 0.1 M ΔH = -2.9E+4 I = 0 M: $log_{10}(\beta)$ = 11.09000
Ni^{2+} + H^+ + 2 $(tyrosine)^{2-}$ ⇌ **$NiH(tyrosine)_2^-$**	21.36715	-5.4E+4	1	NiH_2L_2 ⇌ $NiHL_2$ + H $log_{10}(\beta)$ = -9.4 I = 0.1 M ΔH = 2.3E+4 (Original data for ΔH at I = 0.1 M) Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 29.48570 I = 0.1 M ΔH = -7.7E+4 Ni + H + 2 L ⇌ $NiHL_2$ $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.4E+4 I = 0 M: $log_{10}(\beta)$ = 21.36715
Ni^{2+} + 2 H^+ + 2 $(tyrosine)^{2-}$ ⇌ **$NiH_2(tyrosine)_2$ *(aq)***	30.98073	-7.7E+4	1	Ni + 2 HL ⇌ NiH_2L_2 $log_{10}(\beta)$ = 9.4 I = 0.1 M ΔH = -2.5E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.2E+4 Ni + 2 H + 2 L ⇌ NiH_2L_2 $log_{10}(\beta)$ = 29.48570 I = 0.1 M ΔH = -7.7E+4 I = 0 M: $log_{10}(\beta)$ = 30.98073
Ni^{2+} + 3 $(tyrosine)^{2-}$ ⇌ **$Ni(tyrosine)_3^{4-}$**	13.42855	-5.38E+4	1	$NiHL_3$ ⇌ NiL_3 + H $log_{10}(\beta)$ = -10.2 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 0.1 M) Ni + H + 3 L ⇌ $NiHL_3$ $log_{10}(\beta)$ = 23.62855 I = 0.1 M ΔH = -7.88E+4 Ni + 3 L ⇌ NiL_3 $log_{10}(\beta)$ = 13.42855 I = 0.1 M ΔH = -5.38E+4 I = 0 M: $log_{10}(\beta)$ = 13.42855
Ni^{2+} + H^+ + 3 $(tyrosine)^{2-}$ ⇌ **$NiH(tyrosine)_3^{3-}$**	24.48285	-7.88E+4	1	NiH_2L_3 ⇌ $NiHL_3$ + H $log_{10}(\beta)$ = -9.8 I = 0.1 M ΔH = 2.3E+4 (Original data for ΔH at I = 0.1 M) Ni + 2 H + 3 L ⇌ NiH_2L_3 $log_{10}(\beta)$ = 33.42855 I = 0.1 M ΔH = -1.018E+5 Ni + H + 3 L ⇌ $NiHL_3$ $log_{10}(\beta)$ = 23.62855 I = 0.1 M ΔH = -7.88E+4 I = 0 M: $log_{10}(\beta)$ = 24.48285
Ni^{2+} + 2 H^+ + 3 $(tyrosine)^{2-}$ ⇌ **$NiH_2(tyrosine)_3^{2-}$**	34.92358	-1.018E+5	1	NiH_3L_3 ⇌ NiH_2L_3 + H $log_{10}(\beta)$ = -9.2 I = 0.1 M ΔH = 1.8E+4 (Original data for ΔH at I = 0.1 M) Ni + 3 H + 3 L ⇌ NiH_3L_3 $log_{10}(\beta)$ = 42.62855 I = 0.1 M ΔH = -1.198E+5 Ni + 2 H + 3 L ⇌ NiH_2L_3 $log_{10}(\beta)$ = 33.42855 I = 0.1 M ΔH = -1.018E+5 I = 0 M: $log_{10}(\beta)$ = 34.92358
Ni^{2+} + 3 H^+ + 3 $(tyrosine)^{2-}$ ⇌ **$NiH_3(tyrosine)_3^-$**	44.55073	-1.198E+5	1	Ni + 3 HL ⇌ NiH_3L_3 $log_{10}(\beta)$ = 12.5 I = 0.1 M ΔH = -4.18E+4 (Original data for ΔH at I = 0.1 M) 3 H + 3 L ⇌ H_3L_3 $log_{10}(\beta)$ = 30.12855 I = 0.1 M ΔH = -7.8E+4 Ni + 3 H + 3 L ⇌ NiH_3L_3 $log_{10}(\beta)$ = 42.62855 I = 0.1 M ΔH = -1.198E+5 I = 0 M: $log_{10}(\beta)$ = 44.55073

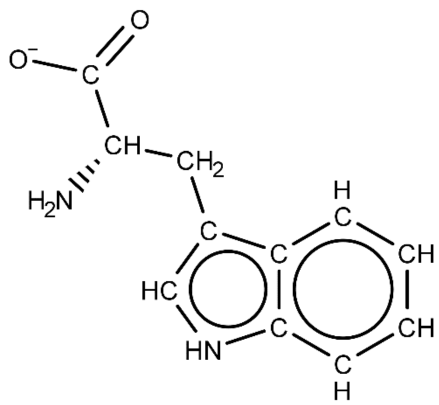
Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Cu(II)$^{2+}$ + (tyrosine)$^{2-}$ ⇌ **Cu(II)(tyrosine) *(aq)***	11.38715		1	Cu(II) + HL ⇌ Cu(II)L + H $\log_{10}(\beta)$ = -7.35 I = 0.1 M Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 17.88285 I = 0.1 M Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 10.53285 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 11.38715
Cu(II)$^{2+}$ + H^{+} + (tyrosine)$^{2-}$ ⇌ **Cu(II)H(tyrosine)$^{+}$**	18.73715	-4.9E+4	1	Cu(II) + HL ⇌ Cu(II)HL $\log_{10}(\beta)$ = 7.84 I = 0.1 M ΔH = -2.3E+4 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 10.04285 I = 0.1 M ΔH = -2.6E+4 Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 17.88285 I = 0.1 M ΔH = -4.9E+4 I = 0 M: $\log_{10}(\beta)$ = 18.73715
Cu(II)$^{2+}$ + 2 (tyrosine)$^{2-}$ ⇌ **Cu(II)(tyrosine)$_2^{2-}$**	16.16000	-5.57E+4	1	Cu(II)HL$_2$ ⇌ Cu(II)L$_2$ + H $\log_{10}(\beta)$ = -10.12 I = 0.1 M ΔH = 2.5E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + H + 2 L ⇌ Cu(II)HL$_2$ $\log_{10}(\beta)$ = 25.42570 I = 0.1 M ΔH = -8.07E+4 Cu(II) + 2 L ⇌ Cu(II)L$_2$ $\log_{10}(\beta)$ = 15.30570 I = 0.1 M ΔH = -5.57E+4 I = 0 M: $\log_{10}(\beta)$ = 16.16000
Cu(II)$^{2+}$ + H^{+} + 2 (tyrosine)$^{2-}$ ⇌ **Cu(II)H(tyrosine)$_2^{-}$**	26.70715	-8.07E+4	1	Cu(II)H$_2$L$_2$ ⇌ Cu(II)HL$_2$ + H $\log_{10}(\beta)$ = -9.36 I = 0.1 M ΔH = 2.4E+4 (Original data for ΔH at I = 0.1 M) Cu(II) + 2 H + 2 L ⇌ Cu(II)H$_2$L$_2$ $\log_{10}(\beta)$ = 34.78570 I = 0.1 M ΔH = -1.047E+5 Cu(II) + H + 2 L ⇌ Cu(II)HL$_2$ $\log_{10}(\beta)$ = 25.42570 I = 0.1 M ΔH = -8.07E+4 I = 0 M: $\log_{10}(\beta)$ = 26.70715
Cu(II)$^{2+}$ + 2 H^{+} + 2 (tyrosine)$^{2-}$ ⇌ **Cu(II)H$_2$(tyrosine)$_2$ *(aq)***	36.28073	-1.047E+5	1	Cu(II) + 2 HL ⇌ Cu(II)H$_2$L$_2$ $\log_{10}(\beta)$ = 14.7 I = 0.1 M ΔH = -5.27E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ H$_2$L$_2$ $\log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.2E+4 Cu(II) + 2 H + 2 L ⇌ Cu(II)H$_2$L$_2$ $\log_{10}(\beta)$ = 34.78570 I = 0.1 M ΔH = -1.047E+5 I = 0 M: $\log_{10}(\beta)$ = 36.28073
Zn^{2+} + (tyrosine)$^{2-}$ ⇌ **Zn(tyrosine) *(aq)***	6.91715	3.5E+3	1	Zn + HL ⇌ ZnL + H $\log_{10}(\beta)$ = -8.2 I = 0.1 M ΔH = 3.7E+4 (Original data for ΔH at I = 0.1 M) Zn + H + L ⇌ ZnHL $\log_{10}(\beta)$ = 14.26285 I = 0.1 M ΔH = -3.35E+4 Zn + L ⇌ ZnL $\log_{10}(\beta)$ = 6.06285 I = 0.1 M ΔH = 3.5E+3 I = 0 M: $\log_{10}(\beta)$ = 6.91715

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Zn^{2+} + H^{+} + $(tyrosine)^{2-}$ ⇌ **$ZnH(tyrosine)^{+}$**	15.11715	-3.35E+4	1	Zn + HL ⇌ ZnHL $log_{10}(\beta)$ = 4.22 I = 0.1 M ΔH = -7.5E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $log_{10}(\beta)$ = 10.04285 I = 0.1 M ΔH = -2.6E+4 Zn + H + L ⇌ ZnHL $log_{10}(\beta)$ = 14.26285 I = 0.1 M ΔH = -3.35E+4 I = 0 M: $log_{10}(\beta)$ = 15.11715
Zn^{2+} + 2 $(tyrosine)^{2-}$ ⇌ **$Zn(tyrosine)_2^{2-}$**	10.88000	-1E+3	1	$ZnHL_2$ ⇌ ZnL_2 + H $log_{10}(\beta)$ = -9.4 I = 0.1 M ΔH = 4E+4 (Original data for ΔH at I = 0.1 M) Zn + H + 2 L ⇌ $ZnHL_2$ $log_{10}(\beta)$ = 19.42570 I = 0.1 M ΔH = -4.1E+4 Zn + 2 L ⇌ ZnL_2 $log_{10}(\beta)$ = 10.02570 I = 0.1 M ΔH = -1E+3 I = 0 M: $log_{10}(\beta)$ = 10.88000
Zn^{2+} + H^{+} + 2 $(tyrosine)^{2-}$ ⇌ **$ZnH(tyrosine)_2^{-}$**	20.70715	-4.1E+4	1	ZnH_2L_2 ⇌ $ZnHL_2$ + H $log_{10}(\beta)$ = -8.91 I = 0.1 M ΔH = 3E+4 (Original data for ΔH at I = 0.1 M) Zn + 2 H + 2 L ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 28.33570 I = 0.1 M ΔH = -7.1E+4 Zn + H + 2 L ⇌ $ZnHL_2$ $log_{10}(\beta)$ = 19.42570 I = 0.1 M ΔH = -4.1E+4 I = 0 M: $log_{10}(\beta)$ = 20.70715
Zn^{2+} + 2 H^{+} + 2 $(tyrosine)^{2-}$ ⇌ **$ZnH_2(tyrosine)_2$** ***(aq)***	29.83073	-7.1E+4	1	Zn + 2 HL ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 8.25 I = 0.1 M ΔH = -1.9E+4 (Original data for ΔH at I = 0.1 M) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 20.08570 I = 0.1 M ΔH = -5.2E+4 Zn + 2 H + 2 L ⇌ ZnH_2L_2 $log_{10}(\beta)$ = 28.33570 I = 0.1 M ΔH = -7.1E+4 I = 0 M: $log_{10}(\beta)$ = 29.83073
Ga^{3+} + H^{+} + $(tyrosine)^{2-}$ ⇌ **$GaH(tyrosine)^{2+}$**	18.35932		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 8.7 I = 3.0 M H + L ⇌ HL $log_{10}(\beta)$ = 11.01046 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 19.71046 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 18.35932
Ga^{3+} + 2 H^{+} + $(tyrosine)^{2-}$ ⇌ **$GaH_2(tyrosine)^{3+}$**	22.19977		1	GaHL + H ⇌ GaH_2L $log_{10}(\beta)$ = 3.3 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 19.71046 I = 3.0 M Ga + 2 H + L ⇌ GaH_2L $log_{10}(\beta)$ = 23.01046 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 22.19977
Cd^{2+} + H^{+} + $(tyrosine)^{2-}$ ⇌ **$CdH(tyrosine)^{+}$**	14.57677		1	Cd + HL ⇌ CdHL $log_{10}(\beta)$ = 3.57 I = 0.5 M (Original data for β at T = 20°C) H + L ⇌ HL $log_{10}(\beta)$ = 9.93322 I = 0.5 M Cd + H + L ⇌ CdHL $log_{10}(\beta)$ = 13.50322 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 14.57677
Cd^{2+} + 2 H^{+} + 2 $(tyrosine)^{2-}$ ⇌ **$CdH_2(tyrosine)_2$** ***(aq)***	27.82516		1	Cd + 2 HL ⇌ CdH_2L_2 $log_{10}(\beta)$ = 6.08 I = 0.5 M (Original data for β at T = 20°C) 2 H + 2 L ⇌ H_2L_2 $log_{10}(\beta)$ = 19.86644 I = 0.5 M Cd + 2 H + 2 L ⇌ CdH_2L_2 $log_{10}(\beta)$ = 25.94644 I = 0.5 M I = 0 M: $log_{10}(\beta)$ = 27.82516

Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+} + H^{+} + (tyrosine)^{2-} \rightleftharpoons$ **$Pb(II)H(tyrosine)^{+}$**	15.14677		1	$Pb(II) + HL \rightleftharpoons Pb(II)HL$ $log_{10}(β) = 4.14$ I = 0.5 M (Original data for β at T = 20°C) $H + L \rightleftharpoons HL$ $log_{10}(β) = 9.93322$ I = 0.5 M $Pb(II) + H + L \rightleftharpoons Pb(II)HL$ $log_{10}(β) = 14.07322$ I = 0.5 M I = 0 M: $log_{10}(β) = 15.14677$
$Pb(II)^{2+} + 2\ H^{+} + 2\ (tyrosine)^{2-} \rightleftharpoons$ **$Pb(II)H_2(tyrosine)_2$ *(aq)***	30.28516		1	$Pb(II) + 2\ HL \rightleftharpoons Pb(II)H_2L_2$ $log_{10}(β) = 8.54$ I = 0.5 M (Original data for β at T = 20°C) $2\ H + 2\ L \rightleftharpoons H_2L_2$ $log_{10}(β) = 19.86644$ I = 0.5 M $Pb(II) + 2\ H + 2\ L \rightleftharpoons Pb(II)H_2L_2$ $log_{10}(β) = 28.40644$ I = 0.5 M I = 0 M: $log_{10}(β) = 30.28516$

2.2.53. Tryptophan

The ligand in its neutral form is L-2-Amino-3-(3-indolyl)propanoic acid (tryptophan; $C_{11}H_{12}N_2O_2$). The ligand L as it is present in the database is the anion $C_{11}H_{11}N_2O_2^{-}$. Its molecular weight is 203.221. Its structural formula is shown on the right.



