

ThermoChimie

Technical report

Track-changes and track-error document: From version 11a to version 12a

J. Rodríguez, E. Colàs and D. García (Amphos 21)



The ThermoChimie database was first developed in 1995 by Andra, the French national radioactive waste management agency. They have since been joined by Radioactive Waste Management (RWM) from the UK, and ONDRAF/NIRAS from Belgium.

ThermoChimie provides an accurate and consistent set of data specifically chosen for use in modelling the behaviour of radionuclides in waste packages, engineered barriers, and both the near surface and deep geosphere. The database can be used to model the speciation and solubility of a wide range of stable and radioactive elements, organics, and solid phases including cements, clay minerals and degradation products (such as zeolites). The database is suitable for use within the range of conditions expected in both near-surface and geological disposal facilities: pH 6-14, ionic strength up to 5M, Eh within the stability fields of water, and temperatures from 15 to 80°C.

ThermoChimie is intended for use across the radioactive waste management community, to support repository performance assessment, research and development activities and decision making. To maximise their utility the data are therefore provided in formats suitable for use with common geochemical modelling codes. The database can be viewed and downloaded from the project website: <https://www.thermochimie-tdb.com/>, where additional information and supporting documents are also available.

In line with the ThermoChimie requirement of traceability, this document provides detail on the changes that have been made to the database during the update from version 11a to version 12a.

ThermoChimie database

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VERSION 1, JULY 2023

Written by: Amphos 21 (Rodriguez, J., Colàs, E.)



Revised by: Amphos 21 (García, D.)

Approved by: ThermoChimie steering committee: Andra (Madé, B.); RWM (Bower, W.); ONDRAF/NIRAS (Brassinnes, S.).

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Prepared by




J. Rodriguez
E. Colàs

Reviewed by



D. García

Validated by



L. Duro

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1 Introduction

The main requirements for ThermoChimie development are self-consistency, comprehensiveness, applicability and traceability¹.

Fulfilling the traceability criteria² involves keeping a record of the changes, updates and improvements made to the database between the different versions. It is also necessary to keep track of the original data sources for every value in the database as well as the processes and calculations used to obtain them.

The following document describes the main changes between version 11a (March 2022) and version 12a (July 2023) of the ThermoChimie database.

This report summarises the differences between both versions; the appendices contain extensive details on the changes that have been implemented.

¹ Further explanations are provided in ThermoChimie guidelines (<https://www.thermochimie-tdb.com/docs/pdf/Guidelines.pdf>).

² For further information on data traceability, the reader is referred to the ThermoChimie guideline 4: Data traceability (<https://www.thermochimie-tdb.com/docs/pdf/Guidelines.pdf>).

2 The ThermoChimie database: Version 12a

ThermoChimie Version 12a is an official, public version. It includes thermodynamic data for the speciation of 53 major, radioactive and toxic elements (Figure 2-1). Data is also available for solid phases, including cement hydrates, clay minerals and other aluminosilicates, such as zeolites. Data on the stability of organic complexes (Acetate, Adipate, Citrate, EDTA, Gluconate, Isosaccharinate, NTA, Oxalate, Phthalate, Malonate, Succinate and Suberate) are also included.

IA												VIII A						
H	IIA											III A	IV A	V A	VIA	VII A	VIII A	He
Li	Be											B	C	N	O	F	Ne	
Na	Mg	IIIB	IVB	VB	VIB	VII B	VIII B		IB	IIB	Al	Si	P	S	Cl	Ar		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	★	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	★★	Rf	Db														
		★	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
		★★	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

X	Already in version 11a
X	New in version 12a

Figure 2-1: Contents of ThermoChimie version 12a.

3 Track-changes: From version 11a to version 12a

From version 11a to version 12a a number of changes and additions have been made to the ThermoChimie database. These changes are mainly related to the inclusion of a new element (Hg) and an extensive revision of thermodynamic data for Citrate, EDTA, Gluconate, Isosaccharinate, NTA, Oxalate, Phthalate, and also TBP and DBP.

After these modifications have been made, the whole database has been recalculated in order to guarantee that the internal calculations are consistent.

The main updates from ThermoChimie version 11a to version 12a are briefly summarised below; extensive details are provided in the appendix.

3.1 Mercury

A thermodynamic data selection for Hg aqueous species and solid compounds has been carried out. The data selection process included a review of the information contained in available literature data, different thermodynamic databases and thermodynamic data compilations. The reliability and consistency of the selection has been verified with alternative data sources, when possible. The final data selection following the ThermoChimie guidelines.

General remarks are summarised below; detailed information is provided in the appendix section 6.

Hg master species and reference state

Mercury has two redox states in aqueous solution, Hg(+II) as Hg^{2+} (formed under oxidising conditions) and Hg(+I) as Hg_2^{2+} (formed under reducing conditions). Liquid mercury (Hg(l)) is the reference state.

Data selection for the primary master species Hg^{2+} and the reference state Hg(l) follow CODATA recommendations (Cox *et al.* 1989). Redox data for $\text{Hg}^{2+}/\text{Hg}_2^{2+}$ reaction have been selected from Bard *et al.* (1985).

Hg oxygen and hydrogen compounds and complexes

Data selection for Hg(II) oxygen and hydrogen compounds and complexes is mainly based on the work by Powell *et al.* (2005). $\text{Hg}_2(\text{OH})^+$ data is based on information from Baes and Mesmer (1976).

Hg halide compounds and complexes

Data selection for Hg halide compounds and complexes is based on the review of the information in Powell *et al.* (2005), Partridge *et al.* (1965), Ciavatta and Grimaldi (1968), Sjöberg (1977), Andersson *et al.* (1974) and Cox *et al.* (1989).

Hg carbonate, sulphate and phosphate compounds and complexes

Information for Hg carbonate, sulphate and phosphate compounds and complexes has been obtained from the revision of the information in Powell *et al.* (2005) and references therein.

Hg sulphide compounds and complexes

Selected thermodynamic data for this system is mainly based on the revision of the work by Benoit *et al.* (1999).

Methylmercury complexes

Methyl (CH_3^-) was not among the organic ligands included in previous ThermoChimie versions. However, methyl plays a critical role in mercury speciation and its environmental behaviour, so a review and data selection for methylmercury complexes has been done.

Thermodynamic information is mainly based on the work of Blanc *et al.* (2018) and references therein (Erni 1977, Alderighi *et al.* 2003, Loux 2007, Skyllberg 2012).

Data selection for the $\text{CH}_4(\text{aq})/\text{CH}_3^-$ reaction is also provided in the Appendix section 7.

3.2 Organics

Isosaccharinate and gluconate

Thermodynamic data for isosaccharinate and gluconate complexes with Mg, Ni, An(III), An(IV), Np(V) and U(VI)³ have been extensively revised and updated taking into account the latest information available in the literature (Kutus *et al.* 2019, González-Siso *et al.* 2018, Tasi *et al.* 2018a and 2018b, Kobayashi *et al.* 2019, Adam *et al.* 2021, Zhang *et al.* 2006, Zhang *et al.* 2009). LFER correlations and analogies have been used to fill in some of the remaining data gaps. Detailed information is provided in the appendix section 8.1.

Oxalate

New information (not included in Hummel *et al.* 2005) for the oxalate system has been reviewed. The data for Np(V) complexation with oxalate have been updated taking into account the information in Maiwald (2019) and Maiwald *et al.* (2020) (appendix section 8.2).

