This memo documents the steps used to create a quality assured thermodynamic database, DATA0.FM2, in accordance with AP-173 revision 1 (Domski and Xiong 2015). The steps are as follows:

1) Copy DATA0.FM1 (Xiong 2011) to DATA0.FM2.
2) Edit DATA0.FM2 and enter all of the fitting and supporting parameters from AP-154, revision 2 (Xiong 2013), AP-155, revision 3 (Xiong 2014), and AP-173, revision 1 as listed in AP-173. Note the analysis plans will be called AP-154, AP-155, and AP-173 without their revision numbers for the remainder of this document.
3) Run the parameter fitting Python scripts using DATA0.FM2 for each of the tasks listed in AP-173.
4) Compare the results with those documented in the analysis reports, and memos, i.e., the original derived parameter values. The original derived values (documented value) were accepted if the results of fitting with DATA0.FM2 were within 10% of the value, which is a deviation from acceptance criteria of AP-173. It was expected that there would be some deviation between the original derived values and those derived with DATA0.FM2 because of the necessity of deriving the parameters in a stepwise fashion.
5) If the difference in the fitted parameter values using DATA0.FM2 was greater than 10%, then the appropriate analysis report, or memo, was updated to reflect the new parameters and DATA0.FM2 was also updated to reflect these changes.

Tables 1, 2, and 3 list the tasks and parameters for AP-154, AP-155, and AP-173, respectively, and compares the values documented in the analysis reports, and memos, in the table column labeled “Documented Value”, with those estimated using the new database DATA0.FM2. A complete listing of the parameter blocks, both fitting and supporting data, that were added to DATA0.FM1 is provided in Appendix A.

Note that the β\(^{(1)}\) and c^± parameters for binary Pitzer interaction parameters are not listed in this memo unless those parameters were specifically derived for inclusion in the database. The reference section provides the analysis reports and memos where complete listings of the parameters included in the QA database may be found, please refer to these references, or the data blocks listed in Appendix A, as a complete source of the parameter values included in DATA0.FM2.

**AP-154 Tasks**
The tasks completed under AP-154 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 1.
Table 1. AP-154 Comparison of the documented parameters with those estimated using DATA0.FM2.

<table>
<thead>
<tr>
<th>AP-154 Task</th>
<th>Chemical Entity</th>
<th>Fitting Parameter</th>
<th>Documented Value</th>
<th>Estimated with DATA0.FM2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>14 &amp; 15</td>
<td>Cerussite</td>
<td>( \text{Log K} )</td>
<td>-3.411</td>
<td>-3.312</td>
<td>Due to the greater than 10% difference for some of the Pitzer parameters it was decided that the Xiong(2014a) would be revised to reflect the values obtained using DATA0.FM2. The reason being the need to maintain consistency with the lead hydroxyl parameters derived under AP-155, Task 3 and 4.1.</td>
</tr>
<tr>
<td>18 &amp; 19(^1)</td>
<td>( \text{Na}^+ - \text{Pb(CO}_3\text{)}_2^{2-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.6245</td>
<td>0.198</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original documented parameters (Xiong 2014b) were retained in DATA0.FM2. Note that an error was found in the ( \text{Mg}^{2+} - \text{PbEDTA}^{2-} ) parameter block that was corrected, and which did not affect the fitted parameters.</td>
</tr>
<tr>
<td></td>
<td>( \text{Na}^+ - \text{Pb(CO}_3\text{)}_2\text{Cl}^- )</td>
<td>( \beta^{(0)} )</td>
<td>0.0191</td>
<td>0.380</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{HCO}_3^- - \text{Pb(CO}_3\text{)}_2^{2-} )</td>
<td>( \theta )</td>
<td>0.108</td>
<td>0.148</td>
<td></td>
</tr>
<tr>
<td>20 &amp; 21</td>
<td>( \text{Na}^+ - \text{PbCl}^- )</td>
<td>( \beta^{(0)} )</td>
<td>0.535</td>
<td>0.514</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original parameters (Xiong 2014c) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td></td>
<td>( \text{Mg}^{2+} - \text{PbCl}^- )</td>
<td>( \beta^{(0)} )</td>
<td>1.975</td>
<td>1.903</td>
<td></td>
</tr>
<tr>
<td>22 &amp; 24</td>
<td>( \text{Mg}^{2+} - \text{PbEDTA}^{2-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.561</td>
<td>0.583</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td></td>
<td>( \text{Mg}^{2+} - \text{Cl}^- \text{PbCl}_3^- )</td>
<td>( \beta^{(0)} )</td>
<td>1.428</td>
<td>1.428</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Mg}^{2+} - \text{EDTA}^{4-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.0100</td>
<td>0.020</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Ca}^{2+} - \text{EDTA}^{4-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.00956</td>
<td>0.00956</td>
<td></td>
</tr>
<tr>
<td>30 &amp; 31(^1)</td>
<td>( \text{Mg}^{2+} - \text{CaEDTA}^{2-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.525</td>
<td>0.300</td>
<td>The values are identical, therefore, the original values (Xiong 2015) were retained in DATA0.FM2. Note that an error was found in the ( \text{Mg}^{2+} / \text{CaEDTA}^{2-} ) parameter block that was corrected, and which did not affect the fit.</td>
</tr>
<tr>
<td></td>
<td>( \text{Ca}^{2+} - \text{MgEDTA}^{4-} )</td>
<td>( \beta^{(0)} )</td>
<td>0.0844</td>
<td>0.640</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Ca}^{2+} - \text{CaEDTA}^{2-} )</td>
<td>( \beta^{(0)} )</td>
<td>-11.156</td>
<td>-11.156</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Na}^+ - \text{CaEDTA}^{2-} )</td>
<td>( \beta^{(0)} )</td>
<td>-0.00956</td>
<td>-0.00956</td>
<td></td>
</tr>
<tr>
<td>28 &amp; 35(^1)</td>
<td>( \text{Mg}^{2+} - \text{Citrate}^{3-} )</td>
<td>( \beta^{(0)} )</td>
<td>3.241</td>
<td>0.933</td>
<td>An error was found in the ( \text{Mg}^{2+} - \text{Citrate}^{3-} ) parameter block that required these parameters to be re-fit. The analysis report and accompanying memos were updated, and DATA0.FM2 was updated to reflect the new values. Note that AP-154 Tasks 20 and 21 were re-run with the updated database and there was no change in the parameters.</td>
</tr>
<tr>
<td></td>
<td>( \text{Mg}^{2+} - \text{MgCitrate}^- )</td>
<td>( \beta^{(0)} )</td>
<td>0.865</td>
<td>1.0915</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Mg}^{2+} - \text{CaCitrate}^- )</td>
<td>( \beta^{(0)} )</td>
<td>0.434</td>
<td>0.376</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{CaCitrate}^- )</td>
<td>( \beta^{(0)} )</td>
<td>-4.973</td>
<td>-5.001</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2012a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td></td>
<td>( \text{Na}^+ - \text{CaCitrate}^- )</td>
<td>( \beta^{(0)} )</td>
<td>-0.131</td>
<td>-0.142</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{Na}^+ - \text{Ca}^{2+} - \text{ClO}_4^- )</td>
<td>( \beta^{(0)} )</td>
<td>-0.00682</td>
<td>-0.00346</td>
<td></td>
</tr>
</tbody>
</table>

\(^1\) During review it was found that the parameter blocks for \( \text{Mg}^{2+} - \text{PbEDTA}^{2-} \), \( \text{Mg}^{2+} - \text{CaEDTA}^{2-} \) and \( \text{Mg}^{2+} - \text{Citrate}^{3-} \) had the alpha(1) set to 2.0 when it should have been 1.4, this was corrected, and had no impact on Tasks 18 and 19, and 30 and 31, however, it did effect Tasks 28 and 35 and new parameters were calculated and the accompanying documentation was updated.
AP-154 Tasks 22 and 24
Task 22 and 24 of AP-154 are not included in Table 1 because the parameters were estimated by manual fitting (Xiong 2011a), and not by the use of the Python script, thus, it was not possible to run the Python script using DATA0.FM2 for parameter comparison purposes. Rather the test cases from Xiong 2011a were run in EQ3/6 using DATA0.FM2 and the output data were plotted together with the experimental data and predicted data of Xiong 2011a in Figure 1. Figure 1 shows that the predicted data of Xiong 2011a, and the predicted data using DATA0.FM2 are very close, therefore, the original parameter values of Xiong were retained in DATA0.FM2.

