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Sandia National Laboratories
Waste Isolation Pilot Plant

An Update to the EQ3/6 Pitzer Thermodynamic Database DATA0.FM1 with the Creation of DATA0.FM4

Work Carried Out under the Analysis Plan for WIPP Near-Field Geochemical Process Modeling, AP 183, Rev. 1.
To be included in the AP-183 records package

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1 INTRODUCTION

The objective of this analysis report is to document the addition of thermodynamic and Pitzer parameters to a current quality assured EQ3/6 thermodynamic database, DATA0.FM1, with the creation of a self-consistent new QA EQ3/6 thermodynamic database, DATA0.FM4. The motivation behind creation of this database is to include systems that were posed of interest and recommended by Environmental Protection Agency (EPA) after the submittal of CRA-2014. This analysis report, as per NP 9-1, is considered a compliance decision analysis.

The new QA database, DATA0.FM4, will include parameters derived under AP-154 revision 2, AP-176, and AP-182 as directed by AP-183, Revision 1. In addition, literature searches were performed to determine the availability of published data that are suitable for WIPP conditions, these data are listed in AP-183, revision 1, and in the following sections. Note that the literature values of Hummel et al., (2005) and Powell et al., (2009) which will be included in DATA0.FM4 were derived using a different aqueous model, the SIT model, and not the Pitzer model which the remainder of the parameters in database were derived. This inconsistency may contribute to model error and greater uncertainty in the results of modeling studies that use this database. By using the currently verified QA EQ3/6 thermodynamic database, DATA0.FMT.R2, also known as DATA0.FM1 (Xiong, 2011) as the starting database additional thermodynamic and Pitzer parameters will be added and tested. Only parameters which were fit to experimental data are able to be tested, the parameters added from the literature are not able to be tested. The final database, DATA0.FM4, will be used for CRA-2019.

Table 1 defines the abbreviations, acronyms, and initialisms used in this report.

Table 1. Abbreviations, Acronyms, and Initialisms

Abbreviation, Acronym, or Initialism	Definition
Ac, acetate	CH_3COO^- or $CH_3CO_2^-$
Brucite	$Mg(OH)_2$
C	carbon
Ca, Ca(II), Ca^{2+}	calcium, calcium in the +II oxidation state, calcium ion
Cerussite	$PbCO_3$
Cit, citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
Cl, Cl(−I), Cl^-	chlorine, chlorine in the −I oxidation state, chloride ion
CMS	(Sandia/WIPP software) Configuration Management System
CO_2	carbon dioxide
CO_3^{2-}	carbonate
cr	crystalline
DB	(thermodynamic) database
CRA-2004	the first WIPP Compliance Recertification Application, submitted to the EPA in March 2004
CRA-2009	the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009
CRA-2014	the third WIPP Compliance Recertification Application, to be submitted to the EPA in March 2014
EDTA	ethylenediaminetetraacetate, $(CH_2COO)_2N(CH_2)_2N(CH_2COO)_2)^{4-}$ or $(CH_2CO_2)_2N(CH_2)_2N(CH_2CO_2)^{4-}$
EPA	(U.S.) Environmental Protection Agency
EQ3/6	a geochemical software package for speciation and solubility calculations (EQ3NR) and reaction-path calculations (EQ6)
earlandite	$Ca_3[C_3H_5O(COO)_3]_2 \cdot 4H_2O$
H or H_2, H^+	hydrogen or hydrogen ion
Halite	NaCl
H_2O	water (aq, g, or contained in solid phases)
hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
Lead oxalate	PbC_2O_4(cr)
litharge	PbO

Table 1 continued on next page

Table 1. Abbreviations, Acronyms, and Initialisms (continued).

Abbreviation, Acronym, or Initialism	Definition
OH, OH^-	hydroxide or hydroxide ion
Ox, oxalate	$(COO)_2^{2-}$ or $C_2O_4^{2-}$
QA	quality assurance
Rev.	revision
whewellite	$CaC_2O_4 \cdot H_2O$
WIPP	Waste Isolation Pilot Plant

2 METHODS

This analysis report documents the steps used to create a quality assured thermodynamic database, DATA0.FM4, in accordance with AP-183 revision 1. For the data derived under AP-154, AP-176, and AP-182 the following steps were followed in updating the database:

1) Copy DATA0.FM1 (Xiong 2011) to a working interim database DATA0.P50.
2) Edit DATA0.P50 and enter all of the parameters, and parameter updates as listed in AP-183. Note the analysis plans will be called AP-154 and AP-183 without their revision numbers for the remainder of this document.
3) Run the parameter fitting Python scripts using DATA0.FM4 for each of the fitted parameters as listed in AP-183.
4) Compare the results with those documented in the analysis reports, and memos, i.e., the original derived parameter values Parameters and simulation using the final interim database will be considered acceptable if they agree to within 10%. If the percent difference exceeds 10%, a new value for lambda will be sought in the interim database. Also, if the 10% criteria is exceeded it will be refitted or the discrepancy will be documented for acceptability. If the percent difference is less than or equal to 10%, the value is acceptable. It was expected that there would be some deviation between the original derived values and those derived with DATA0.FM4 because of the necessity of deriving the parameters in a stepwise fashion.
5) If the difference in the fitted parameter values using DATA0.FM4 was greater than 10%, it will be refit, or the discrepancy will be documented for acceptability. If the percent difference is less than or equal to 10%, the value is acceptable. The literature source values will be directly put into the datablocks of the EQ3/6 database and there will be no testing of these parameters.