EDTA

³ An(III) refers to trivalent lanthanides and actinides as Eu(III), Am(III), Cm(III) and Pu(III). An(IV) refers to tetravalent actinides Th(IV), U(IV), Np(IV), Pu(IV).

New information (not included in Hummel *et al.* 2005) for the EDTA system has been reviewed; detailed information is provided in the appendix section 8.3.

TcO(OH)(Edta)⁻³ has been excluded from the selection in agreement with the discussion and experimental results in DiBlasi *et al.* (2023).

Thermodynamic data for the An(III)-EDTA have been revised taking into account the works by Thakur *et al.* (2009a), Felmy *et al.* (2000) and DiBlasi *et al.* (2022).

The An(IV)-EDTA system has been updated using the information from DiBlasi *et al.* (2021), Rai *et al.* (2008), Xia *et al.* (2003) and Yalçintas *et al.* (2019).

NTA

Data for NTA complexation with Tc, An(III), An(IV), Np(V) and An(VI) have been updated using the information in DiBlasi *et al.* (2023), Mathur *et al.* (2006), Lusk *et al.* (2020), Felmy *et al.* (2000), Bonin *et al.* (2009) and Bonin *et al.* (2016). Detailed information is provided in the appendix section 8.4.

Citrate

Data for Citrate complexation with Tc, An(III), An(IV) and An(VI) have been updated using the information in Wall *et al.* (2013), DiBlasi *et al.* (2023), Brown *et al.* (2014), Thakur *et al.* (2012), Raymond *et al.* (1987), Thakur *et al.* (2009b), Steudtner (2011), Adam *et al.* (2021), Thakur and Van Luik (2014), Willberger (2019) and Berto *et al.* (2012). Detailed information is provided in the appendix section 8.5.

Phthalate

Thermodynamic information on Phthalate complexation with metals and radionuclides is scarce. No changes between ThermoChimie version 11a and version 12a have been made.

TBP and DBP

No data for TBP or DBP species are included in TC vs.11a or version 12a.

4 Track-errors: From version 11a to version 12a

After its release, some errors were identified in previous ThermoChimie database versions. The errors encountered in ThermoChimie version 11a and the corrections applied in ThermoChimie version 12a are summarised below.

Modification of ThermoChimie PhreeqC extraction using Davies ionic strength correction

This correction refers to ThermoChimie extraction into PhreeqC format using the Davies approach.

The `LLNL_AQUEOUS_MODEL_PARAMETERS` data block is used in the eDH (extended Debye-Hückel) approach but not in the Davies approach. Older versions of the XCheck tool extracted this data block into both the eDH and the Davies files. This did not have any effect in PhreeqC versions older than 3.7.0. However, for versions 3.7.0 onwards, the presence of the `LLNL_AQUEOUS_MODEL_PARAMETERS` data block in the extraction process results in an inaccurate application of the ionic strength correction approach if the Davies file was used. This is now corrected; in XCheck tool version 5.1.3 and ThermoChimie version 12a, the `LLNL_AQUEOUS_MODEL_PARAMETERS` data block is no longer extracted into the ThermoChimie Davies PhreeqC file. The Davies ionic strength correction is now correctly applied in the calculations.

Definition of gram formula weight in PhreeqC extraction

This correction refers to ThermoChimie extraction into PhreeqC format.

The `SOLUTION_MASTER_SPECIES` data block is used in PhreeqC to define the correspondence between element names and aqueous primary and secondary master species. The formula and the element gram formula weight are also defined in this data block.

- The gram formula weight for gluconate (Glu) in version 11a was 195.15, which is not accurate. The gram formula weight of element for Glu ($C_6H_{10}O_7^{2-}$) has been corrected to 194.14 in version 12a.
- The gram formula weight for isosaccharinate (Isa) in version 11a was 179.15, which is not accurate. The gram formula weight of element for Isa ($C_6H_{10}O_6^{2-}$) has been corrected to 178.14 in version 12a.
- The formula for the sulphur and silicon primary species should be S and Si, not SO_4 and H_4SiO_4 . A similar problem was encountered for various other species (As formula should be As and not AsO_4 , B formula should be B and not $B(OH)_4$, Cr formula should be Cr and not CrO_4 , U formula should be U and not $UO_2...$). This has been modified in version 12a.

O₂ reaction definition in Geochemist's Workbench

This correction refers to ThermoChimie extraction into Geochemist's Workbench format.

The log K versus temperature array for the $e^-/O_2(g)$ reaction in ThermoChimie version 11a (Figure 4-1) was not fully consistent with the Van't Hoff approach used in the rest of the database.

In version 12, the $e^-/O_2(aq)$ reaction (instead of the $e^-/O_2(g)$ reaction) is defined. The log K versus temperature array is calculated using the Van't Hoff approach (Figure 4-2).

* temperatures				
0.00	25.00	60.00	100.00	
150.00	200.00	250.00	300.00	
e-				
charge=	-1	ion size=	0.0 A	mole wt.= 0.0000 g
3 species in reaction				
0.500 H2O		-0.250 O2 (g)		-1.000 H+
22.76135	20.7757	18.513025	16.4658	
14.473225	12.92125	11.68165	10.67105	

Figure 4-1: $e^-/O_2(g)$ reaction in ThermoChimie version 11a extracted into GWB format. The log K array as a function of temperature was calculated using both enthalpy and heat capacity values.

* temperatures				
0.00	25.00	60.00	100.00	
150.00	200.00	250.00	300.00	
e-				
charge=	-1	ion size=	0.0 A	mole wt.= 0.0000 g
3 species in reaction				
0.500 H2O		-0.250 O2 (aq)		-1.000 H+
23.7405	21.4975	18.9228	16.5717	
14.2579	12.4331	10.9571	9.7387	

Figure 4-2: $e^-/O_2(aq)$ reaction in ThermoChimie version 12 extracted into GWB format with XCheck Tool version 5.1.3. The log K array as a function of temperature is calculated using enthalpy (Van't Hoff approach).

Other errors:

- The correct name of the Green Rust iron solid phase containing chloride ions is "GR-Cl" (with a final letter "L") and not "GR-Cl" (with a final letter "i"). This has been corrected in ThermoChimie version 12a.
- $FeCl_2(aq)$ and $FeCl_3^-$. Lemire et al. (2013) report that high chloride concentrations and/or elevated temperatures are necessary to form $FeCl_2(aq)$. $FeCl_3^-$ is not mentioned in Lemire et al. (2013) nor Lemire et al. (2020). Following the discussion in the NEA review and in order to increase the consistency of the database with the SIT approach, it was decided to eliminate $FeCl_2(aq)$ and $FeCl_3^-$. Due to an error while updating the database, the species were not removed from ThermoChimie version 11a. They are removed from ThermoChimie version 12a.

- The reference for the stability constant of the species $\text{Fe}(\text{HPO}_4)(\text{aq})$ (Eq. 1) is incorrectly quoted as “USGS original”. The correct reference is 20LEM/PAL (Lemire et al. 2020).



- The $\text{ThF}_4(\text{cr})$ data included in ThermoChimie version 11a was not correct. The value of -19.11 corresponds to $\text{ThF}_4(\text{cr,hyd})$ for a reaction written in terms of $\text{HF}(\text{aq})$, not written in terms of F^- . The correct value (Eq. 2) is now implemented in ThermoChimie version 12a.



