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Milestone Report on Test Plan TP 10-01, "Experimental Study of Thermodynamic Parameters of Borate in WIPP Relevant Brines at Sandia National Laboratories Carlsbad Facility"

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DEFINITION OF ABBREVIATIONS, ACRONYMS AND INITIALISMS

Abbreviation or Acronym	Definition
A	pH correction factor
Cit^{3-}	citrate anion, conjugate base of citric acid, $C_6H_5O_7^{3-}$
DI	de-ionized
DDI	deoxygenated de-ionized
EBSD	Electron backscatter diffraction
EDS	Energy dispersive system
$EDTA^{4-}$	ethylenediaminetetraacetate anion, $C_{10}H_{12}N_2O_8^{4-}$
ES&H	Environmental Safety and Health
Fe(II)	ferrous iron
IC	Ion Chromatography
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectroscopy
m	molal (mol/kg H_2O)
M	molar (mol/L)
N_2	nitrogen gas
Ox^{2-}	oxalate anion, $C_2O_4^{2-}$, conjugate base of oxalic acid
QA	quality assurance
SEM	Scanning electron microscope
SNL	Sandia National Laboratories
SNL/CPG	Sandia National Laboratories Carlsbad Programs Group
TP	Test Plan
WIPP	Waste Isolation Pilot Plant
XRD	X-ray diffractometer

1 INTRODUCTION

Experimental studies at Los Alamos National Laboratory (LANL) suggest that borate could potentially complex with Nd(III), an analog to Am(III). Therefore, a comprehensive thermodynamic model involving borate is needed to accurately describe the contributions of borate to the solubility of Am(III) in the WIPP brines, as the WIPP brines, both GWB and ERDA-6, contain significant concentrations of borate.

The purpose of this report is to summarize experimental data obtained to date under Test Plan TP 10-01, "Experimental Study of Thermodynamic Parameters of Borate in WIPP Relevant Brines at Sandia National Laboratories Carlsbad Facility" (Xiong, 2010). The data provided in this summary report addresses the solubility of WIPP-relevant solids and the Pitzer ion-interaction parameters for the aqueous species associated with those solids. Test Plan TP 10-01 supports the Waste Isolation Pilot Plant's (WIPP's) geochemical model used to predict the solubilities of actinide species present in the repository.

In Test Plan TP 10-01, the solubility constants for boracite and hydroboracite, the formation constants for $FeB(OH)_4^+$ and $PbB_4O_7(aq)$, and the Pitzer interaction parameters for the species shown in Table 1-1 were identified for investigation in the initial phase of the test plan. The test plan allows for additional investigations as warranted by examining the results from the initial test phase.

All of the experimental set-ups have been initiated under this test plan. This report documents the experimental set-up and methods used first and foremost. Some of the measurements obtained so far under TP 10-01 are also reported in this report, and this report only contains data for solubility of sodium tetraborate. The rest of the measurements obtained under TP10-01 will be reported in a series of subsequent documents.

Table 1-1 Ion-pairs identified for investigation in Test Plan TP 10-01[a].

1.	$PbB(OH)_4^+$—Cl^-
2.	$PbB(OH)_4^+$—SO_4^{2-}
3.	$Pb[B(OH)_4]_3^-$—Na^+
4.	$Pb[B(OH)_4]_3^-$—Mg^{2+}
5.	$MgB(OH)_4^+$—SO_4^{2-}
6.	$CaB(OH)_4^+$—SO_4^{2-}
7.	$NaB(OH)_4$(aq)—Na^+, Cl^-
8.	$NaB(OH)_4$(aq)—Mg^{2+}, Cl^-
9.	$NaB(OH)_4$(aq)—Na^+, Mg^{2+}
10.	PbB_4O_7(aq)—Na^+, Cl^-
11.	PbB_4O_7(aq)—Mg^{2+}, Cl^-
12.	PbB_4O_7(aq)—Na^+, Mg^{2+}

[a] Based on Table 5 of TP 10-01 (Xiong., 2010)

2 MATERIALS AND METHODS

All supporting solutions were prepared from reagent grade chemicals from Fisher Scientific or its associated vendors, and DI water.