3 RESULTS

3.1 AP-183 Parameters

The following sections summarize the changes and additions that will be included in DATA0.FM4. Files used or created for this exercise include EQ3NR input and output files, Python script results files, an Excel spreadsheet, and the thermodynamic database DATA0.FM4. These files will be stored at: /nfs/data/CVSLIB/WIPP_EXTERNAL/ap183/Files

3.1.1 Organics

Some of the thermodynamic and Pitzer data for the EDTA, citrate, and oxalate systems will be updated and/or expanded compared to that included DATA0.FM1. There will be no changes, or inclusion of additional data, to the lactate and acetate systems as they exist in DATA0.FM1 at this time.

The following tables list all of the reactions and data that will be updated or added to DATA0.FM4. A full listing of the EQ3/6 data blocks as they appear in DATA0.FM4 is included in Appendix I.

Tables 2 and 3 contain the pertinent EDTA parameters that will be updated in DATA0.FM4. See AP-183 for the complete EDTA parameters which will be included in DATA0.FM4, but will remain the same as DATA0.FM1.

Note that the log K values in Table 2 below for $MgHEDTA^{1-}$ and $CaHEDTA^{1-}$ are different than those in Table 1 of AP-183. This difference is caused by the fact that in AP-183 the log K for these reactions is cast in terms of $MgEDTA^{2-}$ and $CaEDTA^{2-}$ which are not the basis species for EDTA. To remedy this the reactions for the dissociation of $MgEDTA^{2-}$ and $CaEDTA^{2-}$ must be added to those for $MgHEDTA^{1-}$ and $CaHEDTA^{1-}$ to cast the reactions in terms of $EDTA^{4-}$. This is a deviation from AP-183, Revision 1.

Table 2. Equilibrium Constants for Reactions with EDTA that will be updated in DATA0.FM4

Reaction	log K	Source
Solid Dissolution Reactions		
$Ca_2EDTA{\bullet}7H_2O(s) \leftrightarrow 2Ca^{2+} + EDTA^{4-} + 7H_2O$	-16.81	Domski (2018)
Aqueous Dissociation Reactions		
$H_4EDTA(aq) \leftrightarrow EDTA^{4-} + 4H^+$	-23.42	Hummel et al. (2005)
$H_3EDTA^- \leftrightarrow EDTA^{4-} + 3H^+$	-21.19	Hummel et al. (2005)
$H_2EDTA^{2-} \leftrightarrow EDTA^{4-} + 2H^+$	-18.04	Hummel et al. (2005)
$HEDTA^{3-} \leftrightarrow EDTA^{4-} + H^+$	-11.24	Hummel et al. (2005)

Reaction	log K	Source
$NaEDTA^{3-} \leftrightarrow Na^{+} + EDTA^{4-}$	-2.80	Hummel et al. (2005)
$MgEDTA^{2-} \leftrightarrow Mg^{2+} + EDTA^{4-}$	-10.90	Hummel et al. (2005)
$MgHEDTA^{1-} \leftrightarrow H^{+} + Mg^{2+} + EDTA^{4-}$	-15.40	Hummel et al. (2005)[A]
$CaEDTA^{2-} \leftrightarrow Ca^{2+} + EDTA^{4-}$	-12.69	Hummel et al. (2005)
$CaHEDTA^{1-} \leftrightarrow H^{+} + Ca^{2+} + EDTA^{4-}$	-16.23	Hummel et al. (2005)[A]

A – New in DATA0.FM4

Table 3. Pitzer Interaction Coefficients (Cation-Anion Interactions) for Ions Containing EDTA that will be updated in DATA0.FM4

I	*j*	α_1/α_2[A]	$\beta^{(0)}$	$\beta^{(1)}$	C^{φ}	Source
Cation-Anion Interactions						
$EDTA^{4-}$	Na^{+}	2.0/12.0	1.10	15.6	0.001	Felmy and Mason (2003)
$EDTA^{4-}$	K^{+}	2.0/12.0	1.10	15.6	0.001	Felmy and Mason (2003)
$NaEDTA^{3-}$	Na^{+}	2.0/12.0	0.59	5.39	0	Felmy and Mason (2003)
$CaEDTA^{2-}$	Na^{+}	2.0/12.0	0.185	2.405	0	Domski (2018a)[B]

A - All values for $\beta^{(2)}$ are 0.
B – New in DATA0.FM4

Table 4 provides updated (Hummel et al, 2005) log K values for the citrate solids phase, and all of the citrate species currently included in DATA0.FM1 as well as some additional species not included DATA0.FM1. Note that all of the citrate Pitzer parameters to be included in DATA0.FM4 will be the same as those included in DATA0.FM1, to see a listing of these values see AP-183.