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Appendices

6 Appendix: Hg data selection

Hg selected data is summarized below.

Table 6-1: Data selection for Hg^{2+} (mercury primary master species).

Species	Hg ²⁺
Formula	Hg ²⁺
$\Delta_f G^\circ$	164.667
$\pm \Delta_f G^\circ$	0.313
$\Delta_f H^\circ$	170.210
$\pm \Delta_f H^\circ$	0.200
S°	-36.190
$\pm S^\circ$	0.800
$\varepsilon M^+/ClO_4^-$	0.34
$\pm \varepsilon M^+/ClO_4^-$	0.03
$\varepsilon M^+/NO_3^-$	-0.10
$\pm \varepsilon M^+/NO_3^-$	0.10
Ref. $\Delta_f H^\circ$	89COX/WAG
Ref. S°	89COX/WAG
Ref. $\varepsilon M^+/ClO_4^-$	97GRE/PLY in 05POW/BRO
Ref. $\varepsilon M^+/NO_3^-$	80CIA in 20GRE/GAO

Table 6-2: Data selection for $Hg(l)$ (mercury reference state).

Species	Hg(l)
Formula	Hg
Coeff. Hg ²⁺	1
Coeff. e ⁻	2
Log K°	28.85
\pm Log K°	0.05
$\Delta_r G^\circ$	-164.667
$\pm \Delta_r G^\circ$	0.313
$\Delta_r H^\circ$	-170.210
$\pm \Delta_r H^\circ$	0.200
$\Delta_r S^\circ$	-18.590
$\pm \Delta_r S^\circ$	0.809
$\Delta_f G^\circ$	0.000
$\pm \Delta_f G^\circ$	0.000
$\Delta_f H^\circ$	0.000
$\pm \Delta_f H^\circ$	0.000
S°	75.900
$\pm S^\circ$	0.120
Ref. $\Delta_f H^\circ$	89COX/WAG
Ref. S°	89COX/WAG

Table 6-3: Data selection for Hg_2^{2+} (mercury secondary master species).

Species	Hg_2^{2+}
Formula	Hg_2^{2+}
Coeff. Hg_2^{2+}	2
Coeff. e^-	2
Log K^0	30.79
\pm Log K^0	
$\Delta_r G^0$	-175.727
$\pm \Delta_r G^0$	
$\Delta_r H^0$	-173.600
$\pm \Delta_r H^0$	
$\Delta_r S^0$	7.134
$\pm \Delta_r S^0$	
$\Delta_f G^0$	153.607
$\pm \Delta_f G^0$	
$\Delta_f H^0$	166.820
$\pm \Delta_f H^0$	
S^0	65.437
$\pm S^0$	
$\epsilon M^+/ClO_4^-$	0.09
$\pm \epsilon M^+/ClO_4^-$	0.02
$\epsilon M^+/NO_3^-$	-0.20
$\pm \epsilon M^+/NO_3^-$	0.10
Ref. $\Delta_r G^0$	85BAR/PAR
Ref. $\Delta_r H^0$	85BAR/PAR
Ref. $\epsilon M^+/ClO_4^-$	80CIA in 20GRE/GAO
Ref. $\epsilon M^+/NO_3^-$	80CIA in 20GRE/GAO

Table 6-4: Data selection for Hg(II)-OH aqueous species.

Species	Hg(OH) ⁺	Hg(OH) ₂ (aq)	Hg(OH) ₃ ⁻	Hg ₂ (OH) ₃ ³⁺	Hg ₃ (OH) ₃ ³⁺
Formula	Hg(OH) ⁺	Hg(OH) ₂	Hg(OH) ₃ ⁻	Hg ₂ (OH) ₃ ³⁺	Hg ₃ (OH) ₃ ³⁺
Coeff. Hg ²⁺	1	1	1	2	3
Coeff. H ₂ O	1	2	3	1	3
Coeff. H ⁺	-1	-2	-3	-1	-3
Log K ^o	-3.40	-5.98	-21.10	-3.33	-6.42
± Log K ^o	0.08	0.06	0.30	0.03	0.15
Δ _r G ^o	19.407	34.134	120.439	19.008	36.645
± Δ _r G ^o	0.457	0.342	1.712	0.171	0.856
Δ _r H ^o		51.500			
± Δ _r H ^o		1.800			
Δ _r S ^o		58.246			
± Δ _r S ^o		6.146			
Δ _f G ^o	-53.066	-275.479	-426.314	111.202	-180.774
± Δ _f G ^o	0.555	0.471	1.745	0.650	1.277
Δ _f H ^o		-349.950			
± Δ _f H ^o		1.813			
S ^o		161.955			
± S ^o		6.283			
ε M ⁺ /ClO ₄ ⁻	0.06				
± ε M ⁺ /ClO ₄ ⁻	0.05				
Ref. Log K ^o	05POW/BRO	05POW/BRO	05POW/BRO	76BAE/MES	76BAE/MES
Ref. Δ _r H ^o		05POW/BRO			
Ref. ε M ⁺ /ClO ₄ ⁻	05POW/BRO				

Table 6-5: Data selection for solid Hg(II) oxide.

Species	HgO(s)
Formula	HgO(s)
Coeff. Hg ²⁺	1
Coeff. H ₂ O	1
Coeff. H ⁺	-2
Log K ⁰	-2.37
± Log K ⁰	0.08
Δ _r G ⁰	13.528
± Δ _r G ⁰	0.457
Δ _r H ⁰	25.300
± Δ _r H ⁰	0.200
Δ _r S ⁰	39.484
± Δ _r S ⁰	1.672
Δ _f G ⁰	-58.945
± Δ _f G ⁰	0.555
Δ _f H ⁰	-90.320
± Δ _f H ⁰	0.286
S ⁰	73.244
± S ⁰	2.097
Ref. Log K ⁰	05POW/BRO
Ref. Δ _r H ⁰	05POW/BRO

Table 6-6: Data selection for Hg(I)-OH aqueous species.

Species	Hg ₂ (OH) ⁺
Formula	Hg ₂ (OH) ⁺
Coeff. Hg ₂ ²⁺	1
Coeff. H ₂ O	1
Coeff. H ⁺	-1
Log K ⁰	-5.00
± Log K ⁰	0.30
Δ _r G ⁰	28.540
± Δ _r G ⁰	1.712
Δ _f G ⁰	-54.993
± Δ _f G ⁰	
Ref. Log K ⁰	76BAE/MES

Table 6-7: Data selection for Hg(II)-Cl aqueous species.