2.1 Solid Materials

Solids of interest were either purchased or synthesized. Solutions for synthesis were prepared using appropriate reagent grade commercial salts. Solid starting materials will be analyzed with the Brucker D8 X-ray diffractometer (XRD) and the JEOL JSM 5900LV scanning electron microscope (SEM) with a ThermoNORAN Vantage electron backscatter diffraction (EBSD) and energy dispersive system (EDS).

2.2 Ion Concentration Measurements

Hydrogen ion concentrations (pcH) will be determined with pH readings measured with a Ross pH electrode with correction factors, *A's* (Roselle, 2011). Concentrations of anions such as chloride will be determined by using the DIONEX 3000 ion chromatograph (IC).

2.3 Total Boron, Iron, and Lead Concentrations

Elemental concentrations of interest will be determined by using the Perkin Elmer Optima DV 3300 inductively coupled plasma atomic emission spectroscopy (ICP-AES). Specifically, ICP-AES has been used to measure the total boron, total iron, and total lead concentrations.

3 RESULTS

The following sections describe the preparation and results to date for determination of solubility and formation constants of the borate species and for ion-pairs listed in Table 1-1 in the order therein. For those experiments in which there are experimental results to be reported, each section has two types of tables; one to describe the experimental set-ups and the other to tabulate results to date. For the experiments in which experimental results are not reported at this time, tables of the first type are presented.

3.1 Experimental determination of solubility constants of boracite and hydroboracite

A literature review regarding solubility constants of boracite and hydroboracite indicate that reliable data for them are not available in the published literature. Anovitz and Hemingway (2002) gave a value of –6178.4 kJ mol^{-1} for Gibbs free energy of formation of boracite. However, they derive this value from the unpublished data. The objective of this set of experiments is to determine the solubility constants of $Mg_3B_7O_{13}Cl$ (boracite) and $CaMgB_6O_8(OH)_6 \cdot 3H_2O$ (hydroboracite) (Task 1 TP 10-01). These two chemicals are not commercially available. We have tried to synthesize them. XRD patterns indicate that there are significant amounts of boric acid remaining in the final products. A new synthesis recipe with $LiBO_2$ has been located. We are working to synthesize them with the new recipe.

Table 3-1. Preparation of experimental set-ups for investigation of solubility constants of boracite and hydroboracite.

Set-up ID	$Mg_3B_7O_{13}Cl$ (g)	$MgCl_2$ (m)	Reference

3.2 Experimental Determination of the formation constant of $FeB(OH)_4^+$

The formation constant of $FeB(OH)_4^+$ is not available in the literature. Iron could be one of the ions that complexes strongly with borate and therefore competes with the actinides for complexation with borate. The objective of this set of experiments is to determine the formation constant of $FeB(OH)_4^+$ (Task 2 TP 10-01).

The experimental set-up for determination of the formation constant of $FeB(OH)_4^+$ is listed in Table 3–2. In Table 3-2, the experimental set-ups including initial brine molalities and mass of solid materials are shown. The solid phase, $Fe_2Cl(OH)_3$, was synthesized. Brines were prepared from DI water, reagent grade H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved iron concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as boron) are to be determined.

Table 3-2 Preparation of experimental set-ups for investigation of formation constant of $FeB(OH)_4^+$

Set-up ID	$Fe_2Cl(OH)_3$ (g)	H_3BO_3(m)	Reference
$FeB(OH)_4$-0.01B-1	1.516	0.01	WIPP-Borate-1, Page 53
$FeB(OH)_4$-0.02B-1	1.501	0.02	WIPP-Borate-1, Page 53
$FeB(OH)_4$-0.03B-1	1.533	0.03	WIPP-Borate-1, Page 53
$FeB(OH)_4$-0.01B-2	1.518	0.01	WIPP-Borate-1, Page 53
$FeB(OH)_4$-0.02B-2	1.506	0.02	WIPP-Borate-1, Page 53
$FeB(OH)_4$-0.03B-2	1.518	0.03	WIPP-Borate-1, Page 53