Equilibrium reaction	$Log_{10}(β)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$H^{+} + (tryptophan)^{-} \rightleftharpoons$ **H(tryptophan) *(aq)***	9.54358	-4.47E+4	1	Original data for β: $log_{10}(β) = 9.33$, at I = 0.1 M. Original data for ΔH at I = 0.1 M.

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + $(tryptophan)^-$ ⇌ **$H_2(tryptophan)^+$**	11.91358	-4.93E+4	1	HL + H ⇌ H_2L $\log_{10}(\beta)$ = 2.37 I = 0.1 M ΔH = -4.6E+3 (Original data for ΔH at I = 0.1 M) H + L ⇌ HL $\log_{10}(\beta)$ = 9.33 I = 0.1 M ΔH = -4.47E+4 2 H + L ⇌ H_2L $\log_{10}(\beta)$ = 11.70 I = 0.1 M ΔH = -4.93E+4 I = 0 M: $\log_{10}(\beta)$ = 11.91358
$Mn(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Mn(II)(tryptophan)^+$**	2.96715	-4.6E+3	1	Original data for β: $\log_{10}(\beta)$ = 2.54, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
2 $Mn(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Mn(II)(tryptophan)_2$ *(aq)***	5.62073	-9.6E+3	1	Original data for β: $\log_{10}(\beta)$ = 4.98, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
3 $Mn(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Mn(II)(tryptophan)_3^-$**	7.18931		1	Original data for β: $\log_{10}(\beta)$ = 8.0, at I = 3.0 M.
$Fe(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Fe(II)(tryptophan)^+$**	3.37954	-9.2E+3	1	Original data for β: $\log_{10}(\beta)$ = 3.92, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Fe(II)^{2+}$ + 2 $(tryptophan)^-$ ⇌ **$Fe(II)(tryptophan)_2$ *(aq)***	6.57931	-1.8E+4	1	Original data for β: $\log_{10}(\beta)$ = 7.39, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
$Fe(II)^{2+}$ + 3 $(tryptophan)^-$ ⇌ **$Fe(II)(tryptophan)_3^-$**	8.68931		1	Original data for β: $\log_{10}(\beta)$ = 9.5, at I = 3.0 M.
$Fe(III)^{3+}$ + $(tryptophan)^-$ ⇌ **$Fe(III)(tryptophan)^{2+}$**	9.60948		1	Original data for β: $\log_{10}(\beta)$ = 9.0, at I = 1.0 M and 20°C.
$Co(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Co(II)(tryptophan)^+$**	4.92715	-1.1E+4	1	Original data for β: $\log_{10}(\beta)$ = 4.5, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Co(II)^{2+}$ + 2 $(tryptophan)^-$ ⇌ **$Co(II)(tryptophan)_2$ *(aq)***	9.26073	-2.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.62, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Co(II)^{2+}$ + 3 $(tryptophan)^-$ ⇌ **$Co(II)(tryptophan)_3^-$**	11.43931	-3.5E+4	1	Original data for β: $\log_{10}(\beta)$ = 12.25, at I = 3.0 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + $(tryptophan)^-$ ⇌ **$Ni(tryptophan)^+$**	5.90715	-2.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 5.48, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 2 $(tryptophan)^-$ ⇌ **$Ni(tryptophan)_2$ *(aq)***	11.04073	-4.93E+4	1	Original data for β: $\log_{10}(\beta)$ = 10.40, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
Ni^{2+} + 3 $(tryptophan)^-$ ⇌ **$Ni(tryptophan)_3^-$**	14.87073	-7.02E+4	1	Original data for β: $\log_{10}(\beta)$ = 14.23, at I = 0.1 M. Original data for ΔH at I = 3.0 M.
$Cu(II)^{2+}$ + $(tryptophan)^-$ ⇌ **$Cu(II)(tryptophan)^+$**	8.63715	-2.3E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.21, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + 2 $(tryptophan)^-$ ⇌ **$Cu(II)(tryptophan)_2$ *(aq)***	16.14073	-5.43E+4	1	Original data for β: $\log_{10}(\beta)$ = 15.5, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
$Cu(II)^{2+}$ + H^+ + $(tryptophan)^-$ ⇌ **$Cu(II)H(tryptophan)^{2+}$**	10.86927		1	Cu(II)L + H ⇌ Cu(II)HL $\log_{10}(\beta)$ = 2.47 I = 0.15 M (Original data for β at T = 37°C) Cu(II) + L ⇌ Cu(II)L $\log_{10}(\beta)$ = 8.16140 I = 0.15 M Cu(II) + H + L ⇌ Cu(II)HL $\log_{10}(\beta)$ = 10.63140 I = 0.15 M I = 0 M: $\log_{10}(\beta)$ = 10.86927
Zn^{2+} + $(tryptophan)^-$ ⇌ **$Zn(tryptophan)^+$**	5.11715	-1.2E+4	1	Original data for β: $\log_{10}(\beta)$ = 4.69, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 2 $(tryptophan)^-$ ⇌ **$Zn(tryptophan)_2$ *(aq)***	9.58073	-2.4E+4	1	Original data for β: $\log_{10}(\beta)$ = 8.94, at I = 0.1 M. Original data for ΔH at I = 0.1 M.
Zn^{2+} + 3 $(tryptophan)^-$ ⇌ **$Zn(tryptophan)_3^-$**	12.68931		1	Original data for β: $\log_{10}(\beta)$ = 13.5, at I = 3.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ga^{3+} + (tryptophan)$^-$ ⇌ **Ga(tryptophan)$^{2+}$**	7.78931		1	Original data for β: $log_{10}(\beta)$ = 8.60, at I = 3.0 M.
Ga^{3+} + H^+ + (tryptophan)$^-$ ⇌ **GaH(tryptophan)$^{3+}$**	11.54358		1	Ga + HL ⇌ GaHL $log_{10}(\beta)$ = 2.00 I = 3.0 M H + L ⇌ HL $log_{10}(\beta)$ = 9.81381 I = 3.0 M Ga + H + L ⇌ GaHL $log_{10}(\beta)$ = 11.81381 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 11.54358
Cd^{2+} + (tryptophan)$^-$ ⇌ **Cd(tryptophan)$^+$**	3.93954		1	Original data for β: $log_{10}(\beta)$ = 4.48, at I = 3.0 M.
Cd^{2+} + 2 (tryptophan)$^-$ ⇌ **Cd(tryptophan)$_2$ *(aq)***	7.76931		1	Original data for β: $log_{10}(\beta)$ = 8.58, at I = 3.0 M.
Cd^{2+} + 3 (tryptophan)$^-$ ⇌ **Cd(tryptophan)$_3^-$**	11.21931		1	Original data for β: $log_{10}(\beta)$ = 12.03, at I = 3.0 M.
Pb(II)$^{2+}$ + (tryptophan)$^-$ ⇌ **Pb(II)(tryptophan)$^+$**	4.35954		1	Original data for β: $log_{10}(\beta)$ = 4.9, at I = 3.0 M.
Pb(II)$^{2+}$ + 2 (tryptophan)$^-$ ⇌ **Pb(II)(tryptophan) *(aq)***	9.45931		1	Original data for β: $log_{10}(\beta)$ = 10.27, at I = 3.0 M.

2.3. Adsorption

Unlike organic complexation, there is no unifying model for adsorption yet. So the constants in the CHEAQS Next database should be considered calcaulation *examples*. The constants for the adsorption equilibria were arbitrarily selected as described below. To reliably model adsorption, measurements are needed to determine the constants. See also the item "Modelling adsorption" in the help file.

2.3.1. Acid-base equilibria

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
≡S-OH ⇌ (≡S-**O)$^-$** + H^+	-9.5		5	
≡S-OH + H^+ ⇌ **≡S-OH$_2^+$**	7.2		5	

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 in that reference for other examples).

2.3.2. Constants for metals

For the adsorption of Fe(III), Cd, Cu(II), Pb(II) and Mg on silica the following relationship has been established:
$log_{10}(^*K^s_1) = -0.09 + 0.62 \times log_{10}(^*K_1)$ (see page 101 in Schindler & Stumm)
$log_{10}(^*K_1)$ 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_{C1})
So:

$\log_{10}(^*K^s_1)$ $= -0.09 + 0.62 \times (\log_{10}(K_{C1}) - 13.997)$
$= -8.76814 + 0.62 \times \log_{10}(K_{C1})$
This approach has been applied to all cations with a charge of 2 or more (see table below).

Similarly, for $(\equiv S)_2$-M the constants can be derived as follows.
$\log_{10}(^*\beta^s_2)$ $= -0.09 + 0.62 \times \log_{10}(^*\beta_2)$ (see page 101 in Schindler & Stumm)
$\log_{10}(^*\beta^s_2)$ $= -0.09 + 0.62 \times (\log_{10}(K_{C2}) - 27.994)$
$= -17.44628 + 0.62 \times \log_{10}(K_{C2})$

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.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$(\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})^- + H^+$	-9.5		5	
$H^+ + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{H_2}^+$	7.2		5	
$Be^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Be}^+ + H^+$	-4.03163		5	
$Be^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Be} + 2\ H^+$	-6.99263		5	
$Mg^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Mg}^+ + H^+$	-7.16854		5	
$Al^{3+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Al}^{2+} + H^+$	-3.18814		5	
$Al^{3+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Al}^+ + 2\ H^+$	-6.47228		5	
$Ca^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Ca}^+ + H^+$	-7.96214		5	
$Sc^{3+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Sc}^{2+} + H^+$	-2.75414		5	
$Sc^{3+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Sc}^+ + 2\ H^+$	-6.10028		5	
$Cr(III)^{3+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Cr(III)}^{2+} + H^+$	-2.38214		5	
$Cr(III)^{3+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Cr(III)}^+ + 2\ H^+$	-6.10028		5	
$Mn(II)^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Mn(II)}^+ + H^+$	-6.66014		5	
$Mn(II)^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Mn(II)} + 2\ H^+$	-13.85028		5	
$Fe(II)^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Fe(II)}^+ + H^+$	-5.91614		5	
$Fe(II)^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Fe(II)} + 2\ H^+$	-12.85828		5	
$Fe(III)^{3+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Fe(III)}^{2+} + H^+$	-1.44594		5	
$Fe(III)^{3+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Fe(III)}^+ + 2\ H^+$	-3.55828		5	
$Co(II)^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Co(II)}^+ + H^+$	-6.10214		5	
$Co(II)^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Co(II)} + 2\ H^+$	-11.74228		5	
$Co(III)^{3+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Co(III)}^{2+} + H^+$	-0.87597		5	
$Ni^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Ni}^+ + H^+$	-6.22614		5	
$Ni^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Ni} + 2\ H^+$	-11.86628		5	
$Cu(II)^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Cu(II)}^+ + H^+$	-4.73814		5	
$Cu(II)^{2+} + 2\ (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})_2\mathbf{Cu(II)} + 2\ H^+$	-10.81228		5	
$Zn^{2+} + (\equiv S\text{-}OH) \rightleftharpoons (\equiv S\text{-}\mathbf{O})\mathbf{Zn}^+ + H^+$	-5.66814		5	

Equilibrium reaction	Log$_{10}$(β)	ΔH (J/mol)	Literature reference	Remarks / conversions
Zn^{2+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$Zn + 2 H^+	-10.56428		5	
Ga^{3+} + (≡S-OH) ⇌ (≡S-O)Ga^{2+} + H^+	-1.88614		5	
Ga^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Ga^+$ + 2 H^+	-4.24028		5	
Sr^{2+} + (≡S-OH) ⇌ (≡S-O)Sr^+ + H^+	-8.25974		5	
Y^{3+} + (≡S-OH) ⇌ (≡S-O)Y^{2+} + H^+	-4.86214		5	
Y^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Y^+$ + 2 H^+	-10.25428		5	
Zr^{4+} + (≡S-OH) ⇌ (≡S-O)Zr^{3+} + H^+	0.09786		5	
Zr^{4+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Zr^{2+}$ + 2 H^+	-1.14028		5	
Pd^{2+} + (≡S-OH) ⇌ (≡S-O)Pd^+ + H^+	-1.82022		5	
Cd^{2+} + (≡S-OH) ⇌ (≡S-O)Cd^+ + H^+	-6.35014		5	
Cd^{2+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$Cd + 2 H^+	-12.67228		5	
In^{3+} + (≡S-OH) ⇌ (≡S-O)In^{2+} + H^+	-2.52474		5	
In^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$In^+$ + 2 H^+	-4.92228		5	
Sn(II)$^{2+}$ + (≡S-OH) ⇌ (≡S-O)Sn(II)$^+$ + H^+	-2.19614		5	
Sn(II)$^{2+}$ + 2 (≡S-OH) ⇌ (≡S-O)$_2$Sn(II) + 2 H^+	-4.48828		5	
Sn(IV)$^{4+}$ + (≡S-OH) ⇌ (≡S-O)Sn(IV)$^{3+}$ + H^+	0.84186		5	
Sn(IV)$^{4+}$ + 2 (≡S-OH) ⇌ (≡S-O)$_2$Sn(IV)$^{2+}$ + 2 H^+	0.72592		5	
Ba^{2+} + (≡S-OH) ⇌ (≡S-O)Ba^+ + H^+	-8.37134		5	
La^{3+} + (≡S-OH) ⇌ (≡S-O)La^{2+} + H^+	-5.35814		5	
La^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$La^+$ + 2 H^+	-10.87428		5	
Ce^{3+} + (≡S-OH) ⇌ (≡S-O)Ce^{2+} + H^+	-5.23414		5	
Ce^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Ce^+$ + 2 H^+	-10.68828		5	
Pr^{3+} + (≡S-OH) ⇌ (≡S-O)Pr^{2+} + H^+	-5.04494		5	
Pr^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Pr^+$ + 2 H^+	-10.62628		5	
Nd^{3+} + (≡S-OH) ⇌ (≡S-O)Nd^{2+} + H^+	-5.04814		5	
Nd^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Nd^+$ + 2 H^+	-10.56428		5	
Sm^{3+} + (≡S-OH) ⇌ (≡S-O)Sm^{2+} + H^+	-4.98614		5	
Sm^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Sm^+$ + 2 H^+	-10.37828		5	
Eu^{3+} + (≡S-OH) ⇌ (≡S-O)Eu^{2+} + H^+	-4.92094		5	
Eu^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Eu^+$ + 2 H^+	-10.37828		5	
Gd^{3+} + (≡S-OH) ⇌ (≡S-O)Gd^{2+} + H^+	-4.92094		5	
Gd^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Gd^+$ + 2 H^+	-10.25428		5	
Tb^{3+} + (≡S-OH) ⇌ (≡S-O)Tb^{2+} + H^+	-4.98614		5	
Tb^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Tb^+$ + 2 H^+	-10.19228		5	
Dy^{3+} + (≡S-OH) ⇌ (≡S-O)Dy^{2+} + H^+	-4.79694		5	
Dy^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Dy^+$ + 2 H^+	-10.13028		5	
Ho^{3+} + (≡S-OH) ⇌ (≡S-O)Ho^{2+} + H^+	-4.73494		5	
Ho^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Ho^+$ + 2 H^+	-10.06828		5	
Er^{3+} + (≡S-OH) ⇌ (≡S-O)Er^{2+} + H^+	-4.73494		5	
Er^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Er^+$ + 2 H^+	-9.94428		5	
Tm^{3+} + (≡S-OH) ⇌ (≡S-O)Tm^{2+} + H^+	-4.67294		5	
Tm^{3+} + 2 (≡S-OH) ⇌ (≡S-O)$_2$$Tm^+$ + 2 H^+	-9.94428		5	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Yb^{3+} + (≡S-OH) ⇌ (≡S-**O)Yb**$^{2+}$ + H^+	-4.67294		5	
Yb^{3+} + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Yb**$^+$ + 2 H^+	-9.88228		5	
Lu^{3+} + (≡S-OH) ⇌ (≡S-**O)Lu**$^{2+}$ + H^+	-4.67294		5	
Lu^{3+} + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Lu**$^+$ + 2 H^+	-9.82028		5	
Hf^{4+} + (≡S-OH) ⇌ (≡S-**O)Hf**$^{3+}$ + H^+	-0.21214		5	
Hf^{4+} + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Hf**$^{2+}$ + 2 H^+	-1.57428		5	
$Hg(II)^{2+}$ + (≡S-OH) ⇌ (≡S-**O)Hg(II)**$^+$ + H^+	-2.19614		5	
$Hg(II)^{2+}$ + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Hg(II)** + 2 H^+	-3.91168		5	
$Pb(II)^{2+}$ + (≡S-OH) ⇌ (≡S-**O)Pb(II)**$^+$ + H^+	-4.80014		5	
$Pb(II)^{2+}$ + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Pb(II)** + 2 H^+	-10.68828		5	
Bi^{3+} + (≡S-OH) ⇌ (≡S-**O)Bi**$^{2+}$ + H^+	-0.77014		5	
Bi^{3+} + 2 (≡S-OH) ⇌ (≡S-**O)$_2$Bi**$^+$ + 2 H^+	-2.24648		5	
$(U(VI)O_2)^{2+}$ + (≡S-OH) ⇌ (≡S-**O)(U(VI)O$_2$)**$^+$ + H^+	-3.74614		5	