Figure 1. Comparison of the documented fit (Xiong, 2011a) with the DATA0.FM2 fit to the experimental data for AP-154 Task 22 and 24.

AP-154 Tasks 29 and 32
Note that tasks 29 and 32 from AP-154, which were specified by AP-173 to be included in DATA0.FM2 were not included because the parameters from these tasks were included in AP-154 tasks 30 and 31 for the EDTA parameters, and task 23 for the oxalate parameters, this is a deviation from AP-173.

AP-155 Tasks
The tasks completed under AP-155 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 2.

Table 2. AP-155 Comparison of the documented parameters with those estimated using DATA0.FM2.

<table>
<thead>
<tr>
<th>AP-155 Task</th>
<th>Chemical Entity</th>
<th>Fitting Parameter</th>
<th>Documented Value</th>
<th>Estimated with DATA0.FM2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 4.1</td>
<td>Pb(OH)(_2)(aq)</td>
<td>Log K</td>
<td>17.0475</td>
<td>17.0395</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td></td>
<td>Pb(OH)(_3^-)</td>
<td></td>
<td>27.989</td>
<td>27.992</td>
<td></td>
</tr>
<tr>
<td>3, 4.1</td>
<td>Na(^+) - Pb(OH)(_3^-)</td>
<td>(\beta^{(0)})</td>
<td>0.335</td>
<td>0.335</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td></td>
<td>Pb(OH)(_2)(aq) - Cl(^-)</td>
<td>(\lambda)</td>
<td>-0.172</td>
<td>-0.172</td>
<td></td>
</tr>
<tr>
<td>AP-155 Task</td>
<td>Chemical Entity</td>
<td>Fitting Parameter</td>
<td>Documented Value</td>
<td>Estimated with DATA0.FM2</td>
<td>Comments</td>
</tr>
<tr>
<td>------------</td>
<td>----------------</td>
<td>------------------</td>
<td>------------------</td>
<td>--------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>4.4, 4.11</td>
<td>PbCl₂(aq) – Mg²⁺ - Cl⁻</td>
<td>ζ</td>
<td>0.682</td>
<td>0.682</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.2</td>
<td>PbO₂⁻(aq) – Mg²⁺</td>
<td>λ</td>
<td>-0.365</td>
<td>-0.365</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.10</td>
<td>Pb₄O₇(aq) - Na⁺</td>
<td>λ</td>
<td>0.156</td>
<td>0.0836</td>
<td>The value estimated with DATA0.FM2 is outside of the 10% range, however, the original documented value (Xiong 2015a) will be retained in DATA0.FM2 because it was derived in a step-wise manner and to change it would not be consistent with the original fitting scheme.</td>
</tr>
<tr>
<td>4.5</td>
<td>MgSO₄(aq)</td>
<td>Log K</td>
<td>-2.383</td>
<td>-2.389</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.6</td>
<td>Na⁺ - Ca²⁺ - OH⁻</td>
<td>Ψ</td>
<td>-0.0198</td>
<td>-0.0198</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.8</td>
<td>Na_Mg_Tetraborate (A)</td>
<td>Log K</td>
<td>-24.400</td>
<td>-24.420</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.8</td>
<td>Na_Mg_Tetraborate (B)</td>
<td>Log K</td>
<td>-24.990</td>
<td>-25.010</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.9</td>
<td>Na⁺ - Mg(B(OH)₄)²⁻</td>
<td>θ</td>
<td>-0.298</td>
<td>-0.298</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.12</td>
<td>B(OH)₃(aq) – Mg²⁺ - Cl⁻</td>
<td>μ</td>
<td>0.0350</td>
<td>0.0350</td>
<td>The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>4.7 (10)</td>
<td>Na-Tetraborate</td>
<td>Log K</td>
<td>-24.800</td>
<td>-24.800</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
</tbody>
</table>

1 – This task was completed under revision 0 of AP-155 which at the time had this task labeled as Task 10.

AP-173 Parameters

AP-173 specifies additional parameters to be included in DATA0.FM2, these parameters are listed in Table 3.

Information Only
<table>
<thead>
<tr>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydromagnesite (5424) Log $K_{sp}$</td>
<td>Xiong 2015b</td>
</tr>
<tr>
<td>Pitzer binary interaction parameter Na⁺ - Am(EDTA)⁻</td>
<td>Xiong 2013a</td>
</tr>
<tr>
<td>Pitzer binary interaction parameter Am$^{3+}$ - Cl⁻</td>
<td>Domski and Xiong 2015, Xiong 2015c</td>
</tr>
</tbody>
</table>

### Hydromagnesite (5424)

Xiong (2015b) derived the solubility product (log $K_{sp}$) for the Pitzer model according to the following dissolution expression:

\[
(1) \quad \text{Mg}_5(\text{CO}_3)_4(\text{OH})_2\cdot 4\text{H}_2\text{O} + 10\text{H}^+ = 5\text{Mg}^{2+} + 4\text{CO}_2(\text{g}) + 10\text{H}_2\text{O}(\text{l}) \quad \log K_{sp} = 60.61
\]

However, to incorporate this value into the EQ3/6 database it was necessary to recast this expression in terms of the basis species for carbonate which is the bicarbonate ion (HCO$_3^-$). To convert to the basis species, HCO$_3^-$, the following reaction (2) was added to reaction (1), as follows:

\[
(2) \quad 4x(\text{CO}_2(\text{g}) + \text{H}_2\text{O} = \text{H}^+ + \text{HCO}_3^- \quad \log K = -7.8193)
\]

\[
4x(-7.8193) + 60.61 = 29.3328
\]

\[
(3) \quad \text{Mg}_5(\text{CO}_3)_4(\text{OH})_2\cdot 4\text{H}_2\text{O} + 6\text{H}^+ = 5\text{Mg}^{2+} + 4\text{HCO}_3^- + 6\text{H}_2\text{O}(\text{l}) \quad \log K_{sp} = 29.3328
\]

### Na⁺ - Am(EDTA)⁻ Pitzer binary interaction parameter

The following data block was added to DATA0.FM2 as calculated in Xiong (2013a).

```
+-----------------------------------------------+----------------+
| Na⁺                                           | AmEDTA⁻        |
| alpha(1) = 2.0                               |                |
| alpha(2) = 12.0                              |                |
| beta(0)                                       |                |
| a1 = 0.4372                                   |                |
| a2 = 0                                       |                |
| a3 = 0                                       |                |
| a4 = 0                                       |                |
| beta(1)                                       |                |
| a1 = 0.29                                    |                |
| a2 = 0                                       |                |
| a3 = 0                                       |                |
| a4 = 0                                       |                |
| beta(2)                                       |                |
| a1 = 0                                       |                |
| a2 = 0                                       |                |
| a3 = 0                                       |                |
| a4 = 0                                       |                |
| Cphi:                                         |                |
| a1 = -0.01303                                |                |
| a2 = 0                                       |                |
| a3 = 0                                       |                |
| a4 = 0                                       |                |
+-----------------------------------------------+----------------+
* Source: "Calculations of Thermodynamic Parameters in EDTA System for Experimental Data From Carlsbad Environmental Monitoring and Research Center (CEMRC)" ERMS:560761
```
AmHB₄O₇²⁺ - Cl⁻ Pitzer binary interaction parameter

As required by AP-173, the binary Pitzer interaction parameters as documented in Xiong (2015) were included in the DATA0.FM2. The comparison of the documented parameter values (Xiong 2015) with those estimated using DATA0.FM2 is listed in Table 4.