Table 4. Equilibrium Constants for Reactions with Citrate that will be updated in DATA0.FM4

Reaction	log K	Source
Solid Dissociation Reactions		
$Ca_3(Citrate)_2 \cdot 4H_2O(s) \leftrightarrow 3Ca^{+} + 2Citrate^{3-} + 4H_2O$	-17.90	Hummel et al. (2005)[A]
Aqueous Dissociation Reactions		
$H_3Citrate\ (aq) \leftrightarrow Citrate^{3-} + 3H^{+}$	-14.27	Hummel et al. (2005)
$H_2Citrate^{-} \leftrightarrow Citrate^{3-} + 2H^{+}$	-11.14	Hummel et al. (2005)
$HCitrate^{2-} \leftrightarrow Citrate^{3-} + H^{+}$	-6.36	Hummel et al. (2005)
$MgHCitrate\ (aq) \leftrightarrow Mg^{2+} + H^{+} + Citrate^{3-}$	-8.96	Hummel et al. (2005)[B]
$Mg(H_2Citrate)^{+} \leftrightarrow Mg^{2+} + 2H^{+} + Citrate^{3-}$	-12.45	Hummel et al. (2005)[B]
$MgCitrate^{-} \leftrightarrow Mg^{2+} + Citrate^{3-}$	-4.81	Hummel et al. (2005)

Reaction	log K	Source
$CaCitrate^- \leftrightarrow Ca^{2+} + Citrate^{3-}$	-4.80	Hummel et al. (2005)
$CaHCitrate(aq) \leftrightarrow Ca^{2+} + H^+ + Citrate^{3-}$	-9.28	Hummel et al. (2005) [B]
$Ca(H_2Citrate)^+ \leftrightarrow Ca^{2+} + 2H^+ + Citrate^{3-}$	-12.67	Hummel et al. (2005) [B]

A - Value from Hummel et al. (2005) converted to the EQ3/6 basis species reaction by adding a value of -11.14 from $H_2Citrate^-$ value.
B – New in DATA0.FM4

Tables 5 - 7 shows the oxalate data that will be updated, or newly included in the case of glushinskite, in DATA0.FM4. The complete set of oxalate phases, aqueous species, and Pitzer data can be found in AP-183.

Table 5. Equilibrium Constants for Reactions with Oxalate that will be updated in DATA0.FM4

Reaction	log K	Source
Solid Dissolution Reactions		
$MgOxalate{\bullet}2H_2O(s)$ (glushinskite) $\leftrightarrow Mg^{2+} + Oxalate^{2-} + 2H_2O$	-6.41	AP-182 (2019)
Aqueous Dissociation Reactions		
$MgOxalate_2^{2-} \leftrightarrow Mg^{2+} + 2Oxalate^{2-}$	-5.24	Jang and Kim (2016)[A]

A – Derived from thermodynamic data in Choppin et al., (2001).

Table 6. Pitzer Interaction Coefficients (Cation-Anion Interactions) for Ions Containing Oxalate that will be updated in DATA0.FM4

I	*j*	α_1/α_2	$\beta^{(0)}$	$\beta^{(1)}$	C^φ	Source
Cation-Anion Interactions						
$Mg(Oxalate)_2^{2-}$	Na^+	2.0/12.0[A]	0.07	0	0	AP-182(2019)

All values for $\beta^{(2)}$ are 0.
A – This is an exception to AP-183, Revision 1, which erroneously has $\alpha_1 = 1.4$

Table 7. Pitzer Interaction Coefficients (Neutral-Cation; Neutral-Anion Interactions) for Ions Containing Organic Ligands that will be updated in DATA0.FM4

i	*j*	$\lambda_{nc'}$ or $\lambda_{na'}$	Source
Neutral-Cation Interactions			
MgOxalate(aq)	Na^+	0.08	AP-182 (2019)
MgOxalate(aq)	Mg^{2+}	-0.20	AP-182 (2019)

3.1.2 Inorganics

This section, Table 8, will cover the data for hydromagnesite, and the iron and lead systems that will be included in DATA0.FM4. Details regarding this data can be found in AP-183.

Table 8. Equilibrium Constants for Dissolution Reactions for MgO Solids that will be updated in DATA0.FM4

Reaction	log K	Source
Solid Dissolution Reactions		
$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$(hydromagnesite5424) + $6H^+ \leftrightarrow 5Mg^{2+} + 4HCO_3^- + 6H_2O$	31.49	Robie and Hemingway (1973)

The lead system as presented in Powell et al. (2009) (Table 9) will be included in DATA0.FM4. It should be noted that only log K data for lead solids phases and aqueous species will be included, but no lead Pitzer parameters will be included in DATA0.FM4. There is a deviation from AP-183, Revision 1 in the $PbSO_4$(s) and $PbSO_4$(aq) reactions that will be corrected in this analysis report. AP-183 has these reactions cast in terms of bisulfate (HSO_4^-) which is not the basis species for sulfur in EQ3/6, sulfate (SO_4^{2-}) is the EQ3/6 basis species. Therefore, the correct reactions which were included in Powell at al., (2009) are listed in Table 8 and will be included in DATA0.FM4.

Table 9. Equilibrium Constants for Reactions with Lead that will be included in DATA0.FM4

Reaction	log K	Source
Solid Dissolution Reactions		
α-PbO(litharge) + $2H^+ \leftrightarrow Pb^{2+} + H_2O$(l)	12.62	Powell et al. (2009)
$PbCO_3$(cerussite) + $H^+ \leftrightarrow Pb^{2+} + HCO_3^-$	-2.84	Powell et al. (2009)
$Pb_2CO_3Cl_2$(s) + $H^+ \leftrightarrow 2Pb^{2+} + HCO_3^{1-} + 2Cl^-$	0.41	Powell et al. (2009)
$PbSO_4$(s) $\leftrightarrow Pb^{2+} + SO_4^{2-}$	-7.80	Powell et al. (2009)