Species	HgCl⁺	HgCl₂(aq)	HgCl₃⁻	HgCl₄²⁻	Hg(OH)Cl(aq)
Formula	HgCl ⁺	HgCl ₂ (aq)	HgCl ₃ ⁻	HgCl ₄ ²⁻	Hg(OH)Cl(aq)
Coeff. Hg ²⁺	1	1	1	1	1
Coeff. Cl ⁻	1	2	3	4	1
Coeff. H ₂ O					1
Coeff. H ⁺					-1
Log K ^o	7.31	14.00	14.93	15.54	4.27
± Log K ^o	0.04	0.07	0.11	0.17	0.35
Δ _r G ^o	-41.726	-79.912	-85.221	-88.702	-24.373
± Δ _r G ^o	0.228	0.400	0.628	0.970	1.998
Δ _r H ^o	-21.300	-49.100	-48.600	-59.100	
± Δ _r H ^o	0.700	1.000	2.690	3.674	
Δ _r S ^o	68.508	103.344	122.826	99.287	
± Δ _r S ^o	2.470	3.612	9.265	12.745	
Δ _f G ^o	-8.277	-177.681	-314.208	-448.907	-228.064
± Δ _f G ^o	0.404	0.558	0.783	1.120	2.026
Δ _f H ^o	-18.170	-213.050	-379.630	-557.210	
± Δ _f H ^o	0.735	1.039	2.714	3.701	
S ^o	88.918	180.353	256.434	289.493	
± S ^o	2.816	3.958	9.475	12.970	
ε M ⁺ /ClO ₄ ⁻	0.19				
± ε M ⁺ /ClO ₄ ⁻	0.02				
ε Na ⁺ /M ⁻			0.05	0.08	
± ε Na ⁺ /M ⁻			0.07	0.09	
Ref. Log K ^o	05POW/BRO	05POW/BRO	05POW/BRO	05POW/BRO	05POW/BRO
Ref. Δ _r H ^o	05POW/BRO	05POW/BRO	05POW/BRO	05POW/BRO	
Ref. ε M ⁺ /ClO ₄ ⁻	05POW/BRO				
Ref. ε Na ⁺ /M ⁻			05POW/BRO	05POW/BRO	

Table 6-8: Data selection for Hg(II)-Cl solid compounds.

Species	HgCl ₂ (s)
Formula	HgCl ₂
Coeff. Hg ²⁺	1
Coeff. Cl ⁻	2
Log K ^o	14.57
± Log K ^o	
Δ _r G ^o	-83.166
± Δ _r G ^o	
Δ _r G ^o	-180.935
± Δ _r G ^o	
Ref. Log K ^o	74AND/CUM
Comments	As reported in the SPANA default database

Table 6-9: Data selection for Hg(I)-Cl solid compounds.

Species	Hg ₂ Cl ₂ (s)
Formula	Hg ₂ Cl ₂
Coeff. Hg ₂ ²⁺	1
Coeff. Cl ⁻	2
Log K ^o	17.85
± Log K ^o	
Δ _r G ^o	-101.895
± Δ _r G ^o	
Δ _r H ^o	-98.030
± Δ _r H ^o	
Δ _r S ^o	12.963
± Δ _r S ^o	
Δ _r G ^o	-210.725
± Δ _r G ^o	0.471
Δ _r H ^o	-265.370
± Δ _r H ^o	0.400
S ^o	191.600
± S ^o	0.800
Ref. Δ _r H ^o	89COX/WAG
Ref. S ^o	89COX/WAG

Table 6-10: Data selection for Hg(II)-carbonate aqueous species.

Species	Hg(CO ₃)(aq)	Hg(OH)CO ₃ ⁻	Hg(HCO ₃) ⁺
Formula	Hg(CO ₃)	Hg(OH)CO ₃ ⁻	Hg(HCO ₃) ⁺
Coeff. Hg ²⁺	1	1	1
Coeff. CO ₃ ²⁻	1	1	1
Coeff. H ₂ O		1	
Coeff. H ⁺		-1	1
Log K ⁰	11.47	5.33	15.80
± Log K ⁰	0.21	0.13	0.13
Δ _r G ⁰	-65.471	-30.424	-90.187
± Δ _r G ⁰	1.199	0.742	0.742
Δ _f G ⁰	-428.704	-630.797	-453.420
± Δ _f G ⁰	1.299	0.895	0.894
Ref. Log K ⁰	05POW/BRO	05POW/BRO	05POW/BRO

Table 6-11: Data selection for Hg(II)-carbonate solid compounds.

Species	HgCO ₃ :2HgO(s)
Formula	HgCO ₃ :2HgO
Coeff. Hg ²⁺	3
Coeff. CO ₃ ²⁻	1
Coeff. H ₂ O	2
Coeff. H ⁺	-4
Log K ⁰	11.48
± Log K ⁰	0.37
Δ _r G ⁰	-65.528
± Δ _r G ⁰	2.112
Δ _f G ⁰	-573.707
± Δ _f G ⁰	2.345
Ref. Log K ⁰	05POW/BRO

Table 6-12: Data selection for Hg(II)-sulphate aqueous species.

Species	HgSO ₄ (aq)
Formula	HgSO ₄
Coeff. Hg ²⁺	1
Coeff. SO ₄ ²⁻	1
Log K ^o	2.68
± Log K ^o	0.10
Δ _r G ^o	-15.297
± Δ _r G ^o	0.571
Δ _r G ^o	-594.634
± Δ _r G ^o	0.774
Ref. Log K ^o	05POW/BRO
Comments	Corrected to I=0 in p.w.

Table 6-13: Data selection for Hg(II)-sulphide aqueous species.

Species	Hg(HS) ⁺	Hg(HS) ₂ (aq)	HgS(aq)	HgS(HS) ⁻	HgS ₂ ²⁻
Formula	Hg(HS) ⁺	Hg(HS) ₂	HgS	HgS(HS) ⁻	HgS ₂ ²⁻
Coeff. Hg ²⁺	1	1	1	1	1
Coeff. HS ⁻	1	2	1	2	2
Coeff. H ⁺			-1	-1	-2
Log K ^o	30.5	37.5	26.5	32.0	23.5
± Log K ^o					
Δ _r G ^o	-174.094	-214.050	-151.262	-182.656	-134.138
± Δ _r G ^o					
Δ _r G ^o	2.816	-24.897	25.648	6.497	55.015
± Δ _r G ^o					
Ref. Log K ^o	99BEN/GIL	99BEN/GIL	99BEN/GIL	99BEN/GIL	99BEN/GIL

Table 6-14: Data selection for solid HgS.

Species	Cinnabar	Metacinnabar
Formula	HgS	HgS
Coeff. Hg ²⁺	1	1
Coeff. HS ⁻	1	1
Coeff. H ⁺	-1	-1
Log K ^o	39.18	38.56
± Log K ^o	0.54	0.51
Δ _r G ^o	-223.621	-220.106
± Δ _r G ^o	3.061	2.896
Δ _r H ^o	-208.210	-200.610
± Δ _r H ^o	2.588	2.131
Δ _r S ^o	51.690	65.390
± Δ _r S ^o	5.482	6.579
Δ _f G ^o	-46.711	-43.196
± Δ _f G ^o	2.191	1.954
Δ _f H ^o	-54.300	-46.700
± Δ _f H ^o	2.100	1.500
S ^o	82.500	96.200
± S ^o	2.100	4.200
Ref. Δ _f H ^o	95ROB/HEM	95ROB/HEM
Ref. S ^o	95ROB/HEM	95ROB/HEM

Table 6-15: Data selection for Hg(II)-phosphate aqueous species.

Species	HgHPO ₄ (aq)	HgPO ₄ ⁻
Formula	HgHPO ₄	HgPO ₄ ⁻
Coeff. Hg ²⁺	1	1
Coeff. H ₂ PO ₄ ⁻	1	1
Coeff. H ⁺	-1	-2
Log K ^o	2.86	-2.63
± Log K ^o	0.44	0.44
Δ _r G ^o	-16.325	15.012
± Δ _r G ^o	2.512	2.512
Δ _f G ^o	-988.81	-957.473
± Δ _f G ^o	2.977	2.977
Ref. Log K ^o	05POW/BRO	05POW/BRO

Table 6-16: Data selection for Hg(II)-phosphate solid compounds.