3.3 Experimental Determination of the formation constant of PbB_4O_7(aq)

The formation constant of PbB_4O_7(aq) is not available in the literature. In light of borate concentrations in GWB (0.178 m) (or 0.0445 m if it is expressed as $B_4O_7^{2-}$) and ERDA-6 (0.0704 m) (or 0.0176 m if it is expressed as $B_4O_7^{2-}$) (Xiong, 2008) at which tetraborate species are expected to be significant, PbB_4O_7(aq) could be an important species. The objective of this set of experiments is to determine the formation constant of PbB_4O_7(aq) (Task 3 TP 10-01).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-3. The solid phase, PbO, was purchased from MP Biomedicals. Supporting solutions were prepared from DI water, reagent grade $NaClO_4$ (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved lead and boron concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sodium) are to be determined.

Table 3-3. Preparation of experimental set-ups for investigation of the formation constant of $PbB_4O_7(aq)$.

Set-up ID	PbO (g)	$NaClO_4$ (m)	Total B Concentration (m)	Reference
PbB_4O_7-0.1ClO_4-1	2.0003	0.10	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.2ClO_4-1	2.0006	0.20	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.3ClO_4-1	2.0001	0.30	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.4ClO_4-1	2.0004	0.40	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.45ClO_4-1	2.0003	0.45	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.1ClO_4-2	2.0000	0.10	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.2ClO_4-2	2.0003	0.20	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.3ClO_4-2	2.0001	0.30	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.4ClO_4-2	2.0008	0.40	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.45ClO_4-2	2.0009	0.45	N/A	WIPP-Borate-1, Page 20
PbB_4O_7-0.1B_4O_7-1	2.0006	N/A	0.13	WIPP-Borate-1, Page 21
PbB_4O_7-0.2B_4O_7-1	2.0011	N/A	0.27	WIPP-Borate-1, Page 21
PbB_4O_7-0.3B_4O_7-1	2.0001	N/A	0.40	WIPP-Borate-1, Page 21
PbB_4O_7-0.4B_4O_7-1	2.0004	N/A	0.53	WIPP-Borate-1, Page 21
PbB_4O_7-0.45B_4O_7-1	2.0015	N/A	0.60	WIPP-Borate-1, Page 21
PbB_4O_7-0.1B_4O_7-2	2.0001	N/A	0.13	WIPP-Borate-1, Page 21
PbB_4O_7-0.2B_4O_7-2	2.0012	N/A	0.27	WIPP-Borate-1, Page 21
PbB_4O_7-0.3B_4O_7-2	2.0004	N/A	0.40	WIPP-Borate-1, Page 21
PbB_4O_7-0.4B_4O_7-2	2.0008	N/A	0.53	WIPP-Borate-1, Page 21
PbB_4O_7-0.45B_4O_7-2	2.0003	N/A	0.60	WIPP-Borate-1, Page 21

3.4 Experimental Determination of Pitzer Interaction Parameters Relevant to the WIPP Brines

As identified in Table 1-1, there are several Pitzer interaction parameters important to the WIPP brines, which are not in the current WIPP thermodynamic database. These interaction parameters are important for accurate prediction of actinide solubilities in the WIPP brines, which will directly support the future actinide solubility calculations for PA. In these experiments, experimental efforts are focused on determination of the Pitzer interaction parameters between $PbB(OH)_4^+$ and Cl^-, and between $PbB(OH)_4^+$ and SO_4^{2-}. The results for $PbB(OH)_4^+$ will be used as analogs for interaction parameters of $FeB(OH)_4^+$ with Cl^- and SO_4^{2-}. The formation constant of $FeB(OH)_4^+$ will be determined independently as mentioned before. The usage of interaction parameters of $PbB(OH)_4^+$ as analogs for $FeB(OH)_4^+$ is because both lead and iron are transition elements, and $PbB(OH)_4^+$ and $FeB(OH)_4^+$ have the same charge.