2.4. Redox equilibria

Most redox couples are originally 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 reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
CrO_4^{2-} + 8 H^+ + 3 e^- ⇌ Cr^{3+} + 4 H_2O	74.96900		8	$HCrO_4^-$ + 7 H^+ + 3 e^- ⇌ Cr^{3+} + 4 H_2O $\log_{10}(\beta)$ = 68.45900 (Original data: E = 1.350 V) H^+ + $(CrO_4)^{2-}$ ⇌ $H(CrO_4)^-$ $\log_{10}(\beta)$ = 6.51 CrO_4^- + 8 H^+ + 3 e^- ⇌ Cr^{3+} + 4 H_2O $\log_{10}(\beta)$ = 74.96900
MnO_4^- + 8 H^+ + 5 e^- ⇌ Mn^{2+} + 4 H_2O	127.36754		8	Original data: E = 1.507 V
MnO_2 *(s)* + 4 H^+ + 2 e^- ⇌ Mn^{2+} + 2 H_2O	41.37966		8	Original data: E = 1.224 V
Fe^{3+} + e^- ⇌ Fe^{2+}	13.03256		8	Original data: E = 0.771 V
Co^{3+} + e^- ⇌ Co^{2+}	32.45464		8	Original data: E = 1.92 V
Cu^{2+} + e^- ⇌ Cu^+	2.58623		8	Original data: E = 0.153 V
Cu^{2+} + 2 e^- ⇌ Cu *(s)*	11.55858		8	Original data: E = 0.3419 V
Sn^{4+} + 2 e^- ⇌ Sn^{2+}	5.10484		8	Original data: E = 0.151 V
PbO_2 *(s)* + 4 H^+ + 2 e^- ⇌ Pb^{2+} + 2 H_2O	49.18906		8	Original data: E = 1.455 V
NO_3^- + 9 H^+ + 8 e^- ⇌ NH_3 + $3H_2O$	109.956		3	NO_3^- + 10 H^+ + 8 e^- ⇌ NH_4^+ + 3 H_2O $\log_{10}(\beta)$ = 119.2 NH_4^+ ⇌ NH_3 + H $\log_{10}(\beta)$ = -9.244 NO_3^- + 9 H^+ + 8 e^- ⇌ NH_3 + $3H_2O$ $\log_{10}(\beta)$ = 109.956

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$\mathbf{NO_3^-} + 2\ H^+ + 2\ e^- \rightleftharpoons \mathbf{NO_2^-} + H_2O$	28.37886		8	Two similar redox equilibria are available: 1: $NO_3^- + 3\ H^+ + 2\ e^- \rightleftharpoons HNO_2 + H_2O$ E = 0.934 V $log_{10}(\beta)$ = 31.57566 $HNO_2 \rightleftharpoons H^+ + NO_2^-$ $log_{10}(\beta)$ = -3.15 $NO_3^- + 2\ H^+ + 2\ e^- \rightleftharpoons NO_2^- + H_2O$ $log_{10}(\beta)$ = 28.42566 2: $NO_3^- + H_2O + 2\ e^- \rightleftharpoons NO_2^- + 2$ OH- E = 0.01 V $log_{10}(\beta)$ = 0.33807 $2\ H^+ + 2\ OH^- \rightleftharpoons 2\ H_2O$ $log_{10}(\beta)$ = 27.994 $NO_3^- + 2\ H^+ + 2\ e^- \rightleftharpoons H_2O + NO_2^-$ $log_{10}(\beta)$ = 28.33207 Average of these two was entered: (28.42566 + 28.33207) / 2 = 28.37886
$\mathbf{SO_4^{2-}} + 8\ H^+ + 8\ e^- \rightleftharpoons \mathbf{S^{2-}}$	20.12		3	$SO_4^{2-} + 10\ H^+ + 8\ e^- \rightleftharpoons H_2S$ *(aq)* $+ 4\ H_2O$ $log_{10}(\beta)$ = 41.04 $H_2S \rightleftharpoons 2\ H + S$ $log_{10}(\beta)$ = -20.92 $SO_4^{2-} + 8\ H^+ + 8\ e^- \rightleftharpoons S^{2-}$ $log_{10}(\beta)$ = 20.12
$\mathbf{SO_4^{2-}} + 2\ H^+ + 2e^- \rightleftharpoons \mathbf{SO_3^{2-}} + H_2O$	-3.34082		8	Two similar redox equilibria are available: 1: $SO_4^{2-} + 4\ H^+ + 2\ e^- \rightleftharpoons H_2SO_3 + H_2O$ E = 0.172 V $log_{10}(\beta)$ = 5.81479 $H_2SO_3 \rightleftharpoons 2\ H^+ + SO_3^{2-}$ $log_{10}(\beta)$ = -9.05 $SO_4^{2-} + 2\ H^+ + 2\ e \rightleftharpoons SO_3^{2-} + H_2O$ $log_{10}(\beta)$ = -3.23521 2: $SO_4^{2-} + H_2O + 2\ e^- \rightleftharpoons SO_3^{2-} + 2\ OH^-$ E = -0.93 V $log_{10}(\beta)$ = -31.44043 $2\ H^+ + 2\ OH^- \rightleftharpoons 2\ H_2O$ $log_{10}(\beta)$ = 27.994 $SO_4^{2-} + 2\ H^+ + 2\ e^- \rightleftharpoons SO_3^{2-} + H_2O$ $log_{10}(\beta)$ = -3.44643 Average of these two was entered: (-3.23521 + -3.44643) / 2 = -3.34082
$\mathbf{SO_4^{2-}} + 8\ H^+ + 6\ e^- \rightleftharpoons$ ***S (s)***	36.24		6	H_2S *(aq)* $\rightleftharpoons S(s) + 2\ H^+ + 2\ e^-$ $log_{10}(\beta)$ = -4.8 $SO_4^{2-} + 10\ H^+ + 8\ e^- \rightleftharpoons H_2S$ *(aq)* $+ 4\ H_2O$ $log_{10}(\beta)$ = 41.04 $SO_4^{2-} + 8\ H^+ + 6\ e^- \rightleftharpoons S(s)$ $log_{10}(\beta)$ = 36.24

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$\mathbf{AsO_4^{3-}}$ + 4 H^+ + 2 e^- ⇌ $\mathbf{AsO_2^-}$ + 2 H_2O	31.16348		8	Two similar redox equilibria are available: 1: H_3AsO_4 + 2 H^+ + 2 e^- ⇌ $HAsO_2$ + 2 H_2O E = 0.56 V $\log_{10}(\beta)$ = 18.93187 AsO_4^{3-} + 3 H^+ ⇌ H_3AsO_4 $\log_{10}(\beta)$ = 20.70 $HAsO_2$ ⇌ H^+ + AsO_2^- $\log_{10}(\beta)$ = -9.29 AsO_4^{3-} + 4 H^+ + 2 e^- ⇌ AsO_2^- +2 H_2O $\log_{10}(\beta)$ = 30.34187 2: AsO_4^{3-} + 2 H_2O + 2 e^- ⇌ AsO_2^- + 4 OH^- E = -0.71 V $\log_{10}(\beta)$ = -24.00291 4 OH^- + 4 H^+ ⇌ 4 H_2O $\log_{10}(\beta)$ = 55.988 AsO_4^{3-} + 4 H^+ + 2 e^- ⇌ AsO_2^- + 2 H_2O $\log_{10}(\beta)$ = 31.98509 Average of these two was entered: (30.34187 + 31.98509) / 2 = 31.16348
$\mathbf{SeO_4^{2-}}$ + 2 H^+ + 2 e^- ⇌ $\mathbf{SeO_3^{2-}}$	28.78305		8	Two similar redox equilibria are available: 1: SeO_4^{2-} + 4 H^+ + 2 e^- ⇌ H_2SeO_3 + H_2O E = 1.151 V $\log_{10}(\beta)$ = 38.91176 H_2SeO_3 ⇌ 2 H + SeO_3^{2-} $\log_{10}(\beta)$ = -11.03 SeO_4^{2-} + 2 H^+ + 2 e^- ⇌ SeO_3^{2-} $\log_{10}(\beta)$ = 27.88176 2: SeO_4^{2-} + H_2O + 2 e^- ⇌ SeO_3^{2-} + 2 OH^- E = 0.05 V $\log_{10}(\beta)$ = 1.69035 2 H^+ + 2 OH^- ⇌ 2 H_2O $\log_{10}(\beta)$ = 27.994 SeO_4^{2-} + 2 H^+ + 2 e^- ⇌ SeO_3^{2-} $\log_{10}(\beta)$ = 29.68435 Average of these two was entered: (27.88176 + 29.68435) / 2 = 28.78305

2.5. Gases

Equilibrium reaction	$\log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
2 H^+ + $(CO_3)^{2-}$ ⇌ $\mathbf{CO_2}$ ***(g)***	18.147	-4.06E+3	1	2 H + L ⇌ H_2L *(aq)* $\log_{10}(\beta)$ = 16.681 ΔH = -2.376E+4 H_2L *(aq)* ⇌ CO_2 (g) $\log_{10}(\beta)$ = 1.466 ΔH = 1.97E+4 2 H + L ⇌ CO_2 (g) $\log_{10}(\beta)$ = 18.147 ΔH = -4.06E+3
(NH_3) *(aq)* ⇌ $\mathbf{NH_3}$ ***(g)***	-1.8		3	
2 H^+ + S^{2-} ⇌ $\mathbf{H_2S}$ ***(g)***	21.91		1	2 H + L ⇌ H_2L *(aq)* $\log_{10}(\beta)$ = 20.92 H_2L *(aq)* ⇌ H_2S (g) $\log_{10}(\beta)$ = 0.99 2 H + L ⇌ H_2S (g) $\log_{10}(\beta)$ = 21.91
2 H^+ + $(SO_2)^{2-}$ ⇌ $\mathbf{SO_2}$ ***(g)***	8.95	4.84E+4	1	2 H + L ⇌ H_2L *(aq)* $\log_{10}(\beta)$ = 9.04 ΔH = 2.14E+4 H_2L *(aq)* ⇌ SO_2 (g) $\log_{10}(\beta)$ = -0.09 ΔH = 2.7E+4 2 H + L ⇌ SO_2 (g) $\log_{10}(\beta)$ = 8.95 ΔH = 4.84E+4