Reaction	log K	Source
Aqueous Dissociation Reactions		
$PbCl^+ \leftrightarrow Pb^{2+} + Cl^-$	-1.50	Powell et al. (2009)
$PbCl_2(aq) \leftrightarrow Pb^{2+} + 2Cl^-$	-2.10	Powell et al. (2009)
$PbCl_3^- \leftrightarrow Pb^{2+} + 3Cl^-$	-2.00	Powell et al. (2009)
$PbOH^+ + H^+ \leftrightarrow Pb^{2+} + H_2O$	7.46	Powell et al. (2009)
$Pb(OH)_2(aq) + 2H^+ \leftrightarrow Pb^{2+} + 2H_2O(l)$	16.94	Powell et al. (2009)
$Pb(CO_3)(OH)^- + 2H^+ \leftrightarrow Pb^{2+} + HCO_3^{1-} + H_2O(l)$	13.44	Powell et al. (2009)
$Pb(CO_3)Cl^- + H^+ \leftrightarrow Pb^{2+} + HCO_3^- + Cl^-$	3.87	Powell et al. (2009)
$PbCO_3(aq) + H^+ \leftrightarrow Pb^{2+} + HCO_3^-$	3.89	Powell et al. (2009)
$Pb(CO_3)_2^{2-} + 2H^+ \leftrightarrow Pb^{2+} + 2HCO_3^-$	10.55	Powell et al. (2009)
$PbSO_4(aq) \leftrightarrow Pb^{2+} + SO_4^{2-}$	-2.72	Powell et al. (2009)

The iron system as presented by Kim et al., (2017) will be included in DATA0.FM4. Both thermodynamic and Pitzer interaction parameters will be included in the new database some of which was derived by Kim et al., (2017), and some which are literature values. Tables 10 – 13 include all of the thermodynamic and Pitzer interaction data that will be included in DATA0.FM4 for the iron system.

Table 10. Equilibrium Constants for Reactions with Iron that will be included in DATA0.FM4

Reaction	log K	Source
Solid Dissolution Reactions		
$Fe(OH)_2(s) + 2H^+$ (ferrous hydroxide) $\leftrightarrow Fe^{2+} + 2H_2O$	12.89	Kim et al. (2017)
$Fe_2Cl(OH)_3(s) + 3H^+$ (hibbingite) $\leftrightarrow 2Fe^{2+} + Cl^- + 3H_2O$	17.08	Kim et al. (2017)
$FeCO_3(s) + H^+$ (siderite) $\leftrightarrow Fe^{2+} + HCO_3^-$	-0.12	Stumm and Morgan (1996)
$Fe_2CO_3(OH)_2(s) + 3H^+$ (chukanovite) $\leftrightarrow 2Fe^{2+} + HCO_3^- + 2H_2O$	12.32	Kim et al. (2017)
Aqueous Dissociation Reactions		
$FeOH^+ + H^+ \leftrightarrow Fe^{2+} + H_2O$	9.31	Shock et al. (1997)
$Fe(OH)_2(aq) + 2H^+ \leftrightarrow Fe^{2+} + 2H_2O$	20.82	Stumm and Morgan (1996)
$Fe(OH)_3^- + 3H^+ \leftrightarrow Fe^{2+} + 3H_2O$	31.0	Baes and Mesmer (1976)
$FeCO_3(aq) + H^+ \leftrightarrow Fe^{2+} + HCO_3^-$	4.83	Bruno et al. (1992)
$Fe(CO_3)_2^{2-} + 2H^+ \leftrightarrow Fe^{2+} + 2HCO_3^{1-}$	13.89	Kim et al. (2017)

Table 11. Pitzer Interaction Coefficients (Cation-Anion Interactions) for Ions Containing Iron that will be included in DATA0.FM4

i	*j*	$\alpha_1/\alpha_2{}^A$	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^φ	Source
Fe^{2+}	Cl^-	2.0/12.0	0.373	1.135	0	-0.022	Moog et al. (2004)
Na^+	$Fe(CO_3)_2^{-2}$	2.0/12.0	-0.23	6.26	0	0	Kim et al. (2017)

Table 12. Pitzer Interaction Coefficients (Cation-Cation Interactions) for Ions Containing Iron that will be included in DATA0.FM4

i	*j*	$\theta_{cc'}$ or $\theta_{aa'}$	Source
Na^+	Fe^{2+}	0.110	Moog et al. (2004)
Mg^{2+}	Fe^{2+}	0.145	Moog et al. (2004)
K^+	Fe^{2+}	0.0274	Moog et al. (2004)
Ca^{2+}	Fe^{2+}	0.0811	Moog et al. (2004)

Table 13. Pitzer Interaction Coefficients (Cation-Cation-Anion Interactions) for Ions Containing Iron that will be included in DATA0.FM4

i	*j*	*k*	Ψ_{ijk}	Source
Fe^{+2}	Na^+	Cl^-	-0.0161	Moog et al. (2004)
Fe^{+2}	K^+	Cl^-	-0.0252	Moog et al. (2004)
Fe^{+2}	Mg^{+2}	Cl^-	-0.0299	Moog et al. (2004)
Fe^{+2}	Ca^{+2}	Cl^-	-0.0160	Moog et al. (2004)

3.2 Comparison of the Tabulated and Fitted Parameters

To test the ability of the newly minted database, DATA0.FM4, to reproduce the fitted parameter values that were used in its creation the Python scripts for each parameter set were executed and the results compared to the tabulated values. The systems that were run include the Na – Ca – Cl - EDTA system, Na – Mg – Cl – Oxalate system, and the Na – Fe – Cl – CO_3 system. A comparison of the derived parameters using the updated database with those tabulated above are shown in Table 14.