<table>
<thead>
<tr>
<th>Chemical Entity</th>
<th>Parameter</th>
<th>Documented Value</th>
<th>Estimated with DATA0.FM2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>AmHB₄O₇²⁺</td>
<td>Log K</td>
<td>-37.34</td>
<td>-37.34</td>
<td>The values are identical, therefore, the original values (Xiong 2015c) are retained in DATA0.FM2.</td>
</tr>
<tr>
<td>AmHB₄O₇²⁺ - Cl⁻</td>
<td>β⁽θ⁾</td>
<td>0.92</td>
<td>0.92</td>
<td></td>
</tr>
</tbody>
</table>

Files

The files that are to be submitted to the records center are listed in Table 5 and may be found at:
/nfs/data/CVSLIB/WIPP_EXTERNAL/ap173/Files

Table 5. List of files to be submitted to records.

<table>
<thead>
<tr>
<th>File Name</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>DATA0.FM2</td>
<td>QA database</td>
</tr>
<tr>
<td>FM2_additions.txt</td>
<td>Data blocks added to DATA0.FM1</td>
</tr>
<tr>
<td>Results_AP154_Task14-15_rev1.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_Task_18-19.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_Task_20-21.xlsx</td>
<td></td>
</tr>
<tr>
<td>AR_AP154_Task22_Modeling.xlsx</td>
<td>Files which compare the documented parameters with those estimated using DATA0.FM2</td>
</tr>
<tr>
<td>AP154_Task23_Results.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_AP154_Task30.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_AP154_Task28-35.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_AP155_task10_Na2B4O7_Na2SO4.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_AP155_Task10_Na2B4O7_NaCl.xlsx</td>
<td></td>
</tr>
<tr>
<td>Results_AP155.xlsx</td>
<td></td>
</tr>
</tbody>
</table>

References


Xiong, Y.-L. 2014c. “Experimental and Thermodynamic Modeling of PbCit– Interactions in NaCl and MgCl2 Solutions” Carlsbad, NM: Sandia National Laboratories. ERMS: 562836

Xiong, Y.-L. 2015. “Experimental determination of solubilities of lead oxalate (PbC2O4), di-calcium ethylenediaminetetraacetic acid (Ca2EDTA(s)) in MgCl2–H2O system, and earlandite (Ca3[C3H5O(COO)3]2•4H2O) in NaCl–H2O and MgCl2–H2O systems, and their respective Pitzer interaction parameters. Revision 1, Supercedes ERMS 561917” Work Carried Out under Tasks 23, 28, 29, 30, 31 and 35 of AP-154: Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA. To be included in the AP-154 records packageAP-154, Revision 2. Carlsbad, NM: Sandia National Laboratories. ERMS: 564844.


APPENDIX A.

Text and Data Blocks Added to DATA0.FM1

data0.fm2
Pitzer Thermodynamic Database (10/14/2015)
DATA0.FM2 was created from DATA0.FM1 (DATA0.FMT.R2) to include all of the parameters outlined in AP-173, revision 1. This database was created in response to EPA comments of the CRA-2014 and will be used to perform the PABC-2016 calculations.

<table>
<thead>
<tr>
<th>AmHb407++</th>
<th>Cl-</th>
</tr>
</thead>
<tbody>
<tr>
<td>alpha(1)</td>
<td>2.0</td>
</tr>
<tr>
<td>alpha(2)</td>
<td>12.0</td>
</tr>
<tr>
<td>beta(0)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.9163</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>beta(1)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>1.74</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>beta(2)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>Cphi:</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.0196</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
</tbody>
</table>

* Source: AP-173

<table>
<thead>
<tr>
<th>Na+</th>
<th>PbCitrate-</th>
</tr>
</thead>
<tbody>
<tr>
<td>alpha(1)</td>
<td>2.0</td>
</tr>
<tr>
<td>alpha(2)</td>
<td>12.0</td>
</tr>
<tr>
<td>beta(0)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.535</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>beta(1)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.29</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>beta(2)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
<tr>
<td>Cphi:</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>0.0196</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
</tbody>
</table>

* Source: Fitting parameter for Tasks 20 & 21

<table>
<thead>
<tr>
<th>Mg++</th>
<th>PbCitrate-</th>
</tr>
</thead>
<tbody>
<tr>
<td>alpha(1)</td>
<td>2.0</td>
</tr>
<tr>
<td>alpha(2)</td>
<td>12.0</td>
</tr>
<tr>
<td>beta(0)</td>
<td></td>
</tr>
<tr>
<td>a1</td>
<td>1.97</td>
</tr>
<tr>
<td>a2</td>
<td>0.</td>
</tr>
<tr>
<td>a3</td>
<td>0.</td>
</tr>
<tr>
<td>a4</td>
<td>0.</td>
</tr>
</tbody>
</table>
beta(1)  
  a1 = 1.74  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

beta(2)  
  a1 = 0.  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

Cphi:  
  a1 = 0.0771  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

* Source: Fitting parameter for Tasks 20 & 21

+----------------------------------------------------------------

Na+  PbEDTA--

alpha(1) = 2.0  
alpha(2) = 12.0  

beta(0)  
  a1 = 0.6507  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

beta(1)  
  a1 = 1.74  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

beta(2)  
  a1 = 0.  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

Cphi:  
  a1 = 0.0647  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

* Source: Fitting parameter for Tasks 18 & 19

+----------------------------------------------------------------

Mg++  PbEDTA--

alpha(1) = 1.4  
alpha(2) = 12.0  

beta(0)  
  a1 = 1.8399  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

beta(1)  
  a1 = 3.27  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

beta(2)  
  a1 = 0.  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

Cphi:  
  a1 = -0.1501  
  a2 = 0.  
  a3 = 0.  
  a4 = 0. 

