	Scientific Analysis/Calculation Error Resolution Document *Complete only applicable items.*	QA: QA Page 1 of 7

1. Document Number: ANL-WIS-GS-000003	2. Revision/Addendum: 01	3. ERD: 01
4. Title: Qualification of Thermodynamic Data for Geochemical Modeling of Mineral-Water Interactions in Dilute Systems		5. No. of Pages Attached: 6

6. Description of and Justification for Change (Identify affected pages, applicable CRs and TBVs):

This Error Resolution Document (ERD) addresses deficiencies in the documentation of qualification of external source data used as direct input, as originally identified in condition report (CR) 10806, which was closed to CR 10788 as a similar issue. During the extent of condition evaluation, a review of ANL-WIS-GS-000003 REV 01 revealed that most of the information required for the qualification of external data was presented in the document, but some of the documentation requirements of SCI-PRO-001, *Qualification of Unqualified Data*, were omitted or needed clarification. The quality of the data is not in question, only the documentation required by SCI-PRO-001. Therefore, there is no impact on the conclusions of this document or impacts on any other documents, including the text, tables or figures of the License Application because ANL-WIS-GS-000003 REV 01 is the only document impacted by the identified changes. This ERD provides the additional documentation necessary to address the deficiencies.

Table 1 provides a list of the inputs classified as "Direct Input" in the DIRS and were identified as having incomplete or missing documentation for qualification for intended use. Table 1 also contains the resolutions for each input and the location within this ERD where the detailed changes to implement the resolution are described. For many of the references, the inputs were classified as "Direct Input" in the DIRS, but the report indicates that the references were used as "Indirect Input". In those cases, the only change required is a correction to the DIRS report.

	Printed Name	Signature	Date
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Table 1. Resolution to Inadequate Documentation for Qualification

Source and Description of Input	Resolution to Inadequate Documentation	Section or Table in ERD Describing Detailed Changes
Casas et al. 1997 [DIRS 102432] Thermodynamic data of uranyl compounds used as indirect input	DIRS incorrectly identified input as direct input; therefore DIRS is changed	Table 2
Carlos et al. 1995 [DIRS 105213] Statement that zeolite minerals are found at Yucca Mountain	DIRS incorrectly identified input as direct input; therefore DIRS is changed	Table 2
Harvie et al. 1984 [DIRS 118163] Thermodynamic data for Friedl salt and syngenite	Values are not recommended for use within the report (Section 6.3.3.4); therefore the inputs are indirect and DIRS is changed	Table 2
Nriagu 1972 [DIRS 151244] Thermodynamic data for PbH2PO4+	Qualified in Section 4.1.17 of report, but more justification is added	Section I
Jackson and Helgeson 1985 [DIRS 151264] Thermodynamic data used as indirect input	DIRS incorrectly identified input as direct input; therefore DIRS is changed	Table 2
Dellien et al. 1976 [DIRS 151392] Original data source for chromium species and solids	DIRS incorrectly identified input as direct input; therefore DIRS is changed	Table 2
Greenberg and Moller 1989 DIRS 152684] Data for cement phases used as indirect input	DIRS incorrectly identified input as direct input; therefore DIRS is changed	Table 2
Titley 1963 [DIRS 153213] Fe2(MoO4)3 data	Values are not recommended for use within the report (Section 4.1); therefore the inputs are indirect and DIRS is changed. The source is deleted from Table 4-1	Section II, Table 2
Ball and Nordstrom 1998 [DIRS 163015] Chromium solid and aqueous species	Qualified in Section 4.1.20 of report, but more justification is added	Section III
Rai et al. 1987 [DIRS 163369] Chromium solid and aqueous species	Qualified in Section 4.1.20 of report, but more justification is added	Section III
Rai et al. 2004 [DIRS 179582] Chromium solid and aqueous species	Qualified in Section 4.1.20 of report, but more justification is added	Section III
Assaaoudi et al. 1997 [DIRS 177936] Rare earth phosphate compositions	Used as corroborating data (Indirect input); therefore DIRS and text is changed	Section IV, Table 2
Hezel and Ross 1966 [DIRS 177990] Rare earth phosphate compositions	Used as corroborating data (Indirect input); therefore DIRS and text is changed	Section IV, Table 2
Assaaoudi et al. 2000 [DIRS 177992] Rare earth phosphate compositions	Used as corroborating data (Indirect input); therefore DIRS and text is changed	Section IV, Table 2
Hezel and Ross 1967 [DIRS 178227] Rare earth phosphate compositions	Used as corroborating data (Indirect input); therefore DIRS and text is changed	Section IV, Table 2
Assaaoudi et al. 2001 [DIRS 179602] Rare earth phosphate compositions	Qualification text is added	Section IV