Table 14. Comparison of the documented parameters with those estimated using DATA0.FM4

Chemical Entity	Fitting Parameter	Documented Value	Estimated with DATA0.FM4	Comments
$Ca_2EDTA*7H_2O$	Log K	-16.81	-16.81	The EDTA parameters are all identical.
$CaEDTA^{2-}$ / Na^+	$\beta^{(0)}$	0.185	0.185	
	$\beta^{(1)}$	2.405	2.405	
$MgOxalate{\bullet}2H_2O(s)$	Log K	-6.41	-6.41	The oxalate parameters are all identical.
$Mg(Oxalate)_2^{2-}$ / Na^+	$\beta^{(0)}$	0.070	0.070	
MgOxalate(aq) / Mg^{2+}	λ	-0.20	-0.20	
MgOxalate(aq) / Na^+	λ	-0.08	-0.08	
Fe(OH)2(s)	Log K	12.89	12.83	The log K for $Fe(OH)_2(s)$ differs by 0.25%, which is inconsequential. All others match exactly.
$Fe_2Cl(OH)_3(s)$	Log K	17.08	17.08	
$Fe(CO_3)_2^{-2}$	Log K	13.89	13.89	The iron carbonate parameters are all identical.
$Fe(CO_3)_2^{-2}$ / Na^+	$\beta^{(0)}$	-0.23	-0.23	
	$\beta^{(1)}$	6.26	6.26	

4 CONCLUSIONS

The purpose of AP-183, Revision 1 was to create an updated quality-assured self-consistent Pitzer thermodynamic database for EQ3/6 for use on the WIPP project. This goal has been met by updating and adding new data to a previously quality assured database DATA0.FM1 with the creation of DATA0.FM4. The updates include both literature values and values derived from experimental data. Note that the literature values of Hummel et al., (2005) and Powell et al., (2009) which were included in DATA0.FM4 were derived using the SIT model, and not the Pitzer model which the remainder of the parameters in database were derived. This inconsistency may contribute to model error and greater uncertainty in the results of modeling studies that use this database. This new database will be used for CRA-2019 geochemical modeling.