* Source: Fitting parameter for Tasks 18 & 19

+----------------------------------------------------------------

Na+  Pb(CO3)2--

alpha(1) = 2.0  
alpha(2) = 12.0  

beta(0)  
  a1 = 0.1975
\[
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(1) \\
a_1 = 1.74 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(2) \\
a_1 = 0. \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
Cphi: \\
a_1 = -0.2105 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
\]

* Source: Fitting parameter AP-154 Task 14 & 15

\[
\begin{array}{l}
\text{Na}^+ \\
alpha(1) = 2.0 \\
alpha(2) = 12.0 \\
beta(0) \\
a_1 = 0.3799 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(1) \\
a_1 = 0.29 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(2) \\
a_1 = 0. \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
Cphi: \\
a_1 = 0.1921 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
\end{array}
\]

* Source: Fitting parameter AP-154 Task 14 & 15

\[
\begin{array}{l}
\text{Mg}^{++} \\
alpha(1) = 2.0 \\
alpha(2) = 12.0 \\
beta(0) \\
a_1 = 0.987 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(1) \\
a_1 = 1.74 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
beta(2) \\
a_1 = 0. \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
Cphi: \\
a_1 = 0.01 \\
a_2 = 0. \\
a_3 = 0. \\
a_4 = 0. \\
\end{array}
\]

* Source: Xiong 2015 fitting solubility of Na2B4O7.10H2O data in MgCl2 solutions. Based on average 1:2 and 2:1 interactions. * beta(zero), a(1)=0.418; beta(one), a(1)=1.74.
Mg++

alpha(1) = 2.0
alpha(2) = 7.59
beta(0)
a1 = -1.42258
a2 = 0.
a3 = 0.
a4 = 0.
beta(1)
a1 = 14.3542
a2 = 0.
a3 = 0.
a4 = 0.
beta(2)
a1 = 504.233
a2 = 0.
a3 = 0.
a4 = 0.
Cphi:
a1 = -0.62469
a2 = 0.
a3 = 0.
a4 = 0.

* Source: Yin et al., 2007

+----------------------------------------------------------------

MgB(OH)4+- S04--

alpha(1) = 2.0
alpha(2) = 12.0
beta(0)
a1 = 0.7806
a2 = 0.
a3 = 0.
a4 = 0.
beta(1)
a1 = 1.74
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: Xiong (2015)

+----------------------------------------------------------------

Mg++ PbCl3-

alpha(1) = 2.0
alpha(2) = 12.0
beta(0)
a1 = 1.4277
a2 = 0.
a3 = 0.
a4 = 0.
beta(1)
a1 = 1.74
a2 = 0.
a3 = 0.
a4 = 0.
beta(2)
a1 = 0.
a2 = 0.
a3 = 0.
a4 = 0.
Cphi:
a1 = 0.000
a2 = 0.
a3 = 0.
\[ a_4 = 0. \]

* Source: In Felmy et al. (2000), beta(zero), \( a(1) = 0.21 \).

\[ \text{Na}^{+} \text{Pb(Oxalate)}^{2-} \]

\[
\begin{align*}
\alpha(1) &= 2.0 \\
\alpha(2) &= 12.0 \\
\beta(0) &= \\
& a_1 = 0.0 \\
& a_2 = 0 \\
& a_3 = 0 \\
& a_4 = 0. \\
\beta(1) &= \\
& a_1 = -1.86 \\
& a_2 = 0 \\
& a_3 = 0 \\
& a_4 = 0. \\
\beta(2) &= \\
& a_1 = 0 \\
& a_2 = 0 \\
& a_3 = 0. \\
& a_4 = 0. \\
Phi: &= \\
& a_1 = 0.198 \\
& a_2 = 0 \\
& a_3 = 0 \\
& a_4 = 0. \\
\end{align*}
\]

* Source: AP-154 Task 22 & 24

\[ \text{K}^{+} \text{Pb(Oxalate)}^{2-} \]

\[
\begin{align*}
\alpha(1) &= 2.0 \\
\alpha(2) &= 12.0 \\
\beta(0) &= \\
& a_1 = 0.0 \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
\beta(1) &= \\
& a_1 = -1.86 \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
\beta(2) &= \\
& a_1 = 0. \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
Phi: &= \\
& a_1 = 0.198 \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
\end{align*}
\]

* Source: AP-154 Task 22 & 24

\[ \text{Pb}^{2+} \text{ Cl}^{-} \]

\[
\begin{align*}
\alpha(1) &= 2.0 \\
\alpha(2) &= 12.0 \\
\beta(0) &= \\
& a_1 = 0.26 \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
\beta(1) &= \\
& a_1 = 1.64 \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
\beta(2) &= \\
& a_1 = 0. \\
& a_2 = 0. \\
& a_3 = 0. \\
& a_4 = 0. \\
Phi: &= \\
\end{align*}
\]
\begin{verbatim}
\texttt{a1 = 0.088}
\texttt{a2 = 0.}
\texttt{a3 = 0.}
\texttt{a4 = 0.}
\texttt{* Source: 84Millero/Byrne}
\end{verbatim}

\begin{verbatim}
PbCl+ Cl-  
alpha(1) = 2.0  
alpha(2) = 12.0  
beta(0)  
a1 = 0.15  
a2 = 0.  
a3 = 0.  
a4 = 0.  
beta(1)  
a1 = 0.  
a2 = 0.  
a3 = 0.  
a4 = 0.  
Cphi:  
a1 = 0.091  
a2 = 0.  
a3 = 0.  
a4 = 0.  
\end{verbatim}

\begin{verbatim}
\texttt{a1 = -0.0605}
\texttt{a2 = 0.}
\texttt{a3 = 0.}
\texttt{a4 = 0.}  
\texttt{* Source: 84Millero/Byrne has a value of -0.19 for beta(0);}
\texttt{* Cphi evaluated by Xiong (2011)}
\end{verbatim}

\begin{verbatim}
Na+ PbCl3-  
alpha(1) = 2.0  
alpha(2) = 12.0  
beta(0)  
a1 = -0.0605  
a2 = 0.  
a3 = 0.  
a4 = 0.  
beta(1)  
a1 = 0.00  
a2 = 0.  
a3 = 0.  
a4 = 0.  
Cphi:  
a1 = 0.091  
a2 = 0.  
a3 = 0.  
a4 = 0.  
\end{verbatim}

\begin{verbatim}
H+ PbCl3-  
alpha(1) = 2.0  
alpha(2) = 12.0  
beta(0)  
a1 = 0.27  
a2 = 0.  
a3 = 0.  
a4 = 0.  
beta(1)  
a1 = -0.63  
a2 = 0.  
a3 = 0.  
a4 = 0.  
\end{verbatim}
<table>
<thead>
<tr>
<th>Source: OOFelmy et al.</th>
</tr>
</thead>
</table>
| \[\begin{align*}
| \text{Na}^+ + \text{Pb(OH)}_3^- & \rightarrow \text{Na}^+ \cdot \text{Pb(OH)}_3 \\\n| \text{Pb}^2+ + \text{Cl}^- & \rightarrow \text{PbCl}_2 \\\n| \text{Na}^+ + \text{AmEDTA}^- & \rightarrow \text{Na}^+ \cdot \text{AmEDTA} \end{align*}\] |

Source: Xiong (2015), modeling solubility of lead oxide in NaClO₄ and NaCl solutions at high pH ranges.
beta(1)  
  a1 = 0.29  
a2 = 0.  
a3 = 0.  
a4 = 0.  

beta(2)  
  a1 = 0.  
a2 = 0.  
a3 = 0.  
a4 = 0.  

βphi:  
a1 = -0.01303  
a2 = 0.  
a3 = 0.  
a4 = 0.  

* Source: "Calculations of Thermodynamic Parameters in EDTA System for Experimental Data From Carlsbad Environmental Monitoring and Research Center (CEMRC)" ERMS:560761  

Na⁺  
  α(1) = 2.0  
  α(2) = 12.0  

β(0)  
  a1 = -0.13133  
a2 = 0.  
a3 = 0.  
a4 = 0.  

β(1)  
  a1 = 0.29  
a2 = 0.  
a3 = 0.  
a4 = 0.  

β(2)  
  a1 = 0.  
a2 = 0.  
a3 = 0.  
a4 = 0.  

Cphi:  
a1 = -0.006818  
a2 = 0.  
a3 = 0.  
a4 = 0.  