2.6. Solids

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Be^{2+} + 2 $(OH)^-$ ⇌ **$Be(OH)_2$** ***(s)***	21.5		1	
Mg^{2+} + 2 $(OH)^-$ ⇌ **$Mg(OH)_2$** ***(s)***	11.1		1	
Al^{3+} + 3 $(OH)^-$ ⇌ **$Al(OH)_3$** ***(s)***	33.7		1	
Ca^{2+} + 2 $(OH)^-$ ⇌ **$Ca(OH)_2$** ***(s)***	5.29	1.7E+4	1	
Sc^{3+} + 3 $(OH)^-$ ⇌ **ScO_2H** ***(s)***	29.7		1	
$Cr(III)^{3+}$ + 3 $(OH)^-$ ⇌ **$Cr(III)(OH)_3$** ***(s)***	30.2		1	
$Mn(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Mn(II)(OH)_2$** ***(s)***	12.8		1	
$Fe(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Fe(II)(OH)_2$** ***(s)***	15.1		1	
2 $Fe(III)^{3+}$ + 6 $(OH)^-$ ⇌ **$Fe(III)_2O_3$** ***(s)***	85.4		1	
$Co(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Co(II)(OH)_2$** ***(s)***	15.7		1	
$Co(III)^{3+}$ + 3 $(OH)^-$ ⇌ **$Co(III)(OH)_3$** ***(s)***	44.4		1	
Ni^{2+} + 2 $(OH)^-$ ⇌ **$Ni(OH)_2$** ***(s)***	17.2		1	
2 $Cu(I)^+$ + 2 $(OH)^-$ ⇌ **$Cu(I)_2O$** ***(s)***	29.4		1	
$Cu(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Cu(II)O$** ***(s)***	19.5		1	
Zn^{2+} + 2 $(OH)^-$ ⇌ **ZnO** ***(s)***	16.76	2.2E+4	1	Original data for ΔH at I = 2.0 M.
2 Ga^{3+} + 6 $(OH)^-$ ⇌ **Ga_2O_3** ***(s)***	79.6		1	
Y^{3+} + 3 $(OH)^-$ ⇌ **$Y(OH)_3$** ***(s)***	25.9		1	
Zr^{4+} + 4 $(OH)^-$ ⇌ **$Zr(OH)_4$** ***(s)***	54.1		1	
Pd^{2+} + 2 $(OH)^-$ ⇌ **$Pd(OH)_2$** ***(s)***	31.44073		1	Original data for β: $log_{10}(\beta)$ = 30.8, at I = 0.1 M.
2 Ag^+ + 2 $(OH)^-$ ⇌ **Ag_2O** ***(s)***	15.42	-3.3E+4	1	
Cd^{2+} + 2 $(OH)^-$ ⇌ **$Cd(OH)_2$** ***(s)***	14.35	-1.7E+4	1	
In^{3+} + 3 $(OH)^-$ ⇌ **$In(OH)_3$** ***(s)***	36.9		1	
$Sn(II)^{2+}$ + 2 $(OH)^-$ ⇌ **$Sn(II)O$** ***(s)***	26.2		1	
Ba^{2+} + 2 $(OH)^-$ ⇌ **$Ba(OH)_2(H_2O)_8$** ***(s)***	3.6	-5.73E+4	1	
La^{3+} + 3 $(OH)^-$ ⇌ **$La(OH)_3$** ***(s)***	22.2		1	
Ce^{3+} + 3 $(OH)^-$ ⇌ **$Ce(OH)_3$** ***(s)***	23.9		1	
Pr^{3+} + 3 $(OH)^-$ ⇌ **$Pr(OH)_3$** ***(s)***	24.4		1	
Nd^{3+} + 3 $(OH)^-$ ⇌ **$Nd(OH)_3$** ***(s)***	26.0		1	
Sm^{3+} + 3 $(OH)^-$ ⇌ **$Sm(OH)_3$** ***(s)***	25.9		1	
Eu^{3+} + 3 $(OH)^-$ ⇌ **$Eu(OH)_3$** ***(s)***	26.5		1	
Gd^{3+} + 3 $(OH)^-$ ⇌ **$Gd(OH)_3$** ***(s)***	26.9		1	
Tb^{3+} + 3 $(OH)^-$ ⇌ **$Tb(OH)_3$** ***(s)***	26.3		1	
Dy^{3+} + 3 $(OH)^-$ ⇌ **$Dy(OH)_3$** ***(s)***	25.9		1	
Ho^{3+} + 3 $(OH)^-$ ⇌ **$Ho(OH)_3$** ***(s)***	26.6		1	
Er^{3+} + 3 $(OH)^-$ ⇌ **$Er(OH)_3$** ***(s)***	26.6		1	
Tm^{3+} + 3 $(OH)^-$ ⇌ **$Tm(OH)_3$** ***(s)***	26.7		1	
Yb^{3+} + 3 $(OH)^-$ ⇌ **$Yb(OH)_3$** ***(s)***	26.6		1	
Lu^{3+} + 3 $(OH)^-$ ⇌ **$Lu(OH)_3$** ***(s)***	27.0		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Hf^{4+} + 4 $(OH)^-$ ⇌ **$Hf(OH)_4$** *(s)*	54.8		1	
$Hg(II)^{2+}$ + 2 $(OH)^-$ ⇌ **Hg(II)O** *(s)*	25.44	-8.95E+04	1	Original data for ΔH at I = 3.0 M.
$Pb(II)^{2+}$ + 2 $(OH)^-$ ⇌ **Pb(II)O** *(s)*	15.3		1	
2 Bi^{3+} + 6 $(OH)^-$ ⇌ **Bi_2O_3** *(s)*	10.8		1	
$(U(VI)O_2)^{2+}$ + 2 $(OH)^-$ ⇌ **$(U(VI)O_2)(OH)_2(H_2O)$** *(s)*	22.0		1	
H^+ + Ag^+ + 2 $(H_2BO_3)^-$ ⇌ **$AgH(H_2BO_3)_2$** *(s)*	13.97200		1	Ag + 2 $H(H_2BO_3)$ ⇌ H + $AgH(H_2BO_3)_2$ $log_{10}(\beta)$ = -4.5 I = 3.0 M 2 H + 2 (H_2BO_3) ⇌ 2 $H(H_2BO_3)$ $log_{10}(\beta)$ = 19.01246 I = 3.0 M Ag + H + 2 (H_2BO_3) ⇌ $AgH(H_2BO_3)_2$ $log_{10}(\beta)$ = 14.51246 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 13.97200
Mg^{2+} + Ca^{2+} + 2 $(CO_3)^{2-}$ ⇌ **$CaMg(CO_3)_2$** *(s)*	16.7		6	
Mg^{2+} + $(CO_3)^{2-}$ ⇌ **$Mg(CO_3)$** *(s)*	7.46	-2.0E+04	1	
4 Mg^{2+} + 2 $(OH)^-$ + 3 $(CO_3)^{2-}$ ⇌ **$Mg_4(CO_3)_3(OH)_2(H_2O)_3$** *(s)*	29.5		6	
Ca^{2+} + $(CO_3)^{2-}$ ⇌ **$Ca(CO_3)$** *(s)*	8.48	1.0E+04	1	
$Mn(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Mn(II)(CO_3)$** *(s)*	11		1	
$Fe(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Fe(II)(CO_3)$** *(s)*	10.8	1.6E+04	1	
$Co(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Co(II)(CO_3)$** *(s)*	11.2		1	
Ni^{2+} + $(CO_3)^{2-}$ ⇌ **$Ni(CO_3)$** *(s)*	11.2		1	
$Cu(II)^{2+}$ + $(CO_3)^{2-}$ ⇌ **$Cu(II)(CO_3)$** *(s)*	11.5		1	
2 $Cu(II)^{2+}$ + 2 $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Cu(II)_2(CO_3)(OH)_2$** *(s)*	33.3	-1.88E+05	1	Original data for ΔH at I = 0.7 M.
3 $Cu(II)^{2+}$ + 2 $(OH)^-$ + 2 $(CO_3)^{2-}$ ⇌ **$Cu(II)_3(CO_3)_2(OH)_2$** *(s)*	44.9		1	
Zn^{2+} + $(CO_3)^{2-}$ ⇌ **$Zn(CO_3)$** *(s)*	10.8		1	
5 Zn^{2+} + 6 $(OH)^-$ + 2 $(CO_3)^{2-}$ ⇌ **$Zn_5(OH)_6(CO_3)_2$** *(s)*	71.276		6	5 Zn + 8 H_2O + 2 CO_2 (g) ⇌ $Zn_5(OH)_6(CO_3)_2$ + 10 H $log_{10}(\beta)$ = -49.0 4 H + 2 CO_3 ⇌ 2 H_2O + 2 CO_2 (g) $log_{10}(\beta)$ = 36.294 6 H + 6 OH ⇌ 6 H_2O $log_{10}(\beta)$ = 83.982 5 Zn + 6 OH + 2 CO_3 ⇌ $Zn_5(OH)_6(CO_3)_2$ $log_{10}(\beta)$ = 71.276
Sr^{2+} + $(CO_3)^{2-}$ ⇌ **$Sr(CO_3)$** *(s)*	9.27	1E+03	1	
2 Y^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Y_2(CO_3)_3$** *(s)*	33		1	
2 Ag^+ + $(CO_3)^{2-}$ ⇌ **$Ag_2(CO_3)$** *(s)*	11.09		1	
Cd^{2+} + $(CO_3)^{2-}$ ⇌ **$Cd(CO_3)$** *(s)*	12.1		1	
Ba^{2+} + $(CO_3)^{2-}$ ⇌ **$Ba(CO_3)$** *(s)*	8.57	-2E+03	1	
2 La^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$La_2(CO_3)_3$** *(s)*	34.4		1	
2 Ce^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Ce_2(CO_3)_3$** *(s)*	27.04657		1	Original data for β: $log_{10}(\beta)$ = 31.1, at I = 3.0 M.
Nd^{3+} + $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Nd(OH)(CO_3)$** *(s)*	21.39503		1	Original data for β: $log_{10}(\beta)$ = 19.9, at I = 0.1 M.
2 Nd^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Nd_2(CO_3)_3$** *(s)*	33.0		1	
2 Sm^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Sm_2(CO_3)_3$** *(s)*	32.5		1	
Eu^{3+} + $(OH)^-$ + $(CO_3)^{2-}$ ⇌ **$Eu(OH)(CO_3)$** *(s)*	21.69503		1	Original data for β: $log_{10}(\beta)$ = 20.2, at I = 0.1 M.
2 Eu^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Eu_2(CO_3)_3$** *(s)*	32.3		1	
2 Gd^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Gd_2(CO_3)_3$** *(s)*	32.2		1	
2 Dy^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Dy_2(CO_3)_3$** *(s)*	31.5		1	
2 Yb^{3+} + 3 $(CO_3)^{2-}$ ⇌ **$Yb_2(CO_3)_3$** *(s)*	31.1		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Hg(II)^{2+} + (CO_3)^{2-} \rightleftharpoons$ **$Hg(II)(CO_3)$ *(s)***	16.1		3	
$3\ Hg(II)^{2+} + 4\ (OH)^{-} + (CO_3)^{2-} \rightleftharpoons$ **$Hg(II)_3O_2(CO_3)$ *(s)***	67.088		1	$3\ Hg(II) + (CO_3) \rightleftharpoons Hg(II)_3(OH)_4(CO_3)(s) + 4\ H$ $\log_{10}(\beta) = 11.1$ $4\ H + 4\ OH \rightleftharpoons 4\ H_2O$ $\log_{10}(\beta) = 55.988$ $3\ Hg(II) + (CO_3) + 4\ OH \rightleftharpoons Hg(II)_3(OH)_4(CO_3)(s) + 4\ H_2O$ $\log_{10}(\beta) = 67.088$
$Pb(II)^{2+} + (CO_3)^{2-} \rightleftharpoons$ **$Pb(II)(CO_3)$ *(s)***	13.2		1	
$3\ Pb(II)^{2+} + 2\ (OH)^{-} + 2\ (CO_3)^{2-} \rightleftharpoons$ **$Pb(II)_3(CO_3)_2(OH)_2$ *(s)***	46.75227		1	Original data for β: $\log_{10}(\beta) = 43.8$, at I = 0.5 M.
$10\ Pb(II)^{2+} + 8\ (OH)^{-} + 6\ (CO_3)^{2-} \rightleftharpoons$ **$Pb(II)_{10}(CO_3)_6(OH)_6O$ *(s)***	120.736		1	$10\ Pb(II) + 6\ (CO_3) \rightleftharpoons Pb(II)_{10}(OH)_6O(CO_3)_6\ (s) + 8\ H$ $\log_{10}(\beta) = 8.76$ $8\ H + 8\ OH \rightleftharpoons 8\ H_2O$ $\log_{10}(\beta) = 111.976$ $10\ Pb(II) + 6\ (CO_3) + 8\ OH \rightleftharpoons Pb(II)_{10}(OH)_6O(CO_3)_6\ (s) + 8\ H_2O$ $\log_{10}(\beta) = 120.736$
$(U(VI)O_2)^{2+} + (CO_3)^{2-} \rightleftharpoons$ **$(U(VI)O_2)(CO_3)$ *(s)***	14.5		1	
$Ag^{+} + (NO_2)^{-} \rightleftharpoons$ **$Ag(NO_2)$ *(s)***	4.13	-6.20E+04	1	
$2\ Cu(II)^{2+} + 3\ (OH)^{-} + (NO_3)^{-} \rightleftharpoons$ **$Cu(II)_2(NO_3)(OH)_3$ *(s)***	32.74		1	
$Bi^{3+} + 2\ (OH)^{-} + (NO_3)^{-} \rightleftharpoons$ **$Bi(OH)_2(NO_3)$ *(s)***	30.544		1	$Bi + (NO_3) \rightleftharpoons BiO(NO_3) + 2\ H$ $\log_{10}(\beta) = 2.55$ $2\ H + 2\ OH \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.994$ $Bi + 2\ OH + (NO_3) \rightleftharpoons BiO(NO_3)$ $\log_{10}(\beta) = 30.544$
$Li^{+} + F^{-} \rightleftharpoons$ **LiF *(s)***	2.77	-4.6E+3	1	
$Na^{+} + F^{-} \rightleftharpoons$ **NaF *(s)***	0.49	-8E+2	1	
$Mg^{2+} + 2\ F^{-} \rightleftharpoons$ **MgF_2 *(s)***	8.11	8E+3	1	
$Al^{3+} + (OH)^{-} + 2\ F^{-} \rightleftharpoons$ **$AlF_2(OH)$ *(s)***	22.59		1	$Al(OH) + 2\ F \rightleftharpoons AlF_2(OH)$ $\log_{10}(\beta) = 13.59$ $Al + OH \rightleftharpoons Al(OH)$ $\log_{10}(\beta) = 9.00$ $Al + OH + 2\ F \rightleftharpoons AlF_2(OH)$ $\log_{10}(\beta) = 22.59$
$Ca^{2+} + 2\ F^{-} \rightleftharpoons$ **CaF_2 *(s)***	10.5	-1.2E+4	1	
$Sr^{2+} + 2\ F^{-} \rightleftharpoons$ **SrF_2 *(s)***	8.58	-4E+3	1	
$Y^{3+} + 3\ F^{-} \rightleftharpoons$ **YF_3 *(s)***	18.3		1	
$Ba^{2+} + 2\ F^{-} \rightleftharpoons$ **BaF_2 *(s)***	5.82	-4E+3	1	
$La^{3+} + 3\ F^{-} \rightleftharpoons$ **LaF_3 *(s)***	18.7		1	
$Ce^{3+} + 3\ F^{-} \rightleftharpoons$ **CeF_3 *(s)***	19.1		1	
$Pr^{3+} + 3\ F^{-} \rightleftharpoons$ **PrF_3 *(s)***	20.18145		1	Original data for β: $\log_{10}(\beta) = 18.9$, at I = 0.1 M.
$Nd^{3+} + 3\ F^{-} \rightleftharpoons$ **NdF_3 *(s)***	20.3		1	
$Sm^{3+} + 3\ F^{-} \rightleftharpoons$ **SmF_3 *(s)***	19.18145		1	Original data for β: $\log_{10}(\beta) = 17.9$, at I = 0.1 M.
$Eu^{3+} + 3\ F^{-} \rightleftharpoons$ **EuF_3 *(s)***	21.9		1	
$Gd^{3+} + 3\ F^{-} \rightleftharpoons$ **GdF_3 *(s)***	18.08145		1	Original data for β: $\log_{10}(\beta) = 16.8$, at I = 0.1 M.
$Tb^{3+} + 3\ F^{-} \rightleftharpoons$ **TbF_3 *(s)***	17.98145		1	Original data for β: $\log_{10}(\beta) = 16.7$, at I = 0.1 M.
$Dy^{3+} + 3\ F^{-} \rightleftharpoons$ **DyF_3 *(s)***	17.58145		1	Original data for β: $\log_{10}(\beta) = 16.3$, at I = 0.1 M.
$Ho^{3+} + 3\ F^{-} \rightleftharpoons$ **HoF_3 *(s)***	17.08145		1	Original data for β: $\log_{10}(\beta) = 15.8$, at I = 0.1 M.
$Er^{3+} + 3\ F^{-} \rightleftharpoons$ **ErF_3 *(s)***	18		1	
$Tm^{3+} + 3\ F^{-} \rightleftharpoons$ **TmF_3 *(s)***	17.08145		1	Original data for β: $\log_{10}(\beta) = 15.8$, at I = 0.1 M.
$Yb^{3+} + 3\ F^{-} \rightleftharpoons$ **YbF_3 *(s)***	16.28145		1	Original data for β: $\log_{10}(\beta) = 15.0$, at I = 0.1 M.
$Lu^{3+} + 3\ F^{-} \rightleftharpoons$ **LuF_3 *(s)***	16.28145		1	Original data for β: $\log_{10}(\beta) = 15.0$, at I = 0.1 M.
$Pb(II)^{2+} + 2\ F^{-} \rightleftharpoons$ **$Pb(II)F_2$ *(s)***	7.44		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$2\ H^+ + (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{SiO_2}$ ***(s)***	27.04		1	$H_2(H_2SiO_4) \rightleftharpoons SiO_2$ (s) $\log_{10}(\beta) = 4.0$ $2\ H + (H_2SiO_4) \rightleftharpoons H_2(H_2SiO_4)$ $\log_{10}(\beta) = 23.04$ $2\ H + (H_2SiO_4) \rightleftharpoons SiO_2$ (s) $\log_{10}(\beta) = 27.04$
$2\ H^+ + 2\ Mg^{2+} + 3\ (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Mg_2Si_3O_8(H_2O)_{3.5}}$ ***(s)***	51.932		1	$2\ Mg + 3\ H_2(H_2SiO_4) + 4\ OH \rightleftharpoons Mg_2Si_3O_8(H_2O)_{3.5} + 4.5\ H_2O$ $\log_{10}(\beta) = 38.8$ (Original data for β for 50°C) $6\ H + 3\ (H_2SiO_4) \rightleftharpoons 3\ H_2(H_2SiO_4)$ $\log_{10}(\beta) = 69.12$ $4\ H_2O \rightleftharpoons 4\ H + 4\ OH$ $\log_{10}(\beta) = -55.988$ $2\ Mg + 2\ H + 3\ (H_2SiO_4) \rightleftharpoons Mg_2Si_3O_8(H_2O)_{3.5}$ $\log_{10}(\beta) = 51.932$
$Ca^{2+} + (H_2SiO_4)^{2-} \rightleftharpoons \mathbf{Ca(H_2SiO_4)}$ ***(s)***	7.2		1	
$H^+ + Mg^{2+} + (NH_3)$ *(aq)* $+ (PO_4)^{3-} \rightleftharpoons \mathbf{MgNH_4PO_4}$ ***(s)***	21.844		6	$Mg + NH_4 + PO_4 \rightleftharpoons MgNH_4PO_4$ $\log_{10}(\beta) = 12.6$ $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ $Mg + NH_3 + H + PO_4 \rightleftharpoons MgNH_4PO_4$ $\log_{10}(\beta) = 21.844$
$H^+ + Mg^{2+} + (PO_4)^{3-} \rightleftharpoons \mathbf{MgH(PO_4)(H_2O)_3}$ ***(s)***	18.175		1	$Mg + H(PO_4) \rightleftharpoons MgH(PO_4)(H_2O)_3$ $\log_{10}(\beta) = 5.80$ $H + L \rightleftharpoons HL$ $\log_{10}(\beta) = 12.375$ $Mg + (PO_4) + L \rightleftharpoons Mg(PO_4)L$ $\log_{10}(\beta) = 18.175$
$3\ Mg^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Mg_3(PO_4)_2}$ ***(s)***	23.28		1	
$Al^{3+} + (PO_4)^{3-} \rightleftharpoons \mathbf{Al(PO_4)}$ ***(s)***	20.48087		1	Original data for β: $\log_{10}(\beta) = 18.34$, at I = 0.15 M and 37°C.
$3\ Al^{3+} + 3\ (OH)^- + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Al_3(PO_4)_2(OH)_3(H_2O)_5}$ ***(s)***	78.851		7	$3\ Al + 2\ PO_4 + 8\ H_2O \rightleftharpoons Al_3(PO_4)_2(OH)_3(H_2O)5 + 3\ H$ $\log_{10}(\beta) = 36.86$ $3\ OH + 3\ H \rightleftharpoons 3\ H_2O$ $\log_{10}(\beta) = 41.991$ $3\ Al + 2\ PO_4 + 3\ OH \rightleftharpoons Al_3(PO_4)_2(OH)_3(H_2O)_5$ $\log_{10}(\beta) = 78.851$
$10\ Ca^{2+} + 2\ F^- + 6\ (PO_4)^{3-} \rightleftharpoons \mathbf{Ca_{10}(PO_4)_6F_2}$ ***(s)***	118		6	
$H^+ + Ca^{2+} + (PO_4)^{3-} \rightleftharpoons \mathbf{CaH(PO_4)}$ ***(s)***	19.275	-3.1E+4	1	$Ca + H(PO_4) \rightleftharpoons CaH(PO_4)(H_2O)_2$ $\log_{10}(\beta) = 6.90$ ΔH = -1.6E+4 $H + (PO_4) \rightleftharpoons H(PO_4)$ $\log_{10}(\beta) = 12.375$ ΔH = -1.5E+4 $Ca + H + (PO_4) \rightleftharpoons CaH(PO_4)$ $\log_{10}(\beta) = 19.275$ ΔH = -3.1E+4
$4\ H^+ + Ca^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Ca(H_2PO_4)_2(H_2O)}$ ***(s)***	40.296		7	$Ca + 2\ H_2PO_4 + H_2O \rightleftharpoons Ca(H_2PO_4)_2(H_2O)$ $\log_{10}(\beta) = 1.15$ $4\ H + 2\ PO_4 \rightleftharpoons 2\ H_2PO_4$ $\log_{10}(\beta) = 39.146$ $Ca + 4\ H + 2\ PO_4 \rightleftharpoons CaH_4(PO_4)_2$ $\log_{10}(\beta) = 40.296$
$2\ Ca^{2+} + (OH)^- + (PO_4)^{3-} \rightleftharpoons \mathbf{Ca_2(HPO_4)(OH)_2}$ ***(s)***	25.727		6	$Ca_{10}(PO_4)_6(OH)_2 + 6\ H_2O \rightleftharpoons 4\ Ca_2(HPO_4)(OH)_2 + 2\ Ca + 2\ HPO_4$ $\log_{10}(\beta) = -17$ $10\ Ca + 6\ PO_4 + 2\ OH \rightleftharpoons Ca_{10}(PO_4)_6(OH)_2$ $\log_{10}(\beta) = 116.66$ $2\ HPO_4 \rightleftharpoons 2\ PO_4 + 2\ H$ $\log_{10}(\beta) = -24.75$ $2\ OH + 2\ H \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.994$ $8\ Ca + 4\ PO_4 + 4\ OH + 4\ H_2O \rightleftharpoons 4\ Ca_2(HPO_4)(OH)_2$ $\log_{10}(\beta) = 102.904$ Divide by 4: $2\ Ca + PO_4 + OH + H_2O \rightleftharpoons Ca_2(HPO_4)(OH)_2$ $\log_{10}(\beta) = 25.727$
$3\ Ca^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Ca_3(PO_4)_2}$ ***(s)***	28.92	-5.4E+4	1	
$4\ Ca^{2+} + H^+ + 3\ (PO_4)^{3-} \rightleftharpoons \mathbf{Ca_4H(PO_4)_3(H_2O)_3}$ ***(s)***	47.08		1	
$5\ Ca^{2+} + (OH)^- + 3\ (PO_4)^{3-} \rightleftharpoons \mathbf{Ca_5(PO_4)_3(OH)}$ ***(s)***	58.33		1	
$H^+ + Fe(II)^{2+} + (NH_3)$ *(aq)* $+ (PO_4)^{3-} \rightleftharpoons \mathbf{Fe(II)NH_4PO_4}$ ***(s)***	22.244		6	$Fe(II) + NH_4 + PO_4 \rightleftharpoons Fe(II)NH_4PO_4$ $\log_{10}(\beta) = 13$ $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ $Fe(II) + NH_3 + H + PO_4 \rightleftharpoons Fe(II)NH_4PO_4$ $\log_{10}(\beta) = 22.244$
$3\ Fe(II)^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Fe(II)_3(PO_4)_2(H_2O)_8}$ ***(s)***	37.76	-5.06E+03	1	
$Fe(III)^{3+} + (PO_4)^{3-} \rightleftharpoons \mathbf{Fe(III)(PO_4)(H_2O)_2}$ ***(s)***	26.4		1	
$3\ Zn^{2+} + 2\ (PO_4)^{3-} \rightleftharpoons \mathbf{Zn_3(PO_4)_2(H_2O)_4}$ ***(s)***	35.42		1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
Ga^{3+} + $(PO_4)^{3-}$ ⇌ **$Ga(PO_4)$** ***(s)***	22.82844		1	Original data for β: $log_{10}(\beta)$ = 21.0, at I = 1.0 M.
Sr^{2+} + H^{+} + $(PO_4)^{3-}$ ⇌ **$SrH(PO_4)$** ***(s)***	19.295		1	Sr + $H(PO_4)$ ⇌ $SrH(PO_4)$ $log_{10}(\beta)$ = 6.92 (Original data for β for 20°C) H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 12.375 Sr + H + (PO_4) ⇌ $SrH(PO_4)$ $log_{10}(\beta)$ = 19.295
Y^{3+} + $(PO_4)^{3-}$ ⇌ **$Y(PO_4)$** ***(s)***	25.02		1	
3 Ag^{+} + $(PO_4)^{3-}$ ⇌ **$Ag_3(PO_4)$** ***(s)***	17.59		1	
5 Cd^{2+} + 2 H^{+} + 4 $(PO_4)^{3-}$ ⇌ **$Cd_5H_2(PO_4)_4(H_2O)_4$** ***(s)***	70.30613		1	5 Cd + 4 $H(PO_4)$ ⇌ 2 H + $Cd_5H_2(PO_4)_4(H_2O)_4$ log10(β) = 25.4 I = 3.0 M 4 H + 4 (PO_4) ⇌ 4 $H(PO_4)$ log10(β) = 52.74276 I = 3.0 M 5 Cd + 2 H + 4 (PO_4) ⇌ Cd5H2$(PO_4)_4(H_2O)_4$ log10(β) = 78.14276 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 70.30613
In^{3+} + $(PO_4)^{3-}$ ⇌ **$In(PO_4)$** ***(s)***	23.45844		1	Original data for β: $log_{10}(\beta)$ = 21.63, at I = 1.0 M.
Ba^{2+} + H^{+} + $(PO_4)^{3-}$ ⇌ **$BaH(PO_4)$** ***(s)***	19.775		1	Ba + $H(PO_4)$ ⇌ $BaH(PO_4)$ $log_{10}(\beta)$ = 7.4 (Original data for β for 20°C) H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 12.375 Ba + H + (PO_4) ⇌ $BaH(PO_4)$ $log_{10}(\beta)$ = 19.295
La^{3+} + $(PO_4)^{3-}$ ⇌ **$La(PO_4)$** ***(s)***	25.75		1	
Ce^{3+} + $(PO_4)^{3-}$ ⇌ **$Ce(PO_4)$** ***(s)***	26.3		1	
Pr^{3+} + $(PO_4)^{3-}$ ⇌ **$Pr(PO_4)$** ***(s)***	26.4		1	
Nd^{3+} + $(PO_4)^{3-}$ ⇌ **$Nd(PO_4)$** ***(s)***	26.2		1	
Sm^{3+} + $(PO_4)^{3-}$ ⇌ **$Sm(PO_4)$** ***(s)***	26.19		1	
Eu^{3+} + $(PO_4)^{3-}$ ⇌ **$Eu(PO_4)$** ***(s)***	25.96		1	
Gd^{3+} + $(PO_4)^{3-}$ ⇌ **$Gd(PO_4)$** ***(s)***	25.6		1	
Tb^{3+} + $(PO_4)^{3-}$ ⇌ **$Tb(PO_4)$** ***(s)***	25.39		1	
Dy^{3+} + $(PO_4)^{3-}$ ⇌ **$Dy(PO_4)$** ***(s)***	25.2		1	
Ho^{3+} + $(PO_4)^{3-}$ ⇌ **$Ho(PO_4)$** ***(s)***	25.1		1	
Er^{3+} + $(PO_4)^{3-}$ ⇌ **$Er(PO_4)$** ***(s)***	25.1		1	
Tm^{3+} + $(PO_4)^{3-}$ ⇌ **$Tm(PO_4)$** ***(s)***	25		1	
Yb^{3+} + $(PO_4)^{3-}$ ⇌ **$Yb(PO_4)$** ***(s)***	24.9		1	
Lu^{3+} + $(PO_4)^{3-}$ ⇌ **$Lu(PO_4)$** ***(s)***	24.8		1	
H^{+} + $Hg(II)^{2+}$ + $(PO_4)^{3-}$ ⇌ **$Hg(II)H(PO_4)$** ***(s)***	24.39409		1	Hg(II) + $H(PO_4)$ ⇌ $Hg(II)H(PO_4)$ $log_{10}(\beta)$ = 13.1 I = 3.0 M H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 13.18569 I = 3.0 M Hg(II) + H + (PO_4) ⇌ $Hg(II)H(PO_4)$ $log_{10}(\beta)$ = 26.28569 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 24.39409
3 $Hg(II)^{2+}$ + 3 $(OH)^{-}$ + $(PO_4)^{3-}$ ⇌ **$Hg(II)_3(PO_4)(OH)_3$** ***(s)***	62.14464		1	3 Hg(II) + $H(PO_4)$ ⇌ 4 H + $Hg(II)_3(OH)_3(PO_4)$ $log_{10}(\beta)$ = 9.4 I = 3.0 M H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 13.18569 I = 3.0 M 3 H + 3 OH ⇌ 3 H_2O $log_{10}(\beta)$ = 42.80169 I = 3.0 M 3 Hg(II) + (PO_4) + 3 OH ⇌ $Hg(II)_3(OH)_3(PO_4)$ $log_{10}(\beta)$ = 65.38738 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 62.14464