Species	Hg ₃ (PO ₄) ₂ (s)	(HgOH) ₃ PO ₄ (s)	HgHPO ₄ (s)
Formula	Hg ₃ (PO ₄) ₂	(HgOH) ₃ PO ₄	HgHPO ₄
Coeff. Hg ²⁺	3	3	1
Coeff. H ₂ PO ₄ ⁻	2	1	1
Coeff. H ⁺	-4	-5	-1
Coeff. H ₂ O		3	
Log K ⁰	13.01	3.80	7.16
± Log K ⁰	0.98	0.89	0.40
Δ _r G ⁰	-74.261	-21.690	-40.869
± Δ _r G ⁰	5.594	5.080	2.283
Δ _f G ⁰	-1854.564	-1376.261	-1013.354
± Δ _f G ⁰	6.480	5.400	2.787
Ref. Log K ⁰	05POW/BRO	05POW/BRO	05POW/BRO

Table 6-17: Data selection for methylmercury aqueous species and gases (table 1 of 2).

Species	CH ₃ Hg ⁺	(CH ₃) ₂ Hg	Hg(CH ₃) ₂ (g)	CH ₃ HgOH(aq)	(CH ₃ Hg) ₂ OH ⁺	CH ₃ HgCl
Formula	CH ₃ Hg ⁺	(CH ₃) ₂ Hg	Hg(CH ₃) ₂ (g)	CH ₃ HgOH	(CH ₃ Hg) ₂ OH ⁺	CH ₃ HgCl
Coeff. Hg ²⁺	1	1	1	1	2	1
Coeff. CH ₄ (aq)	1	2	2	1	2	1
Coeff. Cl ⁻						1
Coeff. H ₂ O				1	1	
Coeff. H ⁺	-1	-2	-2	-2	-2	-1
Log K ⁰	3.00	19.00	8.82	-1.53	3.85	8.45
± Log K ⁰						
Ref. Log K ⁰	18BLA/BUR	18BLA/BUR	18BLA/BUR	18BLA/BUR	18BLA/BUR	18BLA/BUR

Table 6-18: Data selection for methylmercury aqueous species (table 2 of 2).

Species	CH ₃ HgCO ₃ ⁻	CH ₃ HgHCO ₃ (aq)	CH ₃ HgS ⁻	CH ₃ HgSH(aq)	CH ₃ HgSO ₄ ⁻
Formula	CH ₃ HgCO ₃ ⁻	CH ₃ HgHCO ₃	CH ₃ HgS ⁻	CH ₃ HgSH	CH ₃ HgSO ₄ ⁻
Coeff. Hg ²⁺	1	1	1	1	1
Coeff. CH ₄ (aq)	1	1	1	1	1
Coeff. HS ⁻			1	1	
Coeff. SO ₄ ²⁻					1
Coeff. CO ₃ ²⁻	1	1			
Coeff. H ⁺	-1		-2	-1	-1
Log K ⁰	9.10	15.93	7.00	17.50	5.64
± Log K ⁰					
Ref. Log K ⁰	18BLA/BUR	18BLA/BUR	18BLA/BUR	18BLA/BUR	18BLA/BUR

7 Appendix: Methyl data selection

Table 7-1: Data selection for methyl.

Species	CH ₃ ⁻
Formula	CH ₃ ⁻
Coeff. CH ₄ (aq)	1
Coeff. H ⁺	-1
Log K ⁰	-46.00
± Log K ⁰	
Ref. Log K ⁰	18BLA/BUR

8 Appendix: Data selection including organic ligands

The tables below provide a comparison between the data selection in version 12a and version 11a for the complexation of Citrate, EDTA, Gluconate, Isosaccharinate, NTA, Oxalate and Phthalate with several elements of interest.

8.1 Isosaccharinate and gluconate

Table 8-1. Ca-ISA and Ca-GLU compounds and complexes and corresponding Log K° values selected in TC vs. 12a, in comparison with those in TC vs. 11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Ca(HIsa)+	1.70 ± 0.30	Hummel <i>et al.</i> (2005)	1.70 ± 0.30	Hummel <i>et al.</i> (2005)
Ca(Isa)(aq)	-10.40 ± 0.50	Hummel <i>et al.</i> (2005)	-10.40 ± 0.50	Hummel <i>et al.</i> (2005)
Ca(HIsa) ₂ (cr)	6.40 ± 0.20	Hummel <i>et al.</i> (2005)	6.40 ± 0.20	Hummel <i>et al.</i> (2005)
Ca(HGlu) ⁺	1.73 ± 0.05	Schubert <i>et al.</i> (1952)	1.73 ± 0.05	Schubert <i>et al.</i> (1952)
Ca(OH)(HGlu)(aq)	-10.40 ± 0.50	Tits <i>et al.</i> (2002)*	-10.40 ± 0.50	Tits <i>et al.</i> (2002)*
Ca(HGlu) ₂ (s)	4.19 ± 0.05	Van Loon <i>et al.</i> (1999)	4.19 ± 0.05	Van Loon <i>et al.</i> (1999)
Mg(HIsa) ⁺	0.81 ± 0.13	Analogy ^{a)}	-	-
Mg(OH)(HIsa)(aq)	-9.10 ± 0.10	Analogy ^{a)}	-	-
Mg(OH) ₂ (HIsa) ⁻	-20.44 ± 0.10	Analogy ^{a)}	-	-
Mg(HGlu) ⁺	0.81 ± 0.13	Kutus <i>et al.</i> (2019)	-	-
Mg(OH)(HGlu)(aq)	-9.10 ± 0.10	Kutus <i>et al.</i> (2019)	-	-
Mg(OH) ₂ (HGlu) ⁻	-20.44 ± 0.10	Kutus <i>et al.</i> (2019)	-	-

*Analogy with Ca(Isa)(aq). Notice that Ca(OH)(HGlu)(aq) ≡ Ca(Glu)(aq)

a) Direct analogy with the corresponding gluconate species

Table 8-2. Al-GLU Complexes and corresponding Log K° values selected in TC vs. 12a, in comparison with those in TC vs. 11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Al(HGlu) ₂ ²⁺	3.2 ± 0.6	Lakatos <i>et al.</i> (2008)	3.2 ± 0.6	Lakatos <i>et al.</i> (2008)
Al(OH)(HGlu) ⁺	-0.39 ± 0.4	Lakatos <i>et al.</i> (2008)	-0.39 ± 0.4	Lakatos <i>et al.</i> (2008)
Al(OH)(HGlu) ₂	2.85 ± 0.5	Lakatos <i>et al.</i> (2008)	2.85 ± 0.5	Lakatos <i>et al.</i> (2008)
Al(OH) ₂ (HGlu)	-4.85 ± 1	Lakatos <i>et al.</i> (2008)	-4.85 ± 1	Lakatos <i>et al.</i> (2008)
Al(OH) ₂ (HGlu) ₂ ⁻	-2.6 ± 0.6	Lakatos <i>et al.</i> (2008)	-2.6 ± 0.6	Lakatos <i>et al.</i> (2008)
Al(OH) ₃ (HGlu) ⁻	-11.11 ± 1.5	Lakatos <i>et al.</i> (2008)	-11.11 ± 1.5	Lakatos <i>et al.</i> (2008)
Al(OH) ₄ (HGlu) ₂ ²⁻	-20.47 ± 1.5	Palmer <i>et al.</i> (2013)	-20.47 ± 1.5	Palmer <i>et al.</i> (2013)