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APPENDIX I Updates and Additions to DATA0.FM1

```
+------------------------------------------------------------------------
elements
+------------------------------------------------------------------------
Fe         55.84500
Pb        207.20000
+------------------------------------------------------------------------
basis species
+------------------------------------------------------------------------
Fe++
     charge  =    2.0
****
     1 element(s):
      1.0000 Fe
****
+------------------------------------------------------------------------
Pb++
     charge  =    2.0
****
     1 element(s):
      1.0000 Pb
****
+------------------------------------------------------------------------

+------------------------------------------------------------------------
ca combinations: beta(n)(ca) and Cphi(ca) [optional: alpha(n)(ca)]
+------------------------------------------------------------------------
Ca++                          EDTA----
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 5.39
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+------------------------------------------------------------------
Mg++                          CaEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
```

```
    a4 = 0.
  beta(1)
    a1 = 7.21
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+-----------------------------------------------------------------
Mg++                          MgEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 7.27
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+-----------------------------------------------------------------
Na+                           NaEDTA---
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.59
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 5.39
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.
```

```
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Felmy & Mason(2003)
+-----------------------------------------------------------------
Na+                          Mg(Oxalate)2--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.07
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-182
+-----------------------------------------------------------------
Fe++                         Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.37324
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.13499
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.02152
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-----------------------------------------------------------------
Na+                          Fe(CO3)2--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = -0.23
    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
  beta(1)
    a1 = 6.26
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Kim et al (2017)
+-------------------------------------------------------------
Na+                          EDTA----
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 1.10
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 15.6
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.001
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Felmy & Mason(2003)
+-------------------------------------------------------------------
Na+                          CaEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.185
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 2.405
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
```

```
    a3 = 0.
    a4 = 0.
* Source: Domski (2018)
+-----------------------------------------------------------------
Na+                          EDTA----
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 1.10
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 15.6
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.001
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Felmy & Mason(2003)
+-----------------------------------------------------------------
K+                           EDTA----
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 1.10
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 15.6
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.001
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Felmy & Mason(2003)
+-----------------------------------------------------------------
K+                           CaEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.185
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
```

```
    a1 = 2.41

    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.00
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski (2018)
*-----------------------------------------------------------------
* cc' combinations first, then aa' combinations
*-----------------------------------------------------------------
Na+                         Fe++
  theta:
    a1 = 0.10945
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-----------------------------------------------------------------
Mg++                        Fe++
  theta:
    a1 = 0.145
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)15
+-----------------------------------------------------------------
K+                          Fe++
  theta:
    a1 = 0.0274
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)15
+-----------------------------------------------------------------
Ca++                        Fe++
  theta:
    a1 = 0.0811
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
*-----------------------------------------------------------------
* nc combinations first, then na combinations
*-----------------------------------------------------------------
MgOxalate(aq)               Na+
  lambda:
    a1 = 0.08
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-182
+-----------------------------------------------------------------
MgOxalate(aq)               Mg++
  lambda:
```

```
    a1 = -0.20
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-182
*-------------------------------------------------------------
* cc'a combinations
*-------------------------------------------------------------
Fe++                        Na+                         Cl-
  psi:
    a1 = -0.01605
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-------------------------------------------------------------
Fe++                        K+                          Cl-
  psi:
    a1 = -0.0252
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-------------------------------------------------------------
Fe++                        Mg++                        Cl-
  psi:
    a1 = -0.0299
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-------------------------------------------------------------
Fe++                        Ca++                        Cl-
  psi:
    a1 = -0.0160
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Moog et al. (2004)
+-----------------------------------------------------------------
aqueous species
+-----------------------------------------------------------------
PbCl+                       PbCl+
     charge  =   1.0
****
     2 element(s):
      1.0000 Pb             1.0000 Cl
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCl+                    1.0000  Pb++
     1.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -1.5000    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+-------------------------------------------------------------
PbCl2(aq)                   PbCl2(aq)
     charge  =   0.0
****
     2 element(s):
      1.0000 Pb             2.0000 Cl
```

```
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCl2(aq)                1.0000  Pb++
     2.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.1000    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
PbCl3-                     PbCl3-
     charge  =    -1.0
****
     2 element(s):
      1.0000 Pb              3.0000 Cl
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCl3-                   1.0000  Pb++
     3.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.0000    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
PbOH+                      PbOH+
     charge  =    1.0
****
     3 element(s):
      1.0000 Pb              1.0000 H              1.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  PbOH+                   -1.0000  H+
     1.0000  Pb++                     1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     7.4600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al. (2009)
+---------------------------------------------------------------
Pb(OH)2(aq)                Pb(OH)2(aq)
     charge  =    0.0
****
     3 element(s):
      1.0000 Pb              2.0000 H              2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pb(OH)2(aq)             -2.0000  H+
     1.0000  Pb++                     2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    16.9400    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al. (2009)
+---------------------------------------------------------------
PbCO3(aq)                  PbCO3(aq)
     charge  =    0.0
****
     3 element(s):
      1.0000 Pb              1.0000 C              3.0000 O
****
```

```
     4 species in aqueous dissociation reaction:
    -1.0000  PbCO3(aq)                -1.0000  H+
     1.0000  Pb++                      1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    3.8900   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
Pb(CO3)2--                 Pb(CO3)2--
     charge  =  -2.0
****
     3 element(s):
      1.0000 Pb             2.0000 C             6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pb(CO3)2--               -2.0000  H+