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
3 $Hg(II)^{2+}$ + 2 $(PO_4)^{3-}$ ⇌ **$Hg(II)_3(PO_4)_2$ *(s)***	46.91795		1	3 Hg(II) + 2 HL ⇌ 2 H + $Hg(II)_3L_2$ $log_{10}(\beta)$ = 24.6 I = 3.0 M 2 H + 2 L ⇌ 2 HL $log_{10}(\beta)$ = 26.37138 I = 3.0 M 3 Hg(II) + 2 L ⇌ $Hg(II)_3L_2$ $log_{10}(\beta)$ = 50.97138 I = 3.0 M I = 0 M: $log_{10}(\beta)$ = 46.91795
H^+ + $Pb(II)^{2+}$ + $(PO_4)^{3-}$ ⇌ **$Pb(II)H(PO_4)$ *(s)***	23.805		1	Pb(II) + $H(PO_4)$ ⇌ $Pb(II)H(PO_4)$ $log_{10}(\beta)$ = 11.43 H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 12.375 Pb(II) + H + (PO_4) ⇌ $Pb(II)H(PO_4)$ $log_{10}(\beta)$ = 23.805
3 $Pb(II)^{2+}$ + 2 $(PO_4)^{3-}$ ⇌ **$Pb(II)_3(PO_4)_2$ *(s)***	43.53		1	Original data for β at 37°C.
5 $Pb(II)^{2+}$ + $(OH)^-$ + 3 $(PO_4)^{3-}$ ⇌ **$Pb(II)_5(PO_4)_3(OH)$ *(s)***	76.856		7	5 Pb + 3 H_2PO_4 + H_2O ⇌ $Pb_5(PO_4)_3OH$ + 7 H $log_{10}(\beta)$ = 4.14 6 H + 3 PO_4 ⇌ 3 H_2PO_4 $log_{10}(\beta)$ = 58.719 OH + H ⇌ H_2O $log_{10}(\beta)$ = 13.997 5 Pb + 3 PO_4 + OH ⇌ $Pb_5(PO_4)_3OH$ $log_{10}(\beta)$ = 76.856
H^+ + $(U(VI)O_2)^{2+}$ + $(PO_4)^{3-}$ ⇌ **$(U(VI)O_2)H(PO_4)$ *(s)***	24.225		1	(UO_2) + $H(PO_4)$ ⇌ $(UO_2)H(PO_4)$ $log_{10}(\beta)$ = 11.85 H + (PO_4) ⇌ $H(PO_4)$ $log_{10}(\beta)$ = 12.375 (UO_2) + H + (PO_4) ⇌ $(UO_2)H(PO_4)$ $log_{10}(\beta)$ = 24.225
3 $(U(VI)O_2)^{2+}$ + 2 $(PO_4)^{3-}$ ⇌ **$(U(VI)O_2)_3(PO_4)_2$ *(s)***	49.4		1	
Be^{2+} + S^{2-} ⇌ **BeS *(s)***	-5.48		1	Be + H_2S ⇌ 2 H + BeS *(s)* $log_{10}(\beta)$ = -26.4 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Be + S ⇌ BeS *(s)* $log_{10}(\beta)$ = -5.48
Mg^{2+} + S^{2-} ⇌ **MgS *(s)***	-3.78		1	Mg + H_2S ⇌ 2 H + MgS *(s)* $log_{10}(\beta)$ = -24.7 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Mg + S ⇌ MgS *(s)* $log_{10}(\beta)$ = -3.78
Ca^{2+} + S^{2-} ⇌ **CaS *(s)***	2.72		1	Ca + H_2S ⇌ 2 H + CaS *(s)* $log_{10}(\beta)$ = -18.2 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Ca + S ⇌ CaS *(s)* $log_{10}(\beta)$ = 2.72
$Mn(II)^{2+}$ + S^{2-} ⇌ **Mn(II)S *(s)***	13.92		1	Mn(II) + H_2S ⇌ 2 H + Mn(II)S *(s)* $log_{10}(\beta)$ = -7 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Mn(II) + S ⇌ Mn(II)S *(s)* $log_{10}(\beta)$ = 13.92
$Fe(II)^{2+}$ + S^{2-} ⇌ **Fe(II)S *(s)***	17.92		1	Fe(II) + H_2S ⇌ 2 H + Fe(II)S *(s)* $log_{10}(\beta)$ = -3 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Fe(II) + S ⇌ Fe(II)S *(s)* $log_{10}(\beta)$ = 17.92
$Co(II)^{2+}$ + S^{2-} ⇌ **Co(II)S *(s)***	25.62		1	Co(II) + H_2S ⇌ 2 H + Co(II)S *(s)* $log_{10}(\beta)$ = 4.7 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Co(II) + S ⇌ Co(II)S *(s)* $log_{10}(\beta)$ = 25.62
Ni^{2+} + S^{2-} ⇌ **NiS *(s)***	26.62		1	Ni + H_2S ⇌ 2 H + NiS *(s)* $log_{10}(\beta)$ = 5.7 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Ni + S ⇌ NiS *(s)* $log_{10}(\beta)$ = 26.62
2 $Cu(I)^+$ + S^{2-} ⇌ **$Cu(I)_2S$ *(s)***	48.82		1	2 Cu(I) + H_2S ⇌ 2 H + $Cu(I)_2S$ *(s)* $log_{10}(\beta)$ = 27.9 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 2 Cu(I) + S ⇌ $Cu(I)_2S$ *(s)* $log_{10}(\beta)$ = 48.82
$Cu(II)^{2+}$ + S^{2-} ⇌ **Cu(II)S *(s)***	36.12		1	Cu(II) + H_2S ⇌ 2 H + Cu(II)S *(s)* $log_{10}(\beta)$ = 15.2 2 H + S ⇌ H_2S $log_{10}(\beta)$ = 20.92 Cu(II) + S ⇌ Cu(II)S *(s)* $log_{10}(\beta)$ = 36.12