Therefore, the interaction parameters of $PbB(OH)_4^+$ will be good analogs for $FeB(OH)_4^+$. The objective of these experiments is to determine the Pitzer interaction parameters for the species interactions shown in Table 1-1 (Task 4 TP 10-01).

3.4.1 $PbB(OH)_4^+$—Cl^- Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$PbB(OH)_4^+$—Cl^-" (Item 1, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-4. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, reagent grade NaCl (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved lead and boron concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as chloride) are to be determined.

Table 3-4. Preparation of experimental set-ups for investigation of $PbB(OH)_4^+$—Cl^- Interactions.

Set-up ID	PbO (g)	NaCl (m)	H_3BO_3(m)	Reference
$PbB(OH)_4$-0.01Cl-1	2.0019	0.010	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-0.1Cl-1	2.0023	0.10	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-1.0Cl-1	2.0045	1.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-2.0Cl-1	2.0017	2.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-3.0Cl-1	2.0013	3.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-4.0Cl-1	2.0018	4.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-5.0Cl-1	1.9999	5.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-0.01Cl-2	2.0065	0.010	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-0.1Cl-2	2.0047	0.10	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-1.0Cl-2	2.0020	1.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-2.0Cl-2	2.0092	2.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-3.0Cl-2	2.0021	3.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-4.0Cl-2	2.0040	4.0	0.0010	WIPP-Borate-1, Page 8
$PbB(OH)_4$-5.0Cl-2	2.0006	5.0	0.0010	WIPP-Borate-1, Page 8

3.4.2 $PbB(OH)_4^+$—SO_4^{2-} Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$PbB(OH)_4^+$—SO_4^{2-}" (Item 2, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-5. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, Na_2SO_4 (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sulfate, and borate) are to be determined.

Table 3-5 Preparation of experimental set-ups for investigation of $PbB(OH)_4^+$–Cl^- Interactions.

Set-up ID	PbO (g)	Na_2SO_4 (m)	H_3BO_3(m)	Reference
$PbB(OH)_4$-0.01SO_4-1	1.9955	0.010	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-0.1SO_4-1	2.0033	0.10	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-0.5SO_4-1	1.9988	0.50	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.0SO_4-1	2.0038	1.0	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.5SO_4-1	2.0046	1.5	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.8SO_4-1	2.0069	1.8	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-0.01SO_4-2	2.0013	0.010	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-0.1SO_4-2	2.0034	0.10	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-0.5SO_4-2	2.0081	0.50	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.0SO_4-2	2.0087	1.0	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.5SO_4-2	2.0010	1.5	0.0010	WIPP-Borate-1, Page 9
$PbB(OH)_4$-1.8SO_4-2	2.0072	1.8	0.0010	WIPP-Borate-1, Page 9

3.4.3 $Pb[B(OH)_4]_3^-$—Na^+ Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$Pb[B(OH)_4]_3^-$—Na^+" (Item 3, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-6. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, NaCl (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sulfate, and borate) are to be determined.

Table 3-6 Preparation of experimental set-ups for investigation of $Pb[B(OH)_4]_3^-$—Na^+ Interactions.

Set-up ID	PbO (g)	NaCl (m)	H_3BO_3(m)	Reference
PbB3-0.01Na-1	2.0129	0.010	0.03	WIPP-Borate-1, Page 10
PbB3-0.1Na-1	2.0045	0.10	0.03	WIPP-Borate-1, Page 10
PbB3-1.0Na-1	2.0303	1.0	0.03	WIPP-Borate-1, Page 10
PbB3-2.0Na-1	2.0117	2.1	0.03	WIPP-Borate-1, Page 10
PbB3-3.0Na-1	2.0057	3.2	0.03	WIPP-Borate-1, Page 10
PbB3-4.0Na-1	2.0029	4.4	0.03	WIPP-Borate-1, Page 10
PbB3-5.0Na-1	2.0130	5.0	0.03	WIPP-Borate-1, Page 10
PbB3-0.01Na-2	2.0365	0.010	0.03	WIPP-Borate-1, Page 10
PbB3-0.1Na-2	2.0372	0.10	0.03	WIPP-Borate-1, Page 10
PbB3-1.0Na-2	2.0133	1.0	0.03	WIPP-Borate-1, Page 10
PbB3-2.0Na-2	2.0130	2.1	0.03	WIPP-Borate-1, Page 10
PbB3-3.0Na-2	2.0043	3.2	0.03	WIPP-Borate-1, Page 10
PbB3-4.0Na-2	2.0047	4.4	0.03	WIPP-Borate-1, Page 10
PbB3-5.0Na-2	2.0114	5.0	0.03	WIPP-Borate-1, Page 10