     1.0000  Pb++                      2.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   10.5500   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
Pb(CO3)Cl-                 Pb(CO3)Cl-
     charge  =  -1.0
****
     4 element(s):
      1.0000 Pb             1.0000 C             3.0000 O
      1.0000 Cl
****
     5 species in aqueous dissociation reaction:
    -1.0000  Pb(CO3)Cl-               -1.0000  H+
     1.0000  Pb++                      1.0000  HCO3-
     1.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    3.8700   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
Pb(CO3)OH-                 Pb(CO3)OH-
     charge  =  -1.0
****
     4 element(s):
      1.0000 Pb             1.0000 C             4.0000 O
      1.0000 H
****
     5 species in aqueous dissociation reaction:
    -1.0000  Pb(CO3)OH-               -2.0000  H+
     1.0000  Pb++                      1.0000  HCO3-
     1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   13.4400   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
PbSO4(aq)                  PbSO4(aq)
```

```
     charge   =    0.0
****
     3 element(s):
      1.0000 Pb              1.0000 S               4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbSO4(aq)                1.0000  Pb++
     1.0000  SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.7200    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------------
Fe(CO3)2--                Fe(CO3)2(-2)
     charge   =   -2.0
****
     3 element(s):
      2.0000 C               1.0000 Fe              6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Fe(CO3)2--                  -2.0000  H+
     1.0000  Fe++                         2.0000  HCO3-
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
        No_Data    13.8900    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
*
* Source: Kim et al. 2017
+---------------------------------------------------------------------
FeCO3(aq)                 FeCO3(00)
     charge   =    0.0
****
     3 element(s):
      1.0000 C               1.0000 Fe              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  FeCO3(aq)                   -1.0000  H+
     1.0000  Fe++                         1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
        No_Data     4.8300    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Bruno et al 1992
+---------------------------------------------------------------------
FeOH+                     FeOH+
     charge   =    1.0
****
     3 element(s):
      1.0000 H               1.0000 Fe              1.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  FeOH+                       -1.0000  H+
     1.0000  Fe++                         1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     9.3100    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Shock et al 1997
+---------------------------------------------------------------------
Fe(OH)2(aq)               Fe(OH)2(aq)
     charge   =    0.0
```

```
****
     3 element(s):
      1.0000 Fe              2.0000 H              2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Fe(OH)2(aq)              -2.0000  H+
     1.0000  Fe++                      2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    20.8200    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Stumm & Morgan (1996)
+---------------------------------------------------------------------
Fe(OH)3-                  Fe(OH)3-
     charge  =  -1.0
****
     3 element(s):
      1.0000 Fe              3.0000 H              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Fe(OH)3-                   -3.0000  H+
     1.0000  Fe++                        3.0000  H2O
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
        No_Data    31.0000    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Baes and Mesmer (1976)28
+---------------------------------------------------------------------
H3Citrate(aq)             H3C6H5O7(aq)
     charge  =   0.0
****
     3 element(s):
      6.0000 C               8.0000 H              7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  H3Citrate(aq)            3.0000  H+
     1.0000  Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -14.2700    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------------
H2Citrate-                H2C6H5O7-
     charge  =  -1.0
****
     3 element(s):
      6.0000 C               7.0000 H              7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  H2Citrate-               2.0000  H+
     1.0000  Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -11.1400    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------------
HCitrate--                HC6H5O7--
     charge  =  -2.0
****
```

```
     3 element(s):
      6.0000 C              6.0000 H              7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  HCitrate--                1.0000  H+
     1.0000  Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -6.3600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------
CaHCitrate(aq)             CaHC6H5O7
     charge  =   0.0
****
     4 element(s):
      6.0000 C              6.0000 H              1.0000 Ca
      7.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CaHCitrate(aq)            1.0000  Ca++
     1.0000  Citrate---                1.0000  H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -9.2800    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al. (2005) Derived with SIT
Model
+---------------------------------------------------------------
CaH2Citrate+               CaH2C6H5O7+
     charge  =   1.0
****
     4 element(s):
      6.0000 C              7.0000 H              1.0000 Ca
      7.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CaH2Citrate+              1.0000  Ca++
     1.0000  Citrate---                2.0000  H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -12.670    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al. (2005) Derived with SIT
Model
+---------------------------------------------------------------
H4EDTA(aq)                 H4C10H12O8N2(aq)
     charge  =   0.0
****
     4 element(s):
     10.0000 C             16.0000 H              2.0000 N
      8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  H4EDTA(aq)                4.0000  H+
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -23.4200    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al. (2005)
```

```
+------------------------------------------------------------
H3EDTA-                    H3C10H12O8N2-
     charge  =  -1.0
****
     4 element(s):
     10.0000 C             15.0000 H             2.0000 N
      8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  H3EDTA-                  3.0000  H+
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -21.19   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:Hummel et al. (2005) Derived with SIT Model et al. (2005)

+------------------------------------------------------------
H2EDTA--                   H2C10H12O8N2--
     charge  =  -2.0
****
     4 element(s):
     10.0000 C             14.0000 H             2.0000 N
      8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  H2EDTA--                 2.0000  H+
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -18.0400   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:Hummel et al. (2005) Derived with SIT Model et al. (2005)

+------------------------------------------------------------
HEDTA---                   HC10H12O8N2---
     charge  =  -3.0
****
     4 element(s):
     10.0000 C             13.0000 H             2.0000 N
      8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  HEDTA---                 1.0000  H+
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -11.2400   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:Hummel et al. (2005) Derived with SIT Model et al. (2005)
+------------------------------------------------------------
NaEDTA---                  NaC10H12O8N2---
     charge  =  -3.0
****
     5 element(s):
     10.0000 C             12.0000 H             2.0000 N
      8.0000 O              1.0000 Na
****
     3 species in aqueous dissociation reaction:
    -1.0000  NaEDTA---                1.0000 Na+
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
```

```
        No_Data   -2.80000    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source:Hummel et al. (2005) Derived with SIT Model et al. (2005)

+---------------------------------------------------------------
MgHCitrate(aq)              MgHC6H5O7
     charge   =    0.0
****
     4 element(s):
      6.0000 C              6.0000 H              1.0000 Mg
      7.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000   MgHCitrate(aq)            1.0000   Mg++
     1.0000   Citrate---                1.0000   H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -8.9600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------
MgH2Citrate+                MgH2C6H5O7+
     charge   =    1.0
****
     4 element(s):
      6.0000 C              7.0000 H              1.0000 Mg
      7.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000   MgH2Citrate+              1.0000   Mg++
     1.0000   Citrate---                2.0000   H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -8.9600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------
MgCitrate-                  MgC6H5O7-
     charge   =   -1.0
****
     4 element(s):
      6.0000 C              5.0000 H              1.0000 Mg