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Zn^{2+} + S^{2-} \rightleftharpoons \mathbf{ZnS}$ ***(s)***	24.72		1	$Zn + H_2S \rightleftharpoons 2\ H + ZnS$ *(s)* $log_{10}(\beta) = 3.8$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Zn + S \rightleftharpoons ZnS$ *(s)* $log_{10}(\beta) = 24.72$
$Sr^{2+} + S^{2-} \rightleftharpoons \mathbf{SrS}$ ***(s)***	0.02		1	$Sr + H_2S \rightleftharpoons 2\ H + SrS$ *(s)* $log_{10}(\beta) = -20.9$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Sr + S \rightleftharpoons SrS$ *(s)* $log_{10}(\beta) = 0.02$
$2\ Ag^{+} + S^{2-} \rightleftharpoons \mathbf{Ag_2S}$ ***(s)***	50.12		1	$2\ Ag + H_2S \rightleftharpoons 2\ H + Ag_2S$ *(s)* $log_{10}(\beta) = 29.2$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $2\ Ag + S \rightleftharpoons Ag_2S$ *(s)* $log_{10}(\beta) = 50.12$
$Cd^{2+} + S^{2-} \rightleftharpoons \mathbf{CdS}$ ***(s)***	27.92		1	$Cd + H_2S \rightleftharpoons 2\ H + CdS$ (s) $log_{10}(\beta) = 7.0$ $2\ H + S \rightleftharpoons H2S$ $log_{10}(\beta) = 20.92$ $Cd + S \rightleftharpoons CdS$ (s) $log_{10}(\beta) = 27.02$
$2\ In^{3+} + 3\ S^{2-} \rightleftharpoons \mathbf{In_2S_3}$ ***(s)***	78.97896		1	$2\ In + 3\ H_2S \rightleftharpoons 6\ H + In_2S_3$ $log_{10}(\beta) = 15$ I = 1.0 M (Original data for β for 20°C) $6\ H + 3\ S \rightleftharpoons 3\ H_2S$ $log_{10}(\beta) = 60.93156$ I = 1.0 M $2\ In + 3\ S \rightleftharpoons In_2S_3$ $log_{10}(\beta) = 75.93156$ I = 1.0 M I = 0 M: $log_{10}(\beta) = 78.97896$
$Sn(II)^{2+} + S^{2-} \rightleftharpoons \mathbf{Sn(II)S}$ ***(s)***	25.92		1	$Sn(II) + H_2S \rightleftharpoons 2\ H + Sn(II)S$ *(s)* $log_{10}(\beta) = 5.0$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Sn(II) + S \rightleftharpoons Sn(II)S$ *(s)* $log_{10}(\beta) = 25.92$
$Ba^{2+} + S^{2-} \rightleftharpoons \mathbf{BaS}$ ***(s)***	-2.28		1	$Ba + H_2S \rightleftharpoons 2\ H + BaS$ *(s)* $log_{10}(\beta) = -23.3$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Ba + S \rightleftharpoons BaS$ *(s)* $log_{10}(\beta) = -2.28$
$Hg(II)^{2+} + S^{2-} \rightleftharpoons \mathbf{Hg(II)S}$ ***(s)***	53.02		1	$Hg(II) + H_2S \rightleftharpoons 2\ H + Hg(II)S$ *(s)* $log_{10}(\beta) = 32.1$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Hg(II) + S \rightleftharpoons Hg(II)S$ *(s)* $log_{10}(\beta) = 53.02$
$Pb(II)^{2+} + S^{2-} \rightleftharpoons \mathbf{Pb(II)S}$ ***(s)***	28.82		1	$Pb(II) + H_2S \rightleftharpoons 2\ H + Pb(II)S$ *(s)* $log_{10}(\beta) = 7.9$ $2\ H + S \rightleftharpoons H_2S$ $log_{10}(\beta) = 20.92$ $Pb(II) + S \rightleftharpoons Pb(II)S$ *(s)* $log_{10}(\beta) = 28.82$
$2\ Bi^{3+} + 3\ S^{2-} \rightleftharpoons \mathbf{Bi_2S_3}$ ***(s)***	82.76		1	$2\ Bi + 3\ H_2S \rightleftharpoons 6\ H + Bi_2S_3$ $log_{10}(\beta) = 20$ $6\ H + 3\ S \rightleftharpoons 3\ H_2S$ $log_{10}(\beta) = 62.76$ $2\ Bi + 3\ S \rightleftharpoons Bi_2S_3$ $log_{10}(\beta) = 82.76$
$Ca^{2+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Ca(SO_3)(H_2O)_{0.5}}$ ***(s)***	6.64		1	
$2\ Ag^{+} + (SO_3)^{2-} \rightleftharpoons \mathbf{Ag_2(SO_3)}$ ***(s)***	13.82		1	
$K^{+} + 3\ Fe(III)^{3+} + 6\ (OH)^{-} + 2\ (SO_4)^{2-} \rightleftharpoons \mathbf{KFe(III)_3(SO_4)_2(OH)_6}$ ***(s)***	96.492		7	$Fe(III) + K + 2\ SO_4 + 6\ H_2O \rightleftharpoons KFe_3(SO_4)_2(OH)_6 + 6\ H$ $log_{10}(\beta) = 12.51$ $6\ OH + 6\ H \rightleftharpoons 6\ H_2O$ $log_{10}(\beta) = 83.982$ $Fe(III) + K + 2\ SO_4 + 6\ OH \rightleftharpoons KFe_3(SO_4)_2(OH)_6$ $log_{10}(\beta) = 96.492$
$Ca^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Ca(SO_4)(H_2O)_2}$ ***(s)***	4.61	-1E+3	1	
$4\ Cu(II)^{2+} + 6\ (OH)^{-} + (SO_4)^{2-} \rightleftharpoons \mathbf{Cu(II)_4(SO_4)(OH)_6}$ ***(s)***	68.76	-1.32E+5	1	
$Sr^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Sr(SO_4)}$ ***(s)***	6.62	-2E+3	1	
$2\ Ag^{+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Ag_2(SO_4)}$ ***(s)***	4.82	-1.7E+4	1	
$Ba^{2+} + (SO_4)^{2-} \rightleftharpoons \mathbf{Ba(SO_4)}$ ***(s)***	9.98	-2.3E+4	1	