* Fitting parameter Task 35 AP-154  

Mg²⁺  
  α(1) = 2.0  
  α(2) = 12.0  

β(0)  
  a1 = 0.3760  
a2 = 0.  
a3 = 0.  
a4 = 0.  

β(1)  
  a1 = 1.74  
a2 = 0.  
a3 = 0.  
a4 = 0.  

β(2)  
  a1 = 0.  
a2 = 0.  
a3 = 0.  
a4 = 0.  

Cphi:  
a1 = 0.0  
a2 = 0.  
a3 = 0.  
a4 = 0.  

* Fitting parameter Task 35 AP-154  

Mg²⁺  
  α(1) = 2.0  

Information Only
\[ \alpha(2) = 12.0 \]
\[ \beta(0) \]
\[ a_1 = 1.0915 \]
\[ a_2 = 0. \]
\[ a_3 = 0. \]
\[ a_4 = 0. \]
\[ \beta(1) \]
\[ a_1 = 1.74 \]
\[ a_2 = 0. \]
\[ a_3 = 0. \]
\[ a_4 = 0. \]
\[ \beta(2) \]
\[ a_1 = 0. \]
\[ a_2 = 0. \]
\[ a_3 = 0. \]
\[ a_4 = 0. \]
\[ c_{\phi i} : \]
\[ a_1 = 0.0 \]
\[ a_2 = 0. \]
\[ a_3 = 0. \]
\[ a_4 = 0. \]
\* Source: Xiong (2014) modeling solubility of earlandite in MgCl\(_2\) solutions.

+----------------------------------------------------------------
<table>
<thead>
<tr>
<th>Mg++ Citrate---</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \alpha(1) = 1.4 ]</td>
</tr>
<tr>
<td>[ \alpha(2) = 12.0 ]</td>
</tr>
<tr>
<td>[ \beta(0) ]</td>
</tr>
<tr>
<td>[ a_1 = 0.9330 ]</td>
</tr>
<tr>
<td>[ a_2 = 0. ]</td>
</tr>
<tr>
<td>[ a_3 = 0. ]</td>
</tr>
<tr>
<td>[ a_4 = 0. ]</td>
</tr>
<tr>
<td>[ \beta(1) ]</td>
</tr>
<tr>
<td>[ a_1 = 4.4 ]</td>
</tr>
<tr>
<td>[ a_2 = 0. ]</td>
</tr>
<tr>
<td>[ a_3 = 0. ]</td>
</tr>
<tr>
<td>[ a_4 = 0. ]</td>
</tr>
<tr>
<td>[ \beta(2) ]</td>
</tr>
<tr>
<td>[ a_1 = 0.0 ]</td>
</tr>
<tr>
<td>[ a_2 = 0. ]</td>
</tr>
<tr>
<td>[ a_3 = 0. ]</td>
</tr>
<tr>
<td>[ a_4 = 0. ]</td>
</tr>
<tr>
<td>[ c_{\phi i} : ]</td>
</tr>
<tr>
<td>[ a_1 = 0.0 ]</td>
</tr>
<tr>
<td>[ a_2 = 0. ]</td>
</tr>
<tr>
<td>[ a_3 = 0. ]</td>
</tr>
<tr>
<td>[ a_4 = 0. ]</td>
</tr>
</tbody>
</table>
\* Source: Evaluated from earlandite solubility in MgCl\(_2\).
\begin{align*}
\text{CaEDTA--} & \\
\text{alpha(1)} &= 1.4 \\
\text{alpha(2)} &= 12.0 \\
\text{beta(0)} & \\
\text{a1} &= 0.0844 \\
\text{a2} &= 0. \\
\text{a3} &= 0. \\
\text{a4} &= 0. \\
\text{beta(1)} & \\
\text{a1} &= 3.27 \\
\text{a2} &= 0. \\
\text{a3} &= 0. \\
\text{a4} &= 0. \\
\text{beta(2)} & \\
\text{a1} &= 0. \\
\text{a2} &= 0. \\
\text{a3} &= 0. \\
\text{a4} &= 0. \\
\text{Cphi:} & \\
\text{a1} &= 0.0 \\
\text{a2} &= 0. \\
\text{a3} &= 0. \\
\text{a4} &= 0. \\
\text{source: Xiong (2014)}
\end{align*}
\[
\begin{align*}
\text{Na}^+ & \quad \text{MgB(OH)4}^+ \\
\theta: & \\
a_1 &= -0.2975 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: Xiong (2015), modeling solubility of "Na-Mg-Tetraborate (B)" in MgCl2 solutions} \\
\end{align*}
\]

\[
\begin{align*}
\text{Mg}^{++} & \quad \text{PbCl}^+ \\
\theta: & \\
a_1 &= -0.13 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: 00Felmy, -0.13.} \\
\end{align*}
\]

\[
\begin{align*}
\text{Na}^+ & \quad \text{Pb}^{++} \\
\theta: & \\
a_1 &= 0.10 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: 84Millero/Byrne set to 0; 00Felmy has a value of 0.10} \\
\end{align*}
\]

\[
\begin{align*}
\text{Na}^+ & \quad \text{PbCl}^+ \\
\theta: & \\
a_1 &= 0.000 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: 84Millero/Byrne} \\
\end{align*}
\]

\[
\begin{align*}
\text{HCO}_3^- & \quad \text{Pb(CO}_3^2^- \\
\theta: & \\
a_1 &= 0.1476 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: Fitting parameter AP-154 Task 14 & 15} \\
\end{align*}
\]

\[
\begin{align*}
\text{Cl}^- & \quad \text{PbCl}_3^- \\
\theta: & \\
a_1 &= 0.7371 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: Xiong (2014), modeling lead oxalate solubility in MgCl2 solutions.} \\
\end{align*}
\]

\[
\begin{align*}
\text{SO}_4^{--} & \quad \text{B(OH)4}^- \\
\theta: & \\
a_1 &= 0.1697 \\
a_2 &= 0 \\
a_3 &= 0 \\
a_4 &= 0 \\
\textit{* Source: Evaluated from sodium tetraborate in Na2SO4 solutions.} \\
\textit{In FW86, the value is -0.012. The value for the revised model is 0.1697.} \\
\end{align*}
\]

\[
\begin{align*}
\text{SO}_4^{--} & \quad \text{Pb(OH)3}^- \\
\theta: & \\
a_1 &= -0.4046 \\
\end{align*}
\]
\begin{verbatim}
a2 = 0.
a3 = 0.
a4 = 0.
* Source: Xiong (2015), modeling solubility of lead oxide in Na2SO4 solutions.

+----------------------------------------------------------------
\text{CO}_3^{2-} \rightarrow \text{Pb(CO}_3)_2^{2-}
\theta: 
\begin{align*}
  a1 &= 0.2223 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Source: Fitting parameter AP-154 Task 14 & 15

+----------------------------------------------------------------
\text{PbOxalate(aq)} \rightarrow \text{Na}^+
\lambda: 
\begin{align*}
  a1 &= 0.00 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Source: Setting to zero

+----------------------------------------------------------------
\text{PbCO}_3^{(aq)} \rightarrow \text{Na}^+
\lambda: 
\begin{align*}
  a1 &= 0.0 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}

+----------------------------------------------------------------
\text{B(OH)}_3^{(aq)} \rightarrow \text{Mg}^{2+}
\lambda: 
\begin{align*}
  a1 &= 0.0000E+00 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Source: Xiong 2015 fitting solubility of Na2B4O7.10H2O in MgCl2 solutions

+----------------------------------------------------------------
\text{MgOxalate(aq)} \rightarrow \text{Mg}^{2+}
\lambda: 
\begin{align*}
  a1 &= 0.7454 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Source:

+----------------------------------------------------------------
\text{NaB(OH)}_4^{(aq)} \rightarrow \text{Na}^+
\lambda: 
\begin{align*}
  a1 &= 0.093 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Task 10, AP-155 fit value = 0.093

+----------------------------------------------------------------
\text{PbB}_4\text{O}_7^{(aq)} \rightarrow \text{Mg}^{2+}
\lambda: 
\begin{align*}
  a1 &= -0.3653 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
* Source: Xiong (2015), modeling solubility of lead solubility in MgCl2 solutions with 0.3 m H3BO3.