Table 8-3. Complexes and corresponding Log K° values selected in TC vs. 12a, in comparison with those in TC vs. 11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Ni(HIsa) ⁺	-	-	2.80 ± 0.40	Grive <i>et al.</i> (2012)
Ni(OH)(HIsa)(aq)	-6.50 ± 0.30	González-Siso <i>et al.</i> (2018) and Bruno (2018)	-	-
Ni(OH) ₂ (HIsa) ⁻	-17.60 ± 0.50	González-Siso <i>et al.</i> (2018) and Bruno (2018)	-	-
Ni(OH) ₃ (HIsa) ²⁻	-31.00 ± 0.70	González-Siso <i>et al.</i> (2018) and Bruno (2018)	-26.50 ± 1.00	Grive <i>et al.</i> (2012)

Table 8-4. An(III)-ISA and An(III)-GLU complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Log K° TC vs 11a	Species	Log K° TC vs.12a	Log K° TC vs 11a
Eu(OH) ₂ (HIsa)(aq)	-10.97±0.28 ^{a)}		Eu(OH) ₂ (HGlU)(aq)	-10.97±0.28 ^{a)}	
Am(OH) ₂ (HIsa)(aq)	-10.97±0.28 ^{a)}		Am(OH) ₂ (HGlU)(aq)	-10.97±0.28 ^{a)}	
Cm(OH) ₂ (HIsa)(aq)	-10.97±0.28 ^{a)}		Cm(OH) ₂ (HGlU)(aq)	-10.97±0.28 ^{a)}	
Pu(OH) ₂ (HIsa)(aq)	-10.97 ± 0.28 ^{b)}		Pu(OH) ₂ (HGlU)(aq)	-10.97±0.28 ^{a)}	
Eu(OH) ₃ (HIsa) ⁻	-	-20.9±1.00 ^{c)}			
Am(OH) ₃ (HIsa) ⁻	-	-21.5±1.00 ^{c)}	Am(OH) ₃ (HGlU) ⁻	Deleted	-19.70±1.00 ^{c)}

a) Analogy with Pu(OH)₂(HIsa)(aq)b) Tasi *et al.* (2018a and 2018b)c) Tits *et al.* (2005).**Table 8-5.** An(IV)-ISA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a. Complexes with Ca are not included in the table.

Species	Log K° p.w.	Ref.	Log K° TC vs 11a	Species	Log K° p.w.	Ref.	Log K° TC vs 11a
Th(OH) ₃ (HIsa)	-		-5.65 ± 1.50	Th(OH) ₄ (HIsa) ⁻	-14.70	a)	-13.20 ± 0.60
Th(OH) ₃ (HIsa) ₂ ⁻	-4.90	Rai <i>et al.</i> (2009)	-4.90 ± 0.50	Th(OH) ₄ (HIsa) ₂ ²⁻	-12.5	a)	-10.40 ± 0.60
U(OH) ₃ (HIsa)	-		0.29 ± 1.50	U(OH) ₄ (HIsa) ⁻	-7.60	Kobayashi <i>et al.</i> (2019)	-6.70 ± 0.70
U(OH) ₃ (HIsa) ₂ ⁻	-		2.40 ± 1.50	U(OH) ₄ (HIsa) ₂ ²⁻	-5.40	Kobayashi <i>et al.</i> (2019)	-5.10 ± 0.50
Np(OH) ₃ (HIsa)	-		3.27 ± 0.62	Np(OH) ₄ (HIsa) ⁻	-5.89	b)	-4.06 ± 0.62
Np(OH) ₃ (HIsa) ₂ ⁻	-		5.38 ± 0.62	Np(OH) ₄ (HIsa) ₂ ²⁻	-3.69	b)	-2.20 ± 0.62
Pu(OH) ₃ (HIsa)	-		4.75 ± 1.50	Pu(OH) ₄ (HIsa) ⁻	-5.03	Tasi <i>et al.</i> (2018a,b)	-3.60 ± 1.50
Pu(OH) ₃ (HIsa) ₂ ⁻	-		6.86 ± 1.50	Pu(OH) ₄ (HIsa) ₂ ²⁻	-2.83	b)	0.70 ± 1.50
				Pu(OH) ₅ (HIsa) ₂ ²⁻	-16.92	Tasi <i>et al.</i> (2018a,b)	No data

a) Reevaluated from Rai *et al.* (2009) in TC vs.12a.

b) Estimated from LFER correlations in TC vs.12a.

Table 8-6. An(IV)-GLU complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a. Complexes with Ca are not included in the table.

Species	Log K° TC vs.12a*	Log K° TC vs 11a	Species	Log K° TC vs.12a*	Log K° TC vs 11a
Th(OH) ₃ (HGlU)	-	-6.70 ± 1.00	Th(OH) ₄ (HGlU) ⁻	-14.70	-11.80 ± 0.60
Th(OH) ₃ (HGlU) ₂ ⁻	-4.90	-	Th(OH) ₄ (HGlU) ₂ ²⁻	-12.5	-9.90 ± 0.60
U(OH) ₃ (HGlU)	-	0.29 ± 1.50	U(OH) ₄ (HGlU) ⁻	-7.60	-5.94 ± 0.60
U(OH) ₃ (HGlU) ₂ ⁻	-	-	U(OH) ₄ (HGlU) ₂ ²⁻	-5.40	-
Np(OH) ₃ (HGlU)	-	3.27 ± 0.62	Np(OH) ₄ (HGlU) ⁻	-5.89	-3.70 ± 1.30
Np(OH) ₃ (HGlU) ₂ ⁻	-	-	Np(OH) ₄ (HGlU) ₂ ²⁻	-3.69	-
Pu(OH) ₃ (HGlU) ⁻	-	4.75 ± 1.50	Pu(OH) ₄ (HGlU) ⁻	-5.03	-2.70 ± 1.50
Pu(OH) ₃ (HGlU) ₂ ⁻	-	-	Pu(OH) ₄ (HGlU) ₂ ²⁻	-2.83	-
			Pu(OH) ₅ (HGlU) ₂ ²⁻	-16.92	-

*Analogy with An(IV)-ISA

Table 8-7. Ca-An(IV)-ISA and Ca-An(IV)-GLU complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	References	Log K° TC vs 11a	References
CaTh(OH) ₄ (HIsa) ⁺	-	-	-9.00	Colàs (2014)
CaTh(OH) ₄ (HGlU) ⁺	-	-	-9.00	Colàs (2014)
CaPu(OH) ₄ (HIsa) ⁺	-1.66 ± 0.10	Tasi <i>et al.</i> (2018b)	-	-
CaPu(OH) ₅ (HIsa)(aq)	-12.70 ± 0.08	Tasi <i>et al.</i> (2018b)	-	-