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Pb(II)^{2+} + (SO_4)^{2-} \rightleftharpoons$ **$Pb(II)(SO_4)$** ***(s)***	7.79	-1.2E+4	1	
$Li^{+} + Cl^{-} \rightleftharpoons$ **LiCl** ***(s)***	6.89	-3.6E+4	1	
$Na^{+} + Cl^{-} \rightleftharpoons$ **NaCl** ***(s)***	-1.55		1	
$K^{+} + Cl^{-} \rightleftharpoons$ **KCl** ***(s)***	-0.90		1	
$Cu(I)^{+} + Cl^{-} \rightleftharpoons$ **Cu(I)Cl** ***(s)***	6.73		1	
$2\ Zn^{2+} + 3\ (OH)^{-} + Cl^{-} \rightleftharpoons$ **$Zn_2Cl(OH)_3$** ***(s)***	26.8		3	
$Ag^{+} + Cl^{-} \rightleftharpoons$ **AgCl** ***(s)***	9.750	-6.52E+4	1	
$5\ Pb(II)^{2+} + 3\ (PO_4)^{3-} + Cl^{-} \rightleftharpoons$ **$Pb(II)_5(PO_4)_3Cl$** ***(s)***	83.769		7	$5\ Pb + 3\ H_2PO_4 + Cl \rightleftharpoons Pb_5(PO_4)_3Cl + 6\ H$ $\log_{10}(\beta) = 25.05$ $6\ H + 3\ PO_4 \rightleftharpoons 3H_2PO_4$ $\log_{10}(\beta) = 58.719$ $5\ Pb + 3\ PO_4 + Cl \rightleftharpoons Pb_5(PO_4)_3Cl$ $\log_{10}(\beta) = 83.769$
$Pb(II)^{2+} + 2\ Cl^{-} \rightleftharpoons$ **$Pb(II)Cl_2$** ***(s)***	4.78		1	
$Bi^{3+} + 2\ (OH)^{-} + Cl^{-} \rightleftharpoons$ **BiOCl** ***(s)***	35.796		1	$Bi + L \rightleftharpoons BiOL + 2\ H$ $\log_{10}(\beta) = 7.80$ $2\ H + 2\ OH \rightleftharpoons 2\ H_2O$ $\log_{10}(\beta) = 27.996$ $Bi + 2\ OH + L \rightleftharpoons BiOL + 2\ H_2O$ $\log_{10}(\beta) = 35.796$
$6\ H^{+} + 2\ (VO_4)^{3-} \rightleftharpoons$ **V_2O_5** ***(s)***	61.66	-1.724E+5	1	$2\ VO_2 \rightleftharpoons (V_2O_5)\ (s) + 2\ H$ $\log_{10}(\beta) = 1.36$ ΔH = -3.4E+4 $8\ H + 2\ (VO_4) \rightleftharpoons 2\ VO_2$ $\log_{10}(\beta) = 60.30$ ΔH = -1.384E+5 $6\ H + 2\ (VO_4) \rightleftharpoons (V_2O_5)\ (s)$ $\log_{10}(\beta) = 61.66$ ΔH = -1.724E+5
$3\ H^{+} + (NH_3)$ *(aq)* $+ (VO_4)^{3-} \rightleftharpoons$ **$NH_4(VO_3)$** ***(s)***	35.594	-1.182E+5	1	$NH_4 + H_2(VO_4) \rightleftharpoons (NH_4)VO_3$ $\log_{10}(\beta) = 3.5$ ΔH = -3.00E+4 $NH_3 + H \rightleftharpoons NH_4$ $\log_{10}(\beta) = 9.244$ ΔH = -5.20E+4 $2\ H + (VO_4) \rightleftharpoons H_2(VO_4)$ $\log_{10}(\beta) = 22.85$ ΔH = -3.62E+4 $NH3 + 3\ H + (VO_4) \rightleftharpoons (NH_4)VO_3$ $\log_{10}(\beta) = 35.594$ ΔH = -1.182E+5
$4\ H^{+} + Ca^{2+} + 2\ (VO_4)^{3-} \rightleftharpoons$ **$Ca(VO_3)_2(H_2O)_4$** ***(s)***	55.31896		1	$2\ Ca + V_4O_{12} \rightleftharpoons 2\ Ca(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 8.20$ I = 1.0 M (Original data for β for 20°C) $8\ H + 4\ L \rightleftharpoons V_4O_{12}$ $\log_{10}(\beta) = 97.15576$ I = 1.0 M $2\ Ca + 8\ H + 4\ L \rightleftharpoons 2\ Ca(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 105.35576$ I = 1.0 M divide by 2: $Ca + 4\ H + 2\ L \rightleftharpoons Ca(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 52.67788$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 55.31896$
$3\ Ca^{2+} + 2\ (VO_4)^{3-} \rightleftharpoons$ **$Ca_3(VO_4)_2(H_2O)_4$** ***(s)***	20.52740		1	Original data for β: $\log_{10}(\beta) = 17.48$, at I = 1.0 M and 20°C.
$4\ H^{+} + Sr^{2+} + 2\ (VO_4)^{3-} \rightleftharpoons$ **$Sr(VO_3)_2(H_2O)_4$** ***(s)***	60.21896		1	$2\ Sr + V_4O_{12} \rightleftharpoons 2\ Sr(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 18.0$ I = 1.0 M (Original data for β for 20°C) $8\ H + 4\ L \rightleftharpoons V_4O_{12}$ $\log_{10}(\beta) = 97.15576$ I = 1.0 M $2\ Sr + 8\ H + 4\ L \rightleftharpoons 2\ Sr(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 115.15576$ I = 1.0 M divide by 2: $Sr + 4\ H + 2\ L \rightleftharpoons Sr(VO_3)_2(H_2O)_4$ $\log_{10}(\beta) = 57.57788$ I = 1.0 M I = 0 M: $\log_{10}(\beta) = 60.21896$
$3\ Sr^{2+} + 2\ (VO_4)^{3-} \rightleftharpoons$ **$Sr_3(VO_4)_2(H_2O)_4$** ***(s)***	23.64740		1	Original data for β: $\log_{10}(\beta) = 20.60$, at I = 1.0 M and 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
4 H^+ + Ba^{2+} + 2 $(VO_4)^{3-}$ $\rightleftharpoons$ **$Ba(VO_3)_2(H_2O)_4$ *(s)***	63.13896		1	2 Ba + V_4O_{12} $\rightleftharpoons$ 2 $Ba(VO_3)_2(H_2O)_4$ $\log_{10}(\beta)$ = 23.84 I = 1.0 M (Original data for β for 20°C) 8 H + 4 L $\rightleftharpoons$ V_4O_{12} $\log_{10}(\beta)$ = 97.15576 I = 1.0 M 2 Ba + 8 H + 4 L $\rightleftharpoons$ 2 $Ba(VO_3)_2(H_2O)_4$ $\log_{10}(\beta)$ = 120.99576 I = 1.0 M divide by 2: Ba + 4 H + 2 L $\rightleftharpoons$ $Ba(VO_3)_2(H_2O)_4$ $\log_{10}(\beta)$ = 60.49788 I = 1.0 M I = 0 M: $\log_{10}(\beta)$ = 63.13896
3 Ba^{2+} + 2 $(VO_4)^{3-}$ $\rightleftharpoons$ **$Ba_3(VO_4)_2(H_2O)_4$ *(s)***	27.44740		1	Original data for β: $\log_{10}(\beta)$ = 24.40, at I = 1.0 M and 20°C.
2 H^+ + 2 Na^+ + 2 $(CrO_4)^{2-}$ $\rightleftharpoons$ **$Na_2Cr_2O_7$ *(s)***	12.12		1	2 Na + Cr_2O_7 $\rightleftharpoons$ $Na_2Cr_2O_7(H_2O)_2$ $\log_{10}(\beta)$ = -2.42 2 H + 2 (CrO_4) $\rightleftharpoons$ Cr_2O_7 $\log_{10}(\beta)$ = 14.54 2 Na + 2 H + 2 (CrO_4) $\rightleftharpoons$ $Na_2Cr_2O_7(H_2O)_2$ $\log_{10}(\beta)$ = 12.12
$Cu(II)^{2+}$ + $(CrO_4)^{2-}$ $\rightleftharpoons$ **$Cu(II)(CrO_4)$ *(s)***	5.44		1	
2 Ag^+ + $(CrO_4)^{2-}$ $\rightleftharpoons$ **$Ag_2(CrO_4)$ *(s)***	11.59	-5.8E+4	1	
Ba^{2+} + $(CrO_4)^{2-}$ $\rightleftharpoons$ **$Ba(CrO_4)$ *(s)***	9.67	-6.6E+4	1	
$Pb(II)^{2+}$ + $(CrO_4)^{2-}$ $\rightleftharpoons$ **$Pb(II)(CrO_4)$ *(s)***	12.6	-4.418E+4	1	
Ag^+ + $(MnO_4)^-$ $\rightleftharpoons$ **$Ag(MnO_4)$ *(s)***	9.88	-2.9E+4	1	
4 H^+ + 4 $(H_2AsO_3)^-$ $\rightleftharpoons$ **As_4O_6 *(s)***	40.04		1	4 $H(H_2AsO_3)^-$ $\rightleftharpoons$ As_4O_6 + 6 H_2O $\log_{10}(\beta)$ = 2.76 4 H + 4 (H_2AsO_3) $\rightleftharpoons$ 4 $H(H_2AsO_3)$ $\log_{10}(\beta)$ = 37.28 4 H + 4 (H_2AsO_3) $\rightleftharpoons$ As_4O_6 $\log_{10}(\beta)$ = 40.04
3 Ag^+ + 2 $(OH)^-$ + $(H_2AsO_3)^-$ $\rightleftharpoons$ **Ag_3AsO_3 *(s)***	59.93409		1	3 Ag + (H_2AsO_3) $\rightleftharpoons$ Ag_3AsO_3 + 2 H $\log_{10}(\beta)$ = 31.3 I = 0.1 M 2 H + 2 OH $\rightleftharpoons$ 2 H_2O $\log_{10}(\beta)$ = 27.99336 I = 0.1 M 3 Ag + (H_2AsO_3) + 2 OH $\rightleftharpoons$ Ag_2AsO_3 $\log_{10}(\beta)$ = 59.29336 I = 0.1 M I = 0 M: $\log_{10}(\beta)$ = 59.93409
Sc^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$ScAsO_4$ *(s)***	26.7		1	
Y^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$YAsO_4$ *(s)***	22.6		1	
3 Ag^+ + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$Ag_3(AsO_4)$ *(s)***	23.48145		1	Original data for β: $\log_{10}(\beta)$ = 22.2, at I = 0.1 M and 20°C.
La^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$LaAsO_4$ *(s)***	21.4		1	
Pr^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$PrAsO_4$ *(s)***	22.0		1	
Nd^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$NdAsO_4$ *(s)***	21.9		1	
Sm^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$SmAsO_4$ *(s)***	22.7		1	
Eu^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$EuAsO_4$ *(s)***	22.5		1	
Gd^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$GdAsO_4$ *(s)***	21.7		1	
Tb^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$TbAsO_4$ *(s)***	23.1		1	
Dy^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$DyAsO_4$ *(s)***	23.8		1	
Ho^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$HoAsO_4$ *(s)***	22.9		1	
Er^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$ErAsO_4$ *(s)***	22.5		1	
Tm^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$TmAsO_4$ *(s)***	23.1		1	
Yb^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$YbAsO_4$ *(s)***	22.7		1	
Lu^{3+} + $(AsO_4)^{3-}$ $\rightleftharpoons$ **$LuAsO_4$ *(s)***	22.7		1	
2 Na^+ + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Na_2(SeO_3)(H_2O)_5$ *(s)***	-1.9		1	
Mg^{2+} + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Mg(SeO_3)(H_2O)_6$ *(s)***	5.36		1	Original data for β at 20°C.
$Mn(II)^{2+}$ + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Mn(II)(SeO_3)$ *(s)***	7.27		1	Original data for β at 20°C.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Co(II)^{2+}$ + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Co(II)(SeO_3)$** ***(s)***	7.08		1	Original data for β at 20°C.
$Cu(II)^{2+}$ + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Cu(II)(SeO_3)(H_2O)_2$** ***(s)***	7.78		1	Original data for β at 20°C.
Sr^{2+} + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Sr(SeO_3)$** ***(s)***	6.10		1	Original data for β at 20°C.
2 Ag^{+} + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Ag_2(SeO_3)$** ***(s)***	15.55	-4.47E+4	1	
Ba^{2+} + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Ba(SeO_3)$** ***(s)***	6.57	-1.7E+4	1	
$Hg(II)^{2+}$ + $(SeO_3)^{2-}$ $\rightleftharpoons$ **$Hg(II)(SeO_3)$** ***(s)***	14.63264		1	Original data for β: $log_{10}(\beta)$ = 13.82, at I = 1.0 M.
2 H^{+} + 2 (NH_3) *(aq)* + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$(NH_4)_2(SeO_4)$** ***(s)***	18.038		1	2 (NH_4) + (SeO_4) $\rightleftharpoons$ $(NH_4)_2(SeO_4)$ $log_{10}(\beta)$ = -0.45 2 H + 2 NH_3 $\rightleftharpoons$ 2 NH_4 $log_{10}(\beta)$ = 18.488 2 H + 2 NH_3 + (SeO_4) $\rightleftharpoons$ $(NH_4)_2(SeO_4)$ $log_{10}(\beta)$ = 18.038
2 Li^{+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Li_2(SeO_4)(H_2O)$** ***(s)***	-2.05		1	
Be^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Be(SeO_4)(H_2O)_4$** ***(s)***	2.94		1	
2 Na^{+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Na_2(SeO_4)$** ***(s)***	-1.28		1	
Mg^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Mg(SeO_4)(H_2O)_6$** ***(s)***	1.2		1	
2 K^{+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$K_2(SeO_4)$** ***(s)***	0.73		1	
Ca^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Ca(SeO_4)(H_2O)_2$** ***(s)***	3.02	8.3E+3	1	
$Mn(II)^{2+}$ + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Mn(II)(SeO_4)(H_2O)_5$** ***(s)***	2.05		1	
$Co(II)^{2+}$ + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Co(II)(SeO_4)(H_2O)_6$** ***(s)***	1.53		1	
Ni^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Ni(SeO_4)(H_2O)_6$** ***(s)***	1.52		1	
$Cu(II)^{2+}$ + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Cu(II)(SeO_4)(H_2O)_5$** ***(s)***	2.44		1	
Zn^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Zn(SeO_4)(H_2O)_6$** ***(s)***	1.52		1	
2 Rb^{+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Rb_2(SeO_4)$** ***(s)***	0.97		1	
Sr^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Sr(SeO_4)$** ***(s)***	4.4	-4E+2	1	
2 Ag^{+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Ag_2(SeO_4)$** ***(s)***	8.91	4.35E+4	1	
Cd^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Cd(SeO_4)(H_2O)_2$** ***(s)***	1.85		1	
Ba^{2+} + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Ba(SeO_4)$** ***(s)***	7.46	-2.2E+4	1	
$Pb(II)^{2+}$ + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$Pb(II)(SeO_4)$** ***(s)***	6.84	-1.5E+4	1	
$(U(VI)O_2)^{2+}$ + $(SeO_4)^{2-}$ $\rightleftharpoons$ **$(U(VI)O_2)(SeO_4)$** ***(s)***	2.25		1	
$Cu(I)^{+}$ + Br^{-} $\rightleftharpoons$ **$Cu(I)Br$** ***(s)***	8.3		1	
Ag^{+} + Br^{-} $\rightleftharpoons$ **AgBr** ***(s)***	12.3	-8.45E+4	1	
$Hg(II)^{2+}$ + 2 Br^{-} $\rightleftharpoons$ **$Hg(II)Br_2$** ***(s)***	19.8		3	
$Pb(II)^{2+}$ + 2 Br^{-} $\rightleftharpoons$ **$Pb(II)Br_2$** ***(s)***	5.3		1	
Bi^{3+} + 2 $(OH)^{-}$ + Br^{-} $\rightleftharpoons$ **BiOBr** ***(s)***	35.446		1	Bi + Br $\rightleftharpoons$ BiOBr + 2 H $log_{10}(\beta)$ = 7.45 2 H + 2 OH $\rightleftharpoons$ 2 H_2O $log_{10}(\beta)$ = 27.996 Bi + 2 OH + Br $\rightleftharpoons$ BiOBr + H_2O $log_{10}(\beta)$ = 35.446
2 H^{+} + $(MoO_4)^{2-}$ $\rightleftharpoons$ **MoO_3** ***(s)***	8	5.06E+4	1	
Mg^{2+} + $(MoO_4)^{2-}$ $\rightleftharpoons$ **$Mg(MoO_4)$** ***(s)***	1.85		1	
Ca^{2+} + $(MoO_4)^{2-}$ $\rightleftharpoons$ **$Ca(MoO_4)$** ***(s)***	7.95	2E+3	1	
2 Ag^{+} + $(MoO_4)^{2-}$ $\rightleftharpoons$ **$Ag_2(MoO_4)$** ***(s)***	11.55	-5.27E+4	1	
$Pb(II)^{2+}$ + $(MoO_4)^{2-}$ $\rightleftharpoons$ **$Pb(II)(MoO_4)$** ***(s)***	15.62	-5.393E+4	1	
$Cu(I)^{+}$ + I^{-} $\rightleftharpoons$ **$Cu(I)I$** ***(s)***	12		1	
Pd^{2+} + 2 I^{-} $\rightleftharpoons$ **PdI_2** ***(s)***	31.75948		1	Original data for β: $log_{10}(\beta)$ = 31.15, at I = 1.0 M.
Ag^{+} + I^{-} $\rightleftharpoons$ **AgI** ***(s)***	16.08	-1.10E+5	1	
$Sn(II)^{2+}$ + 2 I^{-} $\rightleftharpoons$ **$Sn(II)I_2$** ***(s)***	3.45472		1	Original data for β: $log_{10}(\beta)$ = 5.08, at I = 4.0 M.