+----------------------------------------------------------------
\text{MgSO}_4^{(aq)} \rightarrow \text{Mg}^{2+}
\lambda: 
\begin{align*}
  a1 &= 0.0 \\
  a2 &= 0 \\
  a3 &= 0 \\
  a4 &= 0
\end{align*}
\end{verbatim}
* Source: Xiong (2015) modeling solubility of brucite in Na$_2$SO$_4$ solutions in presence of boric acid

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb$\text{B}_4\text{O}_7$(aq)</td>
<td>Na$^+$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = 0.1555$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: Xiong (2015) AP-155

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B(OH)$_3$(aq)</td>
<td>Pb$^{++}$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = 0.2925$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: Xiong (2015) modeling lead solubility in boric acid, Set to 0.2925 in analog to H$_4$SiO$_4$/Mg$^{++}$ from 97Aza/Pou.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B(OH)$_3$(aq)</td>
<td>PbB(OH)$_4^+$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = 0.0925$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: Xiong (2015) modeling lead solubility in boric acid. Set to 0.0925 in analog to H$_4$SiO$_4$/Mg$^{++}$ from 97Aza/Pou.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbCl$_2$(aq)</td>
<td>Mg$^{++}$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = -0.071$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: OOFelmy, -0.071. Xiong (2015) modeling

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbCl$_2$(aq)</td>
<td>Na$^+$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = -0.11$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: 84Millero/Byrne has a value of -0.14; OOFelmy has a value of -0.11

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb(OH)$_2$(aq)</td>
<td>Na$^+$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = 0.0$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: Xiong (2015), modeling solubility of lead oxide in NaCl and NaClO$_4$ solutions.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbC$_{03}$(aq)</td>
<td>Cl$^-$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = -0.020$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>Reaction</th>
<th>Ion 1</th>
<th>Ion 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbOxalate(aq)</td>
<td>Cl$^-$</td>
<td></td>
</tr>
<tr>
<td>lambda:</td>
<td>$a_1 = 0.00000$</td>
<td>$a_2 = 0.$</td>
</tr>
</tbody>
</table>

* Source: Setting to 0
$\text{PbOxalate}(aq)$

**Oxalate**

$\lambda$:  
$\begin{align*}
a_1 &= 0.00000 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Setting to 0*

$\text{Pb(OH)}_2(aq)$  

$\lambda$:  
$\begin{align*}
a_1 &= -0.5581 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Xiong (2015), modeling solubility of lead oxide in Na$_2$SO$_4$ solutions.*

$\text{Pb(OH)}_2(aq)$  

$\lambda$:  
$\begin{align*}
a_1 &= -0.1721 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Xiong (2015), modeling solubility of lead oxide in NaCl and NaClO$_4$ solutions.*

$\text{PbCl}_2(aq)$  

$\lambda$:  
$\begin{align*}
a_1 &= -0.14 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Xiong 2011; Both 84Millero/Byrne and 00Pelmy has a value of -0.11*

$\text{PbCl}_2(aq)$

$\lambda$:  
$\begin{align*}
a_1 &= 0. \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: [template only]*

$\text{PbCl}_2(aq)$  

$\lambda$:  
$\begin{align*}
a_1 &= 0.0 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Xiong (2015) modeling lead solubility in NaCl and MgCl$_2$ solutions with boric acid*

$\text{Na}^+ \quad \text{Ca}^{++} \quad \text{ClO}_4$  

$\psi$:  
$\begin{align*}
a_1 &= 0.1574 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$

*Source: Fitting parameter Task 28&35c*

$\text{Na}^+ \quad \text{Ca}^{++} \quad \text{OH}$  

$\psi$:  
$\begin{align*}
a_1 &= -0.0198 \\
a_2 &= 0. \\
a_3 &= 0. \\
a_4 &= 0. \\
\end{align*}$
* Source: Xiong (2015) modeling solubility of portlandite in Na2SO4 solutions with 0.001 m H3BO3.

\[
\begin{align*}
\text{Mg}^{++} & \quad \text{PbCl}^{+} & \quad \text{Cl}^{-} \\
\text{psi}: & & \\
\text{a1} & = -0.4129 & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* Source: Xiong (2015) Evaluated from lead solubility data in MgCl2

\[
\begin{align*}
\text{SO}_4^{--} & \quad \text{B}_4\text{O}_5\text{(OH)}_4^{--} & \quad \text{Na}^{+} \\
\text{psi}: & & \\
\text{a1} & = 0.293 & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* a1 set to 0.00 for fitting
* Set to 0 for FW86 model.

\[
\begin{align*}
\text{Cl}^{-} & \quad \text{PbCl}_3^{-} & \quad \text{Mg}^{++} \\
\text{psi}: & & \\
\text{a1} & = 0.0 & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* Source: Xiong (2015)

\[
\begin{align*}
\text{PbCl}_2\text{(aq)} & \quad \text{Na}^{+} & \quad \text{Cl}^{-} \\
\text{zeta}: & & \\
\text{a1} & = 0. & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* Source: Setting to zero

\[
\begin{align*}
\text{PbOxalate}\text{(aq)} & \quad \text{Na}^{+} & \quad \text{Cl}^{-} \\
\text{zeta}: & & \\
\text{a1} & = 0. & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* Source: Setting to zero

\[
\begin{align*}
\text{PbCO}_3\text{(aq)} & \quad \text{Na}^{+} & \quad \text{Cl}^{-} \\
\text{zeta}: & & \\
\text{a1} & = -0.145 & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]


\[
\begin{align*}
\text{B(OH)}_3\text{(aq)} & \quad \text{Mg}^{++} & \quad \text{Cl}^{-} \\
\text{zeta}: & & \\
\text{a1} & = 0.00793 & \\
\text{a2} & = 0. & \\
\text{a3} & = 0. & \\
\text{a4} & = 0. & \\
\end{align*}
\]

* Source: Xiong (2015) modeling sodium tetraborate in MgCl2+NaCl solutions.
zeta:
a1 = 0.6820
a2 = 0.
a3 = 0.
a4 = 0.
* Source: Xiong (2015) modeling

\* Source: Xiong (2015) modeling lead metaborate hydrate solubility

\* in MgCl2+NaCl mixtures with 0.3 m H3BO3.