Table 2. Changes to DIRS

Source	Input Description	Changes Required
Casas et al. 1997 [DIRS 102432]	Solubility study on becquerelite (mispelled in DIRS)	Change from "Direct Input" to "Indirect Input"
Carlos et al. 1995 [DIRS 105213]	Statement that zeolite minerals are found at Yucca Mountain	Change from "Direct Input" to "Indirect Input"
Harvie et al. 1984 [DIRS 118163]	Thermodynamic data for various solids	Change from "Direct Input" to "Indirect Input"
Jackson and Helgeson 1985 [DIRS 151264]	Thermodynamic data for solids and aqueous species	Change from "Direct Input" to "Indirect Input"
Dellien et al. 1976 [DIRS 151392]	Original data source for for CrO3Cl-, eskolaite (Cr2O3), and CrO2	Change from "Direct Input" to "Indirect Input"
Greenberg and Moller 1989 DIRS 152684]	Selected data for cement phases	Change from "Direct Input" to "Indirect Input"
Titley 1963 [DIRS 153213]	Fe2(MoO4)3 data	Change from "Direct Input" to "Indirect Input"
Ziemniak et al. [DIRS 181408]	Thermodynamic data for chromium species	New reference to add to the DIRS (See Section III)
Assaaoudi et al. 1997 [DIRS 177936]	Data for Rare earth phosphate composition	Change from "Direct Input" to "Indirect Input"
Hezel and Ross 1966 [DIRS 177990]	Structural studies and data for Rare earth phosphate compositions	Change from "Direct Input" to "Indirect Input"
Assaaoudi et al. 2000 [DIRS 177992]	Rare earth phosphate compositions	Change from "Direct Input" to "Indirect Input"
Hezel and Ross 1967 [DIRS 178227]	Structural studies and data for Rare earth phosphate compositions	Change from "Direct Input" to "Indirect Input"
Min et al. [DIRS 177994], p. 2199	Lutetium phosphate composition	New reference to add to the DIRS (See Section IV)

I. Resolution to Nriagu 1972 [DIRS 151244]

This source is qualified in Section 4.1.17 of the report, but additional documentation is required. Therefore, prior use of the data is added as a qualification attribute. See changes to document listed below:

Revise the last sentence of page 4-53 to add bullet (e) as follows (with new text in italics):

> "The use of this datum is justified because (a) a standard, accepted method, solubility determination, was used to obtain it, (b) the datum is published in a peer reviewed journal (*Inorganic Chemistry*), (c) the author is well known for similar studies, (d) the data for both species taken from this source should be used together, as the data were determined from a single, common analysis, and *(e) the prior use of the source in data0.ymp.R0 (DTN: MO0009THRMODYN.001 [DIRS 152576]), which is a qualified database*."

II. Resolution to Titley 1963 [DIRS 153213]

The inputs from this source are not recommended for use within the report (Section 4.1); therefore the input should not be classified as "direct input". See changes to document listed below:

In Table 4-1, page 4-8, make the following revision:

Delete the fourth row (i.e., the row containing "$Fe_2(MoO_4)_3$ data").

In Table 4-1, page 4-10, make the following revision:

Delete footnote "c".

III. Resolution to Ball and Nordstrom 1998 [DIRS 163015], Rai et al. 1987 [DIRS 163369], Rai et al. 2004 [DIRS 179582]

These sources are qualified in Section 4.1.20 of the report, but additional documentation is required. Therefore, corroborating information is added as a qualification attribute. See changes to document listed below:

Revise the last three paragraphs on page 4-63 to add an additional bullet (4) to the end of each paragraph as follows (with new text in italics):

"The data from Ball and Nordstrom (1998 [DIRS 163015]) are justified for the intended use in this analysis report on the grounds that (1) they were published in an international peer-reviewed journal, *Journal of Chemical & Engineering Data,* which is a journal from American Chemical Society, and published since 1959, (2) the data were based on a standard, accepted approach for obtaining thermodynamic data, (3) these data are extensively used on the project as a source in seven other controlled and qualified YMP reports, *and (4) the data are corroborated by data in Rai et al. (1987 [DIRS 163369], Table III) which present identical values*.

The data from Rai et al. (2004 [DIRS 179582]) are justified for the intended use in this analysis report on the grounds that (1) they were published in an international peer-reviewed journal, *Journal of Solution Chemistry,* (2) the data were based on a standard, accepted approach for obtaining thermodynamic data, (3) some of the authors in this study have the reputation of evaluating and producing quality thermodynamic data obtained from chromium solubility experiments, *and (4) the log K input value of –10.93 that is used in the database (Table 4-54) is corroborated by data presented in Ziemniak et al. (1998 [DIRS 181408], Table VIII), which, when calculated, result in a very similar log K value of –10.66.*

The data from Rai et al. (1987 [DIRS 163369]) are justified for the intended use in this analysis report on the grounds that (1) they were published in an international peer-reviewed journal, *Inorganic Chemistry,* (2) the data were based on a standard, accepted approach for obtaining thermodynamic data, (3) some of the authors in this study have the reputation of evaluating and producing quality thermodynamic data obtained from

chromium solubility experiments, *and (4) the data have been subjected to a professional review in Ball and Nordstrom 1998 [DIRS 163015]*."