Equilibrium reaction	$Log_{10}(\beta)$	ΔH (J/mol)	Literature reference	Remarks / conversions
$Hg(II)^{2+}$ + 2 I^- ⇌ **$Hg(II)I_2$** *(s)*	28.75516	-1.71E+5	1	Original data for β: $log_{10}(\beta)$ = 27.95, at I = 0.5 M. Original data for ΔH at I = 0.5 M.
$Pb(II)^{2+}$ + 2 I^- ⇌ **$Pb(II)I_2$** *(s)*	8.1	-6.2E+4	1	
Bi^{3+} + 3 I^- ⇌ **BiI_3** *(s)*	18.00337		1	Original data for β: $log_{10}(\beta)$ = 18.09, at I = 2.0 M and 20°C.
2 H^+ + $(WO_4)^{2-}$ ⇌ **WO_3** *(s)*	14.05	-5.43E+4	1	
2 Ag^+ + $(WO_4)^{2-}$ ⇌ **$Ag_2(WO_4)$** *(s)*	12.12	-6.15E+4	1	
$Pb(II)^{2+}$ + $(WO_4)^{2-}$ ⇌ **$Pb(II)(WO_4)$** *(s)*	16.07	-5.23E+4	1	
$Cu(I)^+$ + $(CN)^-$ ⇌ **Cu(I)(CN)** *(s)*	19.5	1.9E+4	1	
Zn^{2+} + 2 $(CN)^-$ ⇌ **$Zn(CN)_2$** *(s)*	14.68931		1	Original data for β: $log_{10}(\beta)$ = 15.5, at I = 3.0 M.
Ag^+ + $(CN)^-$ ⇌ **Ag(CN)** *(s)*	15.74		1	
Ag^+ + $(acetate)^-$ ⇌ **Ag(acetate)** *(s)*	2.71		1	

2.7. Organic complexation

CHEAQS Next includes three models for organic complexation, developed and published by Tipping and co-workers. These are

- Model V or WHAM-W (Tipping and Hurley, 1992, 1994);
- Model VI or WHAM 6 (Tipping, 1998);
- Model VII (Tipping, 2011).

This document only 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. Of course the original papers contain many more details.

2.7.1. Model V

CHEAQS Next 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$_{10}$(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

2.7.2. Model VI

CHEAQS Next 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$_{10}$(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

	Log$_{10}$(K) for:			
Metal	M-FA	M(OH)-FA	M-HA	M(OH)-HA
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

2.7.3. Model VII

CHEAQS Next 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$_{10}$(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

	$Log_{10}(K)$ for:			
Metal	M-FA	M(OH)-FA	M-HA	M(OH)-HA
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

3. Other information

3.1. Molecular weights

This paragraph contains the molecular weights that are included in the file COMPON.RW64. 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. 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 Prohaska (2022) except where stated otherwise.

Component	Molecular weight	Conversion or remarks
H	1.0080	
Li	6.94	
Be	9.0122	
Na	22.990	
Mg	24.305	
Al	26.982	
K	39.098	
Ca	40.078	
Sc	44.956	
Cr(III)	51.996	
Mn(II)	54.938	
Fe(II)	55.845	
Fe(III)	55.845	
Co(II)	58.933	
Co(III)	58.933	
Ni	58.693	
Cu(I)	63.546	
Cu(II)	63.546	
Zn	65.38	
Ga	69.723	
Rb	85.468	
Sr	87.62	
Y	88.906	
Zr	91.224	
Pd	106.42	
Ag	107.87	
Cd	112.41	
In	114.82	
Sn(II)	118.71	
Sn(IV)	118.71	
Cs	132.91	
Ba	137.33	
La	138.91	
Ce	140.12	
Pr	140.91	
Nd	144.24	
Pm	145	taken from Lide (1999)
Sm	150.36	
Eu	151.96	
Gd	157.25	
Tb	158.93	
Dy	162.50	
Ho	164.93	
Er	167.26	
Tm	168.93	
Yb	173.05	
Lu	174.97	
Hf	178.49	
Pt(II)	195.08	
Hg(II)	200.59	
Pb(II)	207.2	
Bi	208.98	
$(U(VI)O_2)$	270.028	is atomic weight of U + 2 x O

Component	Molecular weight	Conversion or remarks
(OH)	17.007	is atomic weight of O + H
(H_2BO_3)	60.823	is atomic weight of B + 2 x H + 3 x O
(CO_3)	60.008	is atomic weight of C + 3 x O
(NH_3)	17.031	is atomic weight of N + 3 x H
(NO_2)	46.005	is atomic weight of N + 2 x O
(NO_3)	62.004	is atomic weight of N + 3 x O
F	18.998	
(H_2SiO_4)	94.097	is atomic weight of Si + 2 x H + 4 x O
(PO_4)	94.970	is atomic weight of P + 4 x O
S	32.06	
(SO_3)	80.057	is atomic weight of S + 3 x O
(SO_4)	96.056	is atomic weight of S + 4 x O
Cl	35.45	
(VO_4)	114.938	is atomic weight of V + 4 x O
(CrO_4)	115.992	is atomic weight of Cr + 4 x O
(MnO_4)	118.934	is atomic weight of Mn + 4 x O
(H_2AsO_3)	124.935	is atomic weight of As + 2 x H + 3 x O
(AsO_4)	138.918	is atomic weight of As + 4 x O
(SeO_3)	126.968	is atomic weight of Se + 3 x O
(SeO_4)	142.967	is atomic weight of Se + 4 x O
Br	79.904	
(MoO_4)	159.946	is atomic weight of Mo (95.96) + 4 x O
I	126.90	
(WO_4)	247.836	is atomic weight of W + 4 x O
(CN)	26.018	is atomic weight of C + N
(acetate)	59.044	is atomic weight of 2 x C + 3 x H + 2 x O
(catechol)	108.096	is atomic weight of 6 x C + 4 x H + 2 x O
(salicylate)	136.106	is atomic weight of 7 x C + 4 x H + 3 x O
(phthalate)	164.116	is atomic weight of 8 x C + 4 x H + 4 x O
(NTA)	188.115	is atomic weight of 6 x C + 6 x H + N + 7 x O
(citrate)	189.099	is atomic weight of 6 x C + 5 x H + 7 x O
(HEDTA)	275.237	is atomic weight of 10 x C + 15 x H + 2 x N + 7 x O
(EDTA)	288.212	is atomic weight of 10 x C + 12 x H + 2 x N + 8 x O
(DTPA)	388.309	is atomic weight of 14 x C + 18 x H + 3 x N + 10 x O
(glycine)	74.059	is atomic weight of 2 x C + 4 x H + N + 2 x O
(alanine)	88.086	is atomic weight of 3 x C + 6 x H + N + 2 x O
(serine)	104.085	is atomic weight of 3 x C + 6 x H + N + 3 x O
(proline)	114.124	is atomic weight of 5 x C + 8 x H + N + 2 x O
(valine)	116.140	is atomic weight of 5 x C + 10 x H + N + 2 x O
(threonine)	118.112	is atomic weight of 4 x C + 8 x H + N + 3 x O
(cysteine)	119.138	is atomic weight of 3 x C + 5 x H + N + 2 x O + S
(isoleucine)	130.167	is atomic weight of 6 x C + 12 x H + N + 2 x O
(leucine)	130.167	is atomic weight of 6 x C + 12 x H + N + 2 x O
(asparagine)	131.111	is atomic weight of 4 x C + 7 x H + 2 x N + 3 x O
(aspartate)	132.095	is atomic weight of 4 x C + 5 x H + N + 4 x O
(glutamate)	145.114	is atomic weight of 5 x C + 7 x H + N + 4 x O
(glutamine)	145.138	is atomic weight of 5 x C + 9 x H + 2 x N + 3 x O
(lysine)	145.182	is atomic weight of 6 x C + 13 x H + 2 x N + 2 x O
(methionine)	148.200	is atomic weight of 5 x C + 10 x H + N + 2 x O + S
(histidine)	154.149	is atomic weight of 6 x C + 8 x H + 3 x N + 2 x O
(phenylalanine)	164.184	is atomic weight of 9 x C + 10 x H + N + 2 x O
(arginine)	172.188	is atomic weight of 6 x C + 12 x H + 4 x N + 2 x O
(tyrosine)	179.175	is atomic weight of 9 x C + 9 x H + N + 3 x O
(tryptophan)	203.221	is atomic weight of 11 x C + 11 x H + 2 x N + 2 x O
MnO_2 *(s)*	86.936	is atomic weight of Mn + 2 x O
Cu *(s)*	63.546	
PbO_2 *(s)*	239.198	is atomic weight of Pb + 2 x O
S *(s)*	32.06	

3.2. 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.
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 chapter 2.
Data for ΔH is valid for T = 25°C and I = 0 M unless otherwise stated.

Exception: for Pt(II) there is little information in compiled databases. Therefore, for Pt(II) original sources were selected.

3.3. Compatibility of data sources

It is not trivial that data taken from different sources are comparable: many, sometimes undocumented conversions are done and assumptions made. Some data were taken from other sources than the NIST database as well. In this paragraph 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.

Complexes
For Turner *et al.*, the following complexes were checked to confirm compatibility with the NIST-database: Ag(OH), $Ag(OH)_2$, AgF, AgCl, $AgCl_2$, Al(OH), $Al(OH)_2$, $Al(OH)_3$, $Al(OH)_4$ and AlF.
For Morel, the following complexes were checked to confirm compatibility with the NIST-database: Ca(OH), Mg(OH), $Mg_4(OH)_4$, Cr(III)(OH), $H(CO_3)$, $H_2(CO_3)$, $Na(CO_3)$, $H(SO_4)$, $Na(SO_4)$ and $K(SO_4)$.
For Turner & Whitfield, the following complexes were checked to confirm compatibility with the NIST-database: HEDTA, H_2EDTA, NaEDTA, KEDTA, MgEDTA, HNTA, NaNTA, KNTA, MgNTA and CaNTA.

Solids
For Stumm & Morgan, the following solids were checked to confirm compatibility with the NIST-database: $Fe(II)(OH)_2$ and $Fe(III)(OH)_3$.
For Van Riemsdijk & Keizer, the following solids were checked to confirm compatibility with the NIST-database: $CaSO_4$, CdS and Cu(II)S.

Redox couples
For Morel, the following redox couples were checked to confirm compatibility with Lide (1999): Fe(III)/Fe(II) and Cu(II)/Cu(I).
For Stumm & Morgan, the following redox couples were checked to confirm compatibility with Lide (1999): Co(III)/Co(II) and Cu(II)/Cu^0 *(s)*.

3.4. Diameters for MSA-model

For the MSA-model, diameters were taken from Simonin (2017, 2019) and Simonin & Verweij (2022). The diameters are listed in the following tables:

- cations;
- anions;
- chloride complexes;
- bromide complexes;
- iodide complexes.

Cation	Diameter (10^{-10}m)	Source
H^+	4.39	Simonin (2022)
Li^+	4.13	Simonin (2022)
Na^+	2.99	Simonin (2022)
Mg^{2+}	6.01	Simonin (2022)
K^+	2.17	Simonin (2022)
Ca^{2+}	5.58	Simonin (2022)
$Mn(II)^{2+}$	6.600	Simonin (2019)
$Co(II)^{2+}$	6.408	Simonin (2019)
Ni^{2+}	6.322	Simonin (2019)
$Cu(II)^{2+}$	6.218	Simonin (2019)
Zn^{2+}	6.03	Simonin (2017)
Sr^{2+}	5.37	Simonin (2022)
Cd^{2+}	5.59	Simonin (2017)
Ba^{2+}	5.06	Simonin (2022)
$Pb(II)^{2+}$	4.939	Simonin (2019)

Anion	Diameter (10^{-10}m)	Source
Cl^-	3.62	Simonin (2017)
Br^-	3.90	Simonin (2017)
I^-	4.32	Simonin (2017)

Chloride complex	Diameter (10^{-10}m)	Source	Remarks
$Mn(II)Cl^+$	6.523	Simonin (2019)	
$Mn(II)Cl_2$	5.482	Simonin (2019)	No β given in NIST
$Mn(II)Cl_3^-$	5.162	Simonin (2019)	No β given in NIST
$Mn(II)Cl_4^{2-}$	5.352	Simonin (2019)	No β given in NIST
$Co(II)Cl^+$	6.360	Simonin (2019)	
$Co(II)Cl_2$	5.478	Simonin (2019)	No β given in NIST
$Co(II)Cl_3^-$	5.158	Simonin (2019)	No β given in NIST
$Co(II)Cl_4^{2-}$	5.348	Simonin (2019)	No β given in NIST
$NiCl^+$	6.618	Simonin (2019)	
$Cu(II)Cl^+$	6.202	Simonin (2019)	
$Cu(II)Cl_2$	5.513	Simonin (2019)	No β given in NIST
$Cu(II)Cl_3^-$	5.180	Simonin (2019)	No β given in NIST
$Cu(II)Cl_4^{2-}$	5.364	Simonin (2019)	No β given in NIST

$ZnCl^+$	6.418	Simonin (2019)	
$ZnCl_2$ *(aq)*	5.495	Simonin (2019)	
$ZnCl_3^-$	5.177	Simonin (2019)	
$ZnCl_4^{2-}$	5.366	Simonin (2019)	
$CdCl^+$	5.751	Simonin (2019)	
$CdCl_2$ *(aq)*	5.549	Simonin (2019)	
$CdCl_3^-$	5.237	Simonin (2019)	
$CdCl_4^{2-}$	5.422	Simonin (2019)	
$Pb(II)Cl^+$	5.134	Simonin (2019)	
$Pb(II)Cl_2$ *(aq)*	5.658	Simonin (2019)	
$Pb(II)Cl_3^-$	5.343	Simonin (2019)	
$Pb(II)Cl_4^{2-}$	5.516	Simonin (2019)	

Bromide complex	Diameter (10^{-10}m)	Source
$ZnBr^+$	6.44	Simonin (2017)
$CdBr^+$	5.80	Simonin (2017)
$CdBr_2$ *(aq)*	6.00	Simonin (2017)
$CdBr_3^-$	5.81	Simonin (2017)
$CdBr_4^{2-}$	5.88	Simonin (2017)

Iodide complex	Diameter (10^{-10}m)	Source
ZnI^+	6.33	Simonin (2017)
CdI^+	6.01	Simonin (2017)
CdI_2 *(aq)*	6.38	Simonin (2017)
CdI_3^-	6.39	Simonin (2017)
CdI_4^{2-}	6.62	Simonin (2017)

3.5. Literature references

In the table below you will find the numbers as mentioned in Chapter 2, together with the texts used by the program and the short reference. Full references are given below the table.

Number in chapter 2	As displayed by program	Reference mentioned below
1	NIST Database 46 Version 8.0	NIST (2004)
2	Turner et al.	Turner et al. (1981)
3	Morel	Morel (1983)
4	Turner & Whitfield	Turner & Whitfield (1987)
5	after Schindler & Stumm	Schindler & Stumm (1987). See also paragraph 2.3.
6	Stumm & Morgan	Stumm & Morgan (1981)
7	Van Riemsdijk & Keizer	Van Riemsdijk & Keizer (1984)
8	Lide (Handbook)	Lide (1999)
	Tipping (1994)	Tipping (1994)
	Tipping (1998)	Tipping (1998)
	Tipping et al. (2011)	Tipping et al. (2011)
12	Azaroual (2001)	Azaroual et al. (2001)

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3.6. Acknowledgements

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Data for Pt were collected in cooperation with TU Delft.