      7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000   MgCitrate-                1.0000   Mg++
     1.0000   Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -4.8100    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al (2005) Derived with SIT
Model
+---------------------------------------------------------------
MgEDTA--                    MgC10H12O8N2--
     charge   =   -2.0
****
     5 element(s):
     10.0000 C             12.0000 H              1.0000 Mg
      2.0000 N              8.0000 O
****
```

```
     3 species in aqueous dissociation reaction:
    -1.0000  MgEDTA--                  1.0000  Mg++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -10.9000   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al. (2005)
+---------------------------------------------------------------
MgHEDTA-                   MgC10H13O8N2-
     charge  =  -1.0
****
     5 element(s):
     10.0000 C             13.0000 H             1.0000 Mg
      2.0000 N              8.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  MgHEDTA-                  1.0000  Mg++
     1.0000  EDTA----                  1.0000  H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -15.4000   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Hummel et al. (2005) Derived with SIT Model et al. (2005)

+---------------------------------------------------------------
MgOxalate(aq)              MgC2O4(aq)
     charge  =   0.0
****
     3 element(s):
      2.0000 C              1.0000 Mg             4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  MgOxalate(aq)             1.0000  Mg++
     1.0000  Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -3.7931   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Giambalvo
+---------------------------------------------------------------
Mg(Oxalate)2--             Mg(C2O4)2--
     charge  =   -2.0
****
     3 element(s):
      4.0000 C              1.0000 Mg             8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  Mg(Oxalate)2--            1.0000  Mg++
     2.0000  Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -5.2400   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Jang & Kim 2016
+---------------------------------------------------------------
CaEDTA--                   CaC10H12O8N2--
     charge  =  -2.0
****
     5 element(s):
     10.0000 C              1.0000 Ca            12.0000 H
      2.0000 N              8.0000 O
****
```

```
     3 species in aqueous dissociation reaction:
    -1.0000  CaEDTA--                  1.0000  Ca++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -12.6900   No_Data    No_Data
        No_Data   No_Data   No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model(2005)
+---------------------------------------------------------------
CaHEDTA-                  CaHC10H13O8N2-
     charge  =  -1.0
****
     5 element(s):
     10.0000 C              1.0000 Ca           13.0000 H
      2.0000 N              8.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  CaHEDTA-                  1.0000  Ca++
     1.0000  EDTA----                  1.0000  H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -16.2300   No_Data    No_Data

        No_Data   No_Data   No_Data    No_Data
* Source: Hummel et al. (2005) Derived with SIT Model(2005)
+---------------------------------------------------------------
solids
+---------------------------------------------------------------
Pb2CO3Cl2(s)                  Pb2CO3Cl2
     V0PrTr  =   000.000 cm**3/mol [source:         ]
****
     4 element(s):
      2.0000 Pb             1.0000 C             2.0000 Cl
      3.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Pb2CO3Cl2(s)             -1.0000  H+
     2.0000  Pb++                      2.0000  Cl-
     1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   0.41000   No_Data    No_Data
        No_Data   No_Data   No_Data    No_Data
* Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------
PbSO4(s)                      PbSO4
     sp.type =  solid
*    EQ3/6   =
     revised =
*    mol.wt. =
     V0PrTr  =   000.000 cm**3/mol [source:         ]
****
     3 element(s):
      1.0000 Pb             1.0000 S             4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbSO4(s)                  1.0000  SO4--
     1.0000  Pb++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -7.8000   500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
```

```
*
*    Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------------
Cerussite(cr)                  PbCO3(cr)
     V0PrTr  =    000.000 cm**3/mol [source:         ]
****
     3 element(s):
      1.0000 Pb             1.0000 C              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Cerussite(cr)               -1.0000  H+
     1.0000  HCO3-                        1.0000  Pb++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -2.8400   500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
*
*    Source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------------
Litharge                PbO
     V0PrTr  =     00.00 cm**3/mol [source: 78hel/del]
****
     2 element(s):
      1.0000 O              1.0000 Pb
****
     4 species in aqueous dissociation reaction:
    -1.0000  Litharge                    -2.0000  H+
     1.0000  H2O                          1.0000  Pb++
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
        No_Data   12.6200   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* source: Powell et al. (2009) Derived with SIT Model et al (2009) Derived with SIT
Model
+---------------------------------------------------------------------
Ca2EDTA.7H2O(s)                Ca2C10H12O8N2.7H2O
     sp.type =  solid
     V0PrTr  =    000.000 cm**3/mol [source:         ]
****
     5 element(s):
     10.0000 C             26.0000 H             15.0000 O
      2.0000 Ca             2.0000 N
****
     4 species in aqueous dissociation reaction:
    -1.0000  Ca2EDTA.7H2O(s)             2.0000  Ca++
     1.0000  EDTA----                    7.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -16.8100  500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
* source: Domski (2018)
+---------------------------------------------------------------------
MgOxalate.2H2O(s)        MgC2O4.2H2O
     V0PrTr  =      0.000 cm**3/mol [source:          ]
****
     4 element(s):
      2.0000 C              4.0000 H              1.0000 Mg
      6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  MgOxalate.2H2O(s)           1.0000  Mg++
```

```
     2.0000  H2O                          1.0000  Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -6.4100    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Glushinskite from AP-182
+---------------------------------------------------------------------
Siderite                  FeCO3
     sp.type =  solid
     V0PrTr  =    29.378 cm**3/mol
****
     3 element(s):
      1.0000 C              1.0000 Fe             3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Siderite                   -1.0000  H+
     1.0000  Fe++                        1.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -0.1200    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Stumm and Morgan (1996)
+---------------------------------------------------------------------
Chukanovite               Fe2(OH)2CO3
     sp.type =  solid
     V0PrTr  =    0.000 cm**3/mol
****
     4 element(s):
      1.0000 C              2.0000 Fe             5.0000 O
      2.0000 H
****
     5 species in aqueous dissociation reaction:
    -1.0000  Chukanovite                -3.0000  H+
     2.0000  Fe++                        1.0000  HCO3-
     2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    12.3200    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Kim et al (2017)
+---------------------------------------------------------------------
Oxychloride-Fe-3          Fe2Cl(OH)3
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     4 element(s):
      1.0000 Cl             3.0000 H              2.0000 Fe
      3.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Oxychloride-Fe-3           -3.0000  H+
     1.0000  Cl-                         2.0000  Fe++
     3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    17.0800    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Kim et al (2017)
+---------------------------------------------------------------------
Fe(OH)2-Hex               Fe(OH)2
     V0PrTr  =    24.630 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      2.0000 H              1.0000 Fe             2.0000 O
```

```
****
     4 species in aqueous dissociation reaction:
    -1.0000  Fe(OH)2-Hex                  -2.0000  H+
     1.0000  Fe++                          2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    12.8900    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Kim et al (2017)
+---------------------------------------------------------------------
Hydromagnesite5424         Mg5(CO3)4(OH)2.4H2O
     V0PrTr  =    000.000 cm**3/mol [source:          ]
****
     4 element(s):
      4.0000 C              10.0000 H              5.0000 Mg
     18.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Hydromagnesite5424        -6.0000  H+
     5.0000  Mg++                       4.0000  HCO3-
     6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    31.2900    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Robie & Hemmingway (1973)

+---------------------------------------------------------------------
```