Pb  207.20000

-----

\* \* \* \* \* \*

Pb++

charge = 2.0

****

1 element(s):
1.0000 Pb

****

-----

AmHB4O7++

AmHB4O7++

charge = 2.0

****

4 element(s):
1.0000 Am
1.0000 H
4.0000 B

7.0000 O

****

5 species in aqueous dissociation reaction:
-1.0000 AmHB4O7++
1.0000 Am+++ 3.0000 H+
4.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data -37.3416 No Data No Data
No Data No Data No Data No Data

* Source: AP-173

-----

PbEDTA--

PbClOH12O8N2--

charge = -2.0

****

5 element(s):
10.0000 C
1.0000 Pb
12.0000 H
2.0000 N
8.0000 O

****

3 species in aqueous dissociation reaction:
-1.0000 PbEDTA-- 1.0000 Pb++
1.0000 EDTA---

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data 20.0100 No Data No Data
No Data No Data No Data No Data

* Source: 

-----

PbCitrate-

PbC6H5O7-

charge = -1.0

****

4 element(s):
6.0000 C
1.0000 Pb
5.0000 H
7.0000 O

****

3 species in aqueous dissociation reaction:
-1.0000 PbCitrate- 1.0000 Pb++
1.0000 Citrate---

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data 7.28 No Data No Data
Information Only
charge = -2.0

****
3 element(s):
4.0000 C 1.0000 Pb 8.0000 O

****
3 species in aqueous dissociation reaction:
-1.0000 Pb(Oxalate)2-- 1.0000 Pb++
2.0000 Oxalate--

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data -8.0500 No_Data No_Data
No_Data No_Data No_Data No_Data
* Source: Based on experiments in K2C2O4 solutions

3 species in aqueous dissociation reaction:
8.0000 0 -1.0000 Pb(Oxalate)2-- 1.0000 Pb++
2.0000 Oxalate--

charge = 0.0

****
4 element(s):
1.0000 B 4.0000 H 1.0000 Na
4.0000 O

****
3 species in aqueous dissociation reaction:
-1.0000 NaB(OH)4(aq) 1.0000 Na+
1.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data -0.2500 No_Data No_Data
No_Data No_Data No_Data No_Data
* Source: Xiong, 2012, SIT model to extrapolate Reardon (1976)
* conditional formation constants. logK = -0.25. Set to No_Data
* for Felmy and Weare (1986) model.

4 species in aqueous dissociation reaction:
1.0000 NaB(OH)4(aq) 1.0000 Na+
1.0000 B(OH)4-

****
3 element(s):
1.0000 S 1.0000 Mg
4.0000 O

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data -2.3826 No_Data No_Data
No_Data No_Data No_Data No_Data
* Source: Xiong (2005), modeling solubility of brucite in Na2SO4
* solutions with 0.001 H3BO3. From Kratsis et al. (2001),
* -2.38.

charge = 0.0

****
4 element(s):
1.0000 B
4.0000 H
1.0000 Na
4.0000 O

****
5 species in aqueous dissociation reaction:
-1.0000 PbB4O7(aq) 1.0000 Pb++
-9.0000 H2O 2.0000 H+
4.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data -28.1354 No_Data No_Data
No_Data No_Data No_Data No_Data
* Source: Xiong (2015)

charge = -1.0

****
4 element(s):
1.0000 Pb
12.0000 H
12.0000 O
3.0000 B

****
3 species in aqueous dissociation reaction:
-1.0000 Pb(B(OH)4)3- 1.0000 Pb++
3.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data 99.9999 No Data No Data
No Data No Data No Data No Data
* Source: Xiong (2015) modeling solubility of PbO
* in the presence of boric acid.
* Simultaneous fitting three data sets (two from Shchigol
* and one from my work).

PbB(OH)4+ PbB(OH)4+
charge = 1.0

**** 4 element(s):
1.0000 Pb 4.0000 H 4.0000 O
1.0000 B

3 species in aqueous dissociation reaction:
-1.0000 PbB(OH)4+ 1.0000 Pb++
1.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data -2.9500 No Data No Data
No Data No Data No Data No Data
* Source: Xiong (2015) modeling solubility of PbO in NaCl
* solutions in the presence of boric acid.
* Using B dot equation to extrapolate the literature
* value.

Pb(B(OH)4)2(aq) Pb(B(OH)4)2(aq)
charge = 0.0

**** 4 element(s):
1.0000 Pb 8.0000 H 8.0000 O
2.0000 B

3 species in aqueous dissociation reaction:
-1.0000 Pb(B(OH)4)2(aq) 1.0000 Pb++
2.0000 B(OH)4-

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No Data -5.5100 No Data No Data
No Data No Data No Data No Data
* Source: Xiong (2015) modeling solubility of PbO in NaCl
* solutions in the presence of boric acid.
* Using B dot equation to extrapolate the literature
* value.

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 -1.4800 No Data No Data
No Data No Data No Data No Data
* Source: 07Luo/Millero

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  -2.0300  No_Data  No_Data
   No_Data  No_Data  No_Data  No_Data
* Source: 84Millero/Byrne

--------------------------------------------------
PbCl2-  PbCl3-
charge = -1.0
****
2 element(s):
1.0000 Pb  3.0000 Cl

*** 3 species in aqueous dissociation reaction:
-1.0000 PbCl2-  1.0000 Pb++
3.0000 Cl-

* 

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
   No_Data  -1.8600  No_Data  No_Data
   No_Data  No_Data  No_Data  No_Data
* Source: 07Luo/Millero

--------------------------------------------------
PbCl3+  PbCl3-
charge = 1.0
****
3 element(s):
1.0000 Pb  1.0000 H  1.0000 O

*** 4 species in aqueous dissociation reaction:
-1.0000 PbCl3+  -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)

--------------------------------------------------
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  17.0475  No_Data  No_Data
   No_Data  No_Data  No_Data  No_Data
* Source: Powell et al. (2009), 17.04.
*  Xiong (2015), 17.0409

--------------------------------------------------
Pb(OH)3-  Pb(OH)3-
charge = -1.0
****
3 element(s):
1.0000 Pb  3.0000 H  3.0000 O

*** 4 species in aqueous dissociation reaction:
-1.0000 Pb(OH)3-  -3.0000 H+
1.0000 Pb++  3.0000 H2O

* 

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
   No_Data  27.9886  No_Data  No_Data
   No_Data  No_Data  No_Data  No_Data
* Source: Powell et al. (2009), 28.03. Xiong (2015), 28.0210

--------------------------------------------------
AmEDTA-  AmClOH1208N2-
charge = -1.0

****
4 element(s):
12.0000 C  18.0000 H  18.0000 O  3.0000 Ca

4 species in aqueous dissociation reaction:
-1.0000 Earlandite  3.0000 Ca++  2.0000 Citrate---  4.0000 H2O

logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
500.0000 -18.1110  500.0000  500.0000
500.0000  500.0000  500.0000  500.0000

Ca2EDTA(s)  Ca2C10H1208N2
sp.type = solid
* EQ3/6 = hmo
revised = 26-Sept-2012
* mol.wt. = 570.5008 g/mol
V0PrTr = 0.000 cm**3/mol [source: ]

5 element(s):
10.0000 C  12.0000 H  8.0000 O  2.0000 Ca  2.0000 N

3 species in aqueous dissociation reaction:
-1.0000 Ca2EDTA(s)  2.0000 Ca++  1.0000 EDTA---

logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
500.0000 -15.3900  500.0000  500.0000
500.0000  500.0000  500.0000  500.0000

PbOxalate(cr)  PbC204
V0PrTr = 0.000 cm**3/mol [source: ]

3 element(s):
2.0000 C  1.0000 Pb  4.0000 O

3 species in aqueous dissociation reaction:
-1.0000 PbOxalate(cr)  1.0000 Pb++  1.0000 Oxalate--

logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data  -11.1300  No_Data  No_Data
No_Data  No_Data  No_Data  No_Data
* Source: Xiong (2011), evaluated from PbOxalate(cr) solubility in NaCl solutions.