For editorial fixes in Table 4-54,

Remove the "a" superscript from the column header "Chemical Reaction" and from the log K value "9.35".

Add the following reference to Section 8.1 and the DIRS:

181408 Ziemniak, S.E.; Jones, M.E.; and Combs, K.E.S. 1998. "Solubility and Phase Behavior of Cr(III) Oxides in Alkaline Media at Elevated Temperatures." *Journal of Solution Chemistry, 27,* (1), 33-66. [New York, New York]: Plenum Publishing. TIC: 259501.

IV. Resolution to Assaaoudi et al. 1997 [DIRS 177936], Hezel and Ross 1966 [DIRS 177990], Assaaoudi et al. 2000 [DIRS 177992], Hezel and Ross 1967 [DIRS 178227], and Assaaoudi et al. 2001 [DIRS 179602]

All of these sources are indicated as direct inputs in the text and in the DIRS. However, a more accurate description is that only Assaaoudi et al 2001 [DIRS 179602] is direct and all the other sources are used as corroborating references. An additional source (Min et al. 2000 [DIRS 177994]) is added as a direct input, and qualified for intended use. See changes to document listed below:

Revise the last sentence of the last paragraph in Section 4.1.17 (page 4-58) as follows (with new text in italics):

"Structural studies on REE (Rare Earth Element) phosphates (Hezel and Ross 1966 [DIRS 177990]; Hezel and Ross 1967 [DIRS 178227]; Assaaoudi et al. 1997 [DIRS 177936]; Assaaoudi et al. 2000 [DIRS 177992]; Assaaoudi et al. 2001 [DIRS 179602]; *Min et al. 2000 [DIRS 177994]*) are used in Section 6.7.8 to assign values for waters of hydration to REE phosphates for which Spahiu and Bruno (1995 [DIRS 103804]) had indicated "XH2O." *Assaaoudi et al. (2001 [DIRS 179602]) and Min et al. (2000 [DIRS 177994]) are used as direct inputs and are qualified for intended use within Section 6.7.8.*"

Add the following text to the bottom of page 6-168 (before Table 6-76), Section 6.7.8:

"The new stoichiometries for all elements (except lutetium (Lu) and promethium (Pm)) in Table 6-76 are provided by Assaaoudi et al. 2001 [DIRS 179602] and is qualified for intended use because (a) the data is corroborated by Hezel and Ross 1966 [DIRS 177990]; Hezel and Ross 1967 [DIRS 178227]; Assaaoudi et al. 1997 [DIRS 177936]; and Assaaoudi et al. 2000 [DIRS 177992], (b) the data is published in a peer reviewed journal (*Vibrational Spectroscopy*), and (c) the author is well known for similar studies (Assaaoudi et al. 1997 [DIRS 177936]; and Assaaoudi et al. 2000 [DIRS 177992]). The new stoichiometry for Lu is provided by Min et al. 2000 [DIRS 177994] and is qualified for

intended use because (a) the data is corroborated by Hezel and Ross 1966 [DIRS 177990], (b) the data is published in a peer reviewed journal (*Materials Research Bulletin*), and (c) one of the authors (Hikichi) is referenced by similar studies (Assaaoudi et al. 1997 [DIRS 177936]; and Assaaoudi et al. 2000 [DIRS 177992]). Pm is a rare element for which there is very few data on the properties of its compounds, particularly $PmPO_4:nH_2O$. Therefore, the formula $PmPO_4:1.5\ H_2O$ is assumed based on similar elements in the lanthanides row of the periodic table (specifically ranging from lanthanum (La) to terbium (Tb)) where neighboring elements such as Nd and Sm phosphates have 1.5 H_2O of hydration (Hezel and Ross 1966 [DIRS 177990], p. 1956)."

Add the following reference to Section 8.1 and the DIRS:

177994 Min, W.; Daimon, K.; Ota, T.; Matsubara, T.; and Hikichi, Y. 2000. "Synthesis and Thermal Reactions of Rhabdophane-(Yb or Lu)." *Materials Research Bulletin, 35,* 2199-2205. [New York, New York]: Pergamon. TIC: 258628.

Revise the contents of Table 4-1, page 4-9, last row, second cell, with the following:

Delete: "Hezel and Ross 1966 [DIRS 177990]; Hezel and Ross 1967 [DIRS 178227]; Assaaoudi et al. 1997 [DIRS 177936]; Assaaoudi et al. 2000 [DIRS 177992]".

Add: "Min et al. 2000 [DIRS 177994]"