3.4.4 $Pb[B(OH)_4]_3^-$—Mg^{2+} Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$Pb[B(OH)_4]_3^-$—Mg^{2+}" (Item 4, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-7. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, $MgCl_2 \cdot 6H_2O$ (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as chloride, and borate) are to be determined.

Table 3-7 Preparation of experimental set-ups for investigation of $Pb[B(OH)_4]_3^-$—Mg^{2+} Interactions.

Set-up ID	PbO (g)	$MgCl_2$ (m)	H_3BO_3(m)	Reference
PbB3-0.01Mg-1	2.0011	0.010	0.03	WIPP-Borate-1, Page 11
PbB3-0.1Mg-1	2.0123	0.10	0.03	WIPP-Borate-1, Page 11
PbB3-1.0Mg-1	2.0156	1.0	0.03	WIPP-Borate-1, Page 11
PbB3-1.5Mg-1	2.0027	1.5	0.03	WIPP-Borate-1, Page 11
PbB3-2.0Mg-1	2.0009	2.0	0.03	WIPP-Borate-1, Page 11
PbB3-2.5Mg-1	2.0117	2.5	0.03	WIPP-Borate-1, Page 11
PbB3-0.01Mg-2	2.0198	0.010	0.03	WIPP-Borate-1, Page 11
PbB3-0.1Mg-2	2.0160	0.10	0.03	WIPP-Borate-1, Page 11
PbB3-1.0Mg-2	2.0221	1.0	0.03	WIPP-Borate-1, Page 11
PbB3-1.5Mg-2	2.0153	1.5	0.03	WIPP-Borate-1, Page 11
PbB3-2.0Mg-2	2.0118	2.0	0.03	WIPP-Borate-1, Page 11
PbB3-2.5Mg-2	2.0096	2.5	0.03	WIPP-Borate-1, Page 11

3.4.5 $MgB(OH)_4^+$—SO_4^{2-} Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$MgB(OH)_4^+$—SO_4^{2-}" (Item 5, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-8. The solid phase, $Mg(OH)_2$(cr), was purchased from Fisher Scientific. Brines were prepared from DI water, Na_2SO_4 (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sulfate, and borate) are to be determined.

Table 3-8 Preparation of experimental set-ups for investigation of $MgB(OH)_4^+$—SO_4^{2-} Interactions.

Set-up ID	$Mg(OH)_2$ (g)	Na_2SO_4 (m)	H_3BO_3(m)	Reference
$MgB(OH)_4$-0.01SO_4-1	2.0008	0.010	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-0.1SO_4-1	2.0004	0.10	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-0.5SO_4-1	2.0007	0.50	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.0SO_4-1	2.0000	1.0	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.5SO_4-1	2.0007	1.5	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.8SO_4-1	2.0008	1.8	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-0.01SO_4-2	2.0000	0.010	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-0.1SO_4-2	2.0003	0.10	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-0.5SO_4-2	2.0000	0.50	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.0SO_4-2	2.0000	1.0	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.5SO_4-2	2.0007	1.5	0.001	WIPP-Borate-1, Page 13
$MgB(OH)_4$-1.8SO_4-2	2.0001	1.8	0.001	WIPP-Borate-1, Page 13

3.4.6 $CaB(OH)_4^+$—SO_4^{2-} Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "$CaB(OH)_4^+$—SO_4^{2-}" (Item 6, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-9. The solid phase, $Ca(OH)_2$ (Fisher), was purchased from Fisher Scientific. Brines were prepared from DI water, Na_2SO_4 (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Ca concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sulfate, and borate) are to be determined.