Na_Tetraborate  Na2B407.10H2O
V0PrTr = 0.000 cm**3/mol [source: ]

4 element(s):
4.0000 B  20.0000 H  2.0000 Na  17.0000 O

5 species in aqueous dissociation reaction:
-1.0000 Na_Tetraborate  1.0000 H2O
2.0000 Na+  4.0000 B(OH)4-
2.0000 H+

logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
No_Data  -24.8000  No_Data  No_Data
No_Data  No_Data  No_Data  No_Data
* Source: Log K set to 0.00 for fitting
* In Felmy and Weare (1986) model, the value for borax is -24.4918.

Na_Mg_Tetraborate(A)  Na1.8Mg0.1B407.10H2O
V0PrTr = 0.000 cm**3/mol [source: ]

5 element(s):
4.0000 B  20.0000 H  1.8000 Na  17.0000 O  0.1000 Mg
**** 6 species in aqueous dissociation reaction:
-1.0000 Na_Mg_Tetraborate(A) 1.0000 H2O
1.8000 Na+ 4.0000 B(OH)4-
2.0000 H+ 0.1000 Mg++

* **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
  No Data -24.4000 No Data No Data
  No Data No Data No Data No Data
* Source: Xiong (2015) Evaluated from solubility of Na2B4O7:10H2O
  in MgCl2 solutions (log K = -24.4500).

* * *

Na_Mg_Tetraborate(B) Na1.6Mg0.2B4O7.10H2O
V0PrTr = 000.000 cm**3/mol [source: ]

**** 5 element(s):
  4.0000 B 20.0000 H 1.6000 Na
  17.0000 O 0.2000 Mg

**** 6 species in aqueous dissociation reaction:
-1.0000 Na_Mg_Tetraborate(B) 1.0000 H2O
1.6000 Na+ 4.0000 B(OH)4-
2.0000 H+ 0.2000 Mg++

* **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
  No Data -25.7250 -24.9900 No Data No Data
  No Data No Data No Data No Data
* Source: Xiong (2015) Evaluated from solubility of Na2B4O7:10H2O
  in MgCl2 solutions (log K = -24.8000).

* * *

PbMgCl4:6H2O PbMgCl4:6H2O
V0PrTr = 000.000 cm**3/mol [source: ]

**** 5 element(s):
  4.0000 Cl 1.0000 Pb 1.0000 Mg
  12.0000 H 6.0000 O

**** 5 species in aqueous dissociation reaction:
-1.0000 PbMgCl4:6H2O 1.0000 Pb++
4.0000 Cl- 1.0000 Mg++
6.0000 H2O

* **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
  No Data 99.9999 No Data No Data
  No Data No Data No Data No Data
* Source: Felmy et al., 2000, GCA, 64:3615-3628
  No Data -6.0700 No Data No_Data

Pb_Metaborate_hydrate Pb(BO2)2:H2O
sp.type = solid
* EQ3/6 = pis
revised = 01-Jul-2015
* mol.wt. = xxxx g/mol
V0PrTr = 0.0 cm**3/mol [source: ]

**** 4 element(s):
  1.0000 Pb 2.0000 B 5.0000 O
  2.0000 H

**** 4 species in aqueous dissociation reaction:
-1.0000 Pb_Metaborate_hydrate -3.0000 H2O
2.0000 B(OH)4- 1.0000 Pb++

* **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
  No Data -12.1551 No Data No Data
  No_Data No_Data No_Data No_Data
*Source: Xiong (2015)*

---

**Litharge**

PbO

* sp.type = solid polymorph
* EQ3/6 = ymp.R2, ymp.R0, com, ree, alt, sup
* YMP Qualification status = Q
* mol.wt. = 223.199 g/mol
* VOPrTr = 23.910 cm**3/mol [source: 78hel/del]

****

2 element(s):

1.0000 O
1.0000 Pb

****

4 species in aqueous dissociation reaction:

-1.0000 Litharge
1.0000 H2O

-2.0000 H+
1.0000 Pb++

****

logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:

13.6341 12.5914 11.3804 10.2699
9.1675 8.2762 7.5166 6.8252

---

**Hydromagnesite5424**

Mg5(CO3)4(OH)2.4H2O

VOPrTr = 000.000 cm**3/mol [source: ]

****

4 element(s):

4.0000 C
10.0000 H
18.0000 O

5.0000 Mg

****

5 species in aqueous dissociation reaction:

-1.0000 Hydromagnesite5424

5.0000 Mg++
1.0000 H2O

-6.0000 H+
4.0000 HCO3-

****

logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:

No_Data 29.3328 No_Data No_Data
No_Data No_Data No_Data No_Data

* Source: Recalculation of Solubility Constants of Synthetic Hydromagnesite(5424) Using the Pitzer Model
* Note that the reaction in the source was in terms of CO2(g) a non-basis species, to covert to the basis species, HCO3-
* the reaction 4 x(CO2(g) + H2O = H+ + HCO3- logK = -7.8193) was added, 60.61 + 4 x -7.8193 = 29.3328

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date: November 3, 2015

to: SNL WIPP Records Center  
Defense Waste Management Programs

from: Paul S. Domski

subject: Memo of Correction for “Memo AP-173, EQ3/6 Database Update: DATA0.FM2”

The purpose of this memo is document that “Memo AP-173, EQ3/6 Database Update: DATA0.FM2”, file name “AP173_FM2_memo_final.doc”, dated 10/27/2015 has been updated to correct a formatting error in Figure 1 where the Y-axis label would not print properly. The new file, “AP173_FM2_memo_final_fixed_fig.doc” differs from the original only in the way that Figure 1 prints.
AP-154 Tasks 22 and 24
Task 22 and 24 of AP154 are not included in Table 1 because the parameters were estimated by manual fitting (Xiong 2011a), and not by the use of the Python script, thus, it was not possible to run the Python script using DATA0.FM2 for parameter comparison purposes. Rather the test cases from Xiong 2011a were run in EQ3/6 using DATA0.FM2 and the output data were plotted together with the experimental data and predicted data of Xiong 2011a in Figure 1. Figure 1 shows that the predicted data of Xiong 2011a, and the predicted data using DATA0.FM2 are very close, therefore, the original parameter values of Xiong were retained in DATA0.FM2.

Figure 1. Comparison of the documented fit (Xiong, 2011a) with the DATA0.FM2 fit to the experimental data for AP-154 Task 22 and 24.

AP-154 Tasks 29 and 32
Note that tasks 29 and 32 from AP-154, which were specified by AP-173 to be included in DATA0.FM2 were not included because the parameters from these tasks were included in AP-154 tasks 30 and 31 for the EDTA parameters, and task 23 for the oxalate parameters, this is a deviation from AP-173.

AP-155 Tasks
The tasks completed under AP-155 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 2.

Table 2. AP-155 Comparison of the documented parameters with those estimated using DATA0.FM2.

<table>
<thead>
<tr>
<th>AP-155 Task</th>
<th>Chemical Entity</th>
<th>Fitting Parameter</th>
<th>Documented Value</th>
<th>Estimated with DATA0.FM2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 4.1</td>
<td>Pb(OH)(_2)(aq)</td>
<td>Log K</td>
<td>17.0475</td>
<td>17.0395</td>
<td>The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.</td>
</tr>
<tr>
<td>3, 4.1</td>
<td>Pb(OH)(_3)</td>
<td></td>
<td>27.989</td>
<td>27.992</td>
<td></td>
</tr>
<tr>
<td>3, 4.1</td>
<td>Na(^+) - Pb(OH)(_3)</td>
<td>(\beta^{(0)})</td>
<td>0.335</td>
<td>0.335</td>
<td>The values are identical, therefore, the</td>
</tr>
</tbody>
</table>