Table 8-8. Np(V)-gluconate complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
NpO ₂ (HGlU)(aq)	1.68 ± 0.10	Zhang <i>et al.</i> (2006)	-	-
NpO ₂ (HGlU) ₂ ⁻	2.39 ± 0.10	Zhang <i>et al.</i> (2006)	-	-

Table 8-9. U(VI)-ISA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
UO ₂ (HIsa) ⁺	3.70 ± 1.00	Rao <i>et al.</i> (2004)	3.70 ± 1.00	Rao <i>et al.</i> (2004)
UO ₂ (HIsa) ₂	6.60 ± 1.00	Rao <i>et al.</i> (2004)	6.60 ± 1.00	Rao <i>et al.</i> (2004)
UO ₂ (HIsa) ₃ ⁻	8.50 ± 1.00	Rao <i>et al.</i> (2004)	8.50 ± 1.00	Rao <i>et al.</i> (2004)
UO ₂ (OH) ₃ (HIsa) ₂ ³⁻	-14.50 ± 0.10	Kobayashi <i>et al.</i> (2019)	-	-
UO ₂ (OH) ₄ (HIsa) ³⁻	-	-	-28.10 ± 1.00	Gaona <i>et al.</i> (2006)

Table 8-10. U(VI)-GLU complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
UO ₂ (HGlU) ⁺	2.59 ± 0.30	Zhang <i>et al.</i> (2009)	-	-
UO ₂ (OH)(HGlU)(aq)	0.20 ± 0.20	Zhang <i>et al.</i> (2009)	-	-

8.2 Oxalate

Table 8-11. *Np(V)-Ox thermodynamic data selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	TC vs.12a			TC vs 11a		
	Log K°	$\Delta_r H^\circ_m$	$\epsilon(\text{Na}^+, X^-)$	Log K°	$\Delta_r H^\circ_m$	$\epsilon(\text{Na}^+, X^-)$
$\text{NpO}_2(\text{Ox})^-$	3.90±0.10 ^{a)}	-1.300±0.700 ^{b)}	-0.40±0.10 ^{a)}	3.90±0.10 ^{a)}	-	-0.40±0.10 ^{a)}
$\text{NpO}_2(\text{Ox})_2^{3-}$	5.80±0.20 ^{a)}	-8.700±1.400 ^{b)}	-0.30±0.20 ^{a)}	5.80±0.20 ^{a)}	-	-0.30±0.20 ^{a)}

a) Hummel *et al.* (2005)

b) Maiwald *et al.* (2020).

8.3 EDTA

Table 8-12. Tc(IV)-EDTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
TcO(OH)(Edta) ⁻³	-	-	19.00 ± 0.58	Akram and Bourbon (1995)

Table 8-13. An(III)-EDTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs. 11a	References
Eu(HEdta)	21.84 ± 0.27	Analogy Am(HEdta)	-	-
Am(HEdta)	21.84 ± 0.27	Hummel <i>et al.</i> (2005)	21.84 ± 0.27	Hummel <i>et al.</i> (2005)
Cm(HEdta)	21.84 ± 0.27	Analogy Am(HEdta)	-	-
Np(HEdta)	22.02 ± 0.45	Analogy Pu(HEdta)	-	-
Pu(HEdta)	22.02 ± 0.45	Hummel <i>et al.</i> (2005)	22.02 ± 0.45	Hummel <i>et al.</i> (2005)
EuEdta ⁻	19.67 ± 0.11	Analogy Am(Edta) ⁻	-	-
Am(Edta) ⁻	19.67 ± 0.11	Hummel <i>et al.</i> (2005)	19.67 ± 0.11	Hummel <i>et al.</i> (2005)
Cm(Edta) ⁻	19.67 ± 0.11	Analogy Am(Edta) ⁻	-	-
Np(Edta) ⁻	19.90	Hummel <i>et al.</i> (2005)	19.90	Hummel <i>et al.</i> (2005)
Pu(Edta) ⁻	20.18 ± 0.37	Hummel <i>et al.</i> (2005)	20.18 ± 0.37	Hummel <i>et al.</i> (2005)

Table 8-14. An(IV)-EDTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
(Th(OH)(Edta)) ₂ ²⁻	-	-	43.70 ± 0.50	Akram & Bourbon (1995)
(U(OH)(Edta)) ₂ ²⁻	-	-	51.70	Ermolaev & Krot (1963)
Th(HEdta) ⁺	28.70	Akram & Bourbon (1995)	28.70	Akram & Bourbon (1995)
Th(Edta)	26.95 ± 0.20	Akram & Bourbon (1995)	26.95 ± 0.20	Akram & Bourbon (1995)
Th(OH)(Edta) ⁻	19.50 ± 0.42	Akram & Bourbon (1995)	19.50 ± 0.42	Akram & Bourbon (1995)
Th(OH) ₂ Edta ²⁻	11.5 ± 1	Xia <i>et al.</i> (2003)	-	-
Th(OH) ₃ Edta ³⁻	-4 ± 1	Xia <i>et al.</i> (2003)	-	-
U(Edta)	29.50 ± 0.20	Hummel <i>et al.</i> (2005)	29.50 ± 0.20	Hummel <i>et al.</i> (2005)
U(OH)(Edta) ⁻	22.7	Estimated	24.60	Ermolaev & Krot (1963)
U(OH) ₂ (Edta) ²⁻	16.68	Estimated	16.50	Ermolaev & Krot (1963)
U(OH) ₃ (Edta) ³⁻	7.06	Estimated	-	-
Np(Edta)	31.20 ± 0.60	Hummel <i>et al.</i> (2005)	31.20 ± 0.60	Hummel <i>et al.</i> (2005)
Np(OH)Edta ⁻	23.73	Estimated	-	-
Np(OH) ₂ Edta ²⁻	18.24	Estimated	-	-
Np(OH) ₃ Edta ³⁻	8.62	Estimated	-	-
Pu(Edta)	31.80	Hummel <i>et al.</i> (2005)	31.80	Hummel <i>et al.</i> (2005)
Pu(OH)Edta ⁻	23.00 ± 0.30	DiBlasi <i>et al.</i> (2021)	24.44 ± 0.30	Rai <i>et al.</i> (2008)
Pu(OH) ₂ Edta ²⁻	18.02 ± 0.30	DiBlasi <i>et al.</i> (2021)	18.95 ± 0.30	Rai <i>et al.</i> (2008)
Pu(OH) ₃ Edta ³⁻	8.50 ± 0.30	DiBlasi <i>et al.</i> (2021)	9.33 ± 0.30	Rai <i>et al.</i> (2008)

8.4 NTA

Table 8-15. *An(III)-NTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Eu(Nta)(aq)	13.00 ± 0.10	Analogy Am(Nta)(aq)	-	-
Am(Nta)(aq)	13.00 ± 0.10	Akram and Bourbon (1995)	13.00 ± 0.10	Akram and Bourbon (1995)
Cm(Nta)(aq)	13.00 ± 0.10	Analogy Am(Nta)(aq)		
Np(Nta)(aq)	13.00 ± 0.10	Analogy Am(Nta)(aq)	-	-
Pu(Nta)(aq)	13.00 ± 0.10	Analogy Am(Nta)(aq)	-	-
Am(Nta) ₂ ³⁻	-	-	22.00 ± 0.40	Akram and Bourbon (1995)