Table 3-9 Preparation of experimental set-ups for investigation of $CaB(OH)_4^+$—SO_4^{2-}" Interactions.

Set-up ID	$Ca(OH)_2$ (g)	Na_2SO_4 (m)	H_3BO_3(m)	Reference
$CaB(OH)_4$-0.01SO_4-1	2.0006	0.010	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-0.1SO_4-1	2.0007	0.10	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-0.5SO_4-1	2.0000	0.50	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.0SO_4-1	2.0000	1.0	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.5SO_4-1	2.0008	1.5	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.8SO_4-1	2.0000	1.8	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-0.01SO_4-2	2.0009	0.010	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-0.1SO_4-2	2.0008	0.10	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-0.5SO_4-2	2.0009	0.50	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.0SO_4-2	2.0006	1.0	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.5SO_4-2	2.0003	1.5	0.001	WIPP-Borate-1, Page 14
$CaB(OH)_4$-1.8SO_4-2	2.0007	1.8	0.001	WIPP-Borate-1, Page 14

3.4.7 $NaB(OH)_4$(aq)—Na^+, Cl^- Interactions

The objective of this set of experiments is to (2) determine the Pitzer ion-interaction parameters for the ion triplet "$NaB(OH)_4$(aq)—Na^+, Cl^-" (Item 7, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-10. The solid phase, $Na_2B_4O_7 \cdot 10H_2O$, was purchased from Fisher Scientific. Brines were prepared from DI water and NaCl (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved B concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sodium and chloride) are to be determined. Experimental results gathered to date are shown in Table 3-11.

Table 3-10 Preparation of experimental set-ups for investigation of $NaB(OH)_4(aq)$—Na^+, Cl^- Interactions.

Set-up ID	$Na_2B_4O_7•10H_2O$ (g)	NaCl(m)	Reference
$Na_2B_4O_7$-NaCl-0.01-1	5.0024	0.010	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-0.1-1	5.0031	0.10	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-1.0-1	5.0005	1.0	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-2.0-1	5.0094	2.1	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-3.0-1	5.0073	3.2	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-4.0-1	5.0011	4.4	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-5.0-1	5.0086	5.0	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-0.01-2	5.0057	0.010	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-0.1-2	5.0064	0.10	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-1.0-2	5.0098	1.0	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-2.0-2	5.0066	2.1	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-3.0-2	5.0053	3.2	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-4.0-2	5.0097	4.4	WIPP-Borate-1, Page 4
$Na_2B_4O_7$-NaCl-5.0-2	5.0092	5.0	WIPP-Borate-1, Page 4

Table 3-11 Measured data for the solubility of $Na_2B_4O_7•10H_2O$ in NaCl solutions (the "$NaB(OH)_4(aq)$—Na^+, Cl^-" experiment).

Set-up ID	pH [a] (132 days)	Na, m [b] (132 days)	Boron, m [b] (132 days)
$Na_2B_4O_7$-NaCl-0.01-1	9.10	2.50E-01	5.15E-01
$Na_2B_4O_7$-NaCl-0.1-1	8.95	3.03E-01	4.35E-01
$Na_2B_4O_7$-NaCl-1.0-1	8.55	8.89E-01	1.79E-01
$Na_2B_4O_7$-NaCl-2.0-1	8.34	2.02E-00	1.57E-01
$Na_2B_4O_7$-NaCl-3.0-1	8.33	3.07E-00	1.39E-01
$Na_2B_4O_7$-NaCl-4.0-1	8.22	3.54E-00	1.65E-01
$Na_2B_4O_7$-NaCl-5.0-1	8.05	4.58E-00	1.45E-01
$Na_2B_4O_7$-NaCl-0.01-2	9.03	2.56E-01	5.09E-01
$Na_2B_4O_7$-NaCl-0.1-2	8.93	2.96E-01	4.17E-01
$Na_2B_4O_7$-NaCl-1.0-2	8.57	9.91E-01	1.94E-01
$Na_2B_4O_7$-NaCl-2.0-2	8.49	1.95E-00	1.47E-01
$Na_2B_4O_7$-NaCl-3.0-2	8.29	3.05E-00	1.43E-01
$Na_2B_4O_7$-NaCl-4.0-2	8.23	3.56E-00	1.51E-01
$Na_2B_4O_7$-NaCl-5.0-2	8.04	4.63E-00	1.46E-01
Reference	WIPP-Borate-1, Page 30	WIPP-Borate-1, Page 4; WIPP-Borate-1 Supplemental Binder 1, ICP-AES Analysis Date 11/04/2010	WIPP-Borate-1, Pgs 31-33; WIPP-Borate-1 Supplemental Binder 1, ICP-AES Analysis Date 11/08/2010

[a] Measured with pH electrode and pH meter; [b] measured with ICP-AES

3.4.8 $NaB(OH)_4(aq)$—Mg^{2+}, Cl^- Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion triplet "$NaB(OH)_4(aq)$—Mg^{2+}, Cl^-" (Item 8, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-12. The solid phase, $Na_2B_4O_7 \cdot 10H_2O$, was purchased from Fisher Scientific. Brines were prepared from DI water and $MgCl_2 \cdot 6H_2O$ (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved B concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as magnesium and chloride) are to be determined. Experimental results gathered to date are shown in Table 3-13.

Table 3-12 Preparation of experimental set-ups for investigation of $NaB(OH)_4(aq)$—Mg^{2+}, Cl^- Interactions.

Set-up ID	$Na_2B_4O_7 \cdot 10H_2O$ (g)	$MgCl_2$ (m)	Reference
$Na_2B_4O_7$-0.01Mg-1	5.0047	0.010	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-0.1Mg-1	5.0089	0.10	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-1.0Mg-1	5.0012	1.0	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-1.5Mg-1	5.0085	1.5	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-2.0Mg-1	5.0008	2.0	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-2.5Mg-1	5.0043	1.0	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-0.01Mg-2	5.0099	0.010	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-0.1Mg-2	5.0098	0.10	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-1.0Mg-2	5.0067	1.0	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-1.5Mg-2	5.0027	1.5	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-2.0Mg-2	5.0028	2.0	WIPP-Borate-1, Page 5
$Na_2B_4O_7$-2.5Mg-2	5.0032	1.0	WIPP-Borate-1, Page 5

Table 3-13 Measured data for the solubility of $Na_2B_4O_7•10H_2O$ in $MgCl_2$ solutions (the "$NaB(OH)_4(aq)$—Mg^{2+}, Cl^-" experiment).

Set-up ID	pH [a] (135 days)	Na, m [b] (135 days)	Boron, m [b] (135 days)
$Na_2B_4O_7$-0.01Mg-1	9.21	2.47E-01	5.16E-01
$Na_2B_4O_7$-0.1Mg-1	8.86	2.58E-01	4.79E-01
$Na_2B_4O_7$-1.0Mg-1	6.94	2.70E-01	2.44E-01
$Na_2B_4O_7$-1.5Mg-1	7.03	2.70E-01	4.76E-01
$Na_2B_4O_7$-2.0Mg-1	6.97	2.71E-01	4.90E-01
$Na_2B_4O_7$-2.5Mg-1	6.21	2.78E-01	5.18E-01
$Na_2B_4O_7$-0.01Mg-2	9.18	2.49E-01	5.10E-01
$Na_2B_4O_7$-0.1Mg-2	8.88	2.54E-01	4.68E-01
$Na_2B_4O_7$-1.0Mg-2	7.48	2.71E-01	3.02E-01
$Na_2B_4O_7$-1.5Mg-2	7.04	2.63E-01	4.66E-01
$Na_2B_4O_7$-2.0Mg-2	6.99	2.76E-01	4.98E-01
$Na_2B_4O_7$-2.5Mg-2	6.21	2.73E-01	5.20E-01
Reference	WIPP-Borate-1, Page 30	WIPP-Borate-1 Supplemental Binder 1, ICP-AES