Table 8-16. *An(IV)-NTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Th(Nta) ⁺	19.73 ± 0.60	Bonin <i>et al.</i> (2016)	17.15 ± 0.25	Akram and Bourbon (1995)
Th(OH)(Nta)	-		11.20 ± 0.49	Akram and Bourbon (1995)
Th(OH) ₂ (Nta) ⁻	-		7.20 ± 0.48	Akram and Bourbon (1995)
U(Nta) ⁺	20.00 ± 1.00	Akram and Bourbon (1995)	20.00 ± 1.00	Akram and Bourbon (1995)
Np(Nta) ⁺	20.70 ± 0.20	Akram and Bourbon (1995)	20.70 ± 0.20	Akram and Bourbon (1995)
Np(Nta) ₂ ²⁻	-		36.30 ± 0.20	Akram and Bourbon (1995)
Pu(Nta) ⁺	25.72 ± 0.30	Bonin <i>et al.</i> (2016)	21.00 ± 2.00	Akram and Bourbon (1995)

Table 8-17. *Np(V)-NTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
NpO ₂ (HNta) ⁻	11.70 ± 0.40	Akram and Bourbon (1995)	11.70 ± 0.40	Akram and Bourbon (1995)
NpO ₂ (Nta) ²⁻	7.46 ± 0.05	Akram and Bourbon (1995)	7.46 ± 0.05	Akram and Bourbon (1995)
NpO ₂ (OH)(Nta) ³⁻	-	-	-4.70 ± 0.30	Akram and Bourbon (1995)

Table 8-18. *An(VI)-NTA complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
UO ₂ (HNta)	14.50 ± 0.10	De Stefano <i>et al.</i> (2006)	9.00 ± 1.00	Akram and Bourbon (1995)
UO ₂ (Nta) ⁻	10.15 ± 0.10	De Stefano <i>et al.</i> (2006)	10.80 ± 0.09	Akram and Bourbon (1995)
NpO ₂ (Nta) ⁻	-	-	11.00 ± 2.00	Akram and Bourbon (1995)
PuO ₂ (Nta) ⁻	-	-	11.00 ± 2.00	Akram and Bourbon (1995)

8.5 Citrate

Table 8-19. Tc-citrate complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
TcO(OH) ₂ Cit ³⁻	2.80 ± 0.20	Wall <i>et al.</i> (2013)	-	-

Table 8-20. An(III)-citrate complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
Am(HCit) ⁺	12.86 ± 1.00	Hummel <i>et al.</i> (2005)	12.86 ± 1.00	Hummel <i>et al.</i> (2005)
Am(HCit) ₂ ²⁻	23.52 ± 1.00	Hummel <i>et al.</i> (2005)	23.52 ± 1.00	Hummel <i>et al.</i> (2005)
Am(Cit)	8.55 ± 0.20	Hummel <i>et al.</i> (2005)	8.55 ± 0.20	Hummel <i>et al.</i> (2005)
Am(Cit) ₂ ³⁻	13.90 ± 0.10	Hummel <i>et al.</i> (2005)	13.90 ± 0.10	Hummel <i>et al.</i> (2005)
Cm(HCit) ⁺	12.86 ± 1.00	Analogy with Am	-	-
Cm(HCit) ₂ ²⁻	23.52 ± 1.00	Analogy with Am	-	-
Cm(Cit)	8.55 ± 0.20	Analogy with Am	-	-
Cm(Cit) ₂ ³⁻	13.90 ± 0.10	Analogy with Am	-	-
Eu(HCit) ⁺	12.86 ± 1.00	Analogy with Am	-	-
Eu(HCit) ₂ ²⁻	23.52 ± 1.00	Analogy with Am	-	-
Eu(Cit)	8.55 ± 0.20	Analogy with Am	-	-
Eu(Cit) ₂ ³⁻	13.90 ± 0.10	Analogy with Am	-	-
Pu(HCit) ⁺	12.86 ± 1.00	Analogy with Am	-	-
Pu(HCit) ₂ ²⁻	23.52 ± 1.00	Analogy with Am	-	-
Pu(Cit)	8.55 ± 0.20	Analogy with Am	-	-
Pu(Cit) ₂ ³⁻	13.90 ± 0.10	Analogy with Am	-	-

Table 8-21. Th-citrate complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
ThCit ⁺	14.13	Raymond <i>et al.</i> (1987)	16.80 ± 0.30	Akram and Bourbon (1995)
Th(Cit) ₂ ²⁻	24.29	Raymond <i>et al.</i> (1987)	25.80 ± 0.30	Akram and Bourbon (1995)

Table 8-22. U(VI)-citrate complexes and corresponding Log K° values selected in TC vs.12a, in comparison with those in TC vs.11a.

Species	Log K° TC vs.12a	Reference	Log K° TC vs 11a	Reference
(UO ₂) ₂ (Cit) ₂ ²⁻	21.3 ± 0.5	Hummel <i>et al.</i> (2005)	21.3 ± 0.5	Hummel <i>et al.</i> (2005)
UO ₂ (Cit) ⁻	8.96 ± 0.17	Hummel <i>et al.</i> (2005)	8.96 ± 0.17	Hummel <i>et al.</i> (2005)
UO ₂ (HCit)	11.36 ± 1	Hummel <i>et al.</i> (2005)	11.36 ± 1	Hummel <i>et al.</i> (2005)
(UO ₂) ₂ (Cit) ₂ (OH) ₂ ⁴⁻	9.29±0.03	Berto <i>et al.</i> (2012)	-	-
(UO ₂) ₂ (Cit) ₂ (OH) ₃ ³⁻	16.04±0.04	Berto <i>et al.</i> (2012)	-	-
(UO ₂) ₂ (Cit)(OH) ₂ ⁻	5.30±0.01	Berto <i>et al.</i> (2012)	-	-
(UO ₂) ₂ (Cit)(OH)	9.65±0.07	Berto <i>et al.</i> (2012)	-	-

Table 8-23. *U(VI)-citrate interaction coefficients selected in TC vs.12a, in comparison with those in TC vs.11a.*

Species	$\epsilon(\text{MX, Na}^+)$ TC vs.12a	Reference	$\epsilon(\text{MX, Na}^+)$ TC vs 11a	Reference
$(\text{UO}_2)_2(\text{Cit})_2^{2-}$	-0.11 ± 0.09	Hummel <i>et al.</i> (2005)	-0.11 ± 0.09	Hummel <i>et al.</i> (2005)
$\text{UO}_2(\text{Cit})^-$	-	Hummel <i>et al.</i> (2005)	-	Hummel <i>et al.</i> (2005)
$\text{UO}_2(\text{HCit})$	-	Hummel <i>et al.</i> (2005)	-	Hummel <i>et al.</i> (2005)
$(\text{UO}_2)_2(\text{Cit})_2(\text{OH})_2^{4-}$	0.56 ± 0.01	Berto <i>et al.</i> (2012)	-	-
$(\text{UO}_2)_2(\text{Cit})_2(\text{OH})_3^{3-}$	0.70 ± 0.01	Berto <i>et al.</i> (2012)	-	-
$(\text{UO}_2)_2(\text{Cit})(\text{OH})_2^-$	0.60 ± 0.01	Berto <i>et al.</i> (2012)	-	-
$(\text{UO}_2)_2(\text{Cit})(\text{OH})$	-	Berto <i>et al.</i> (2012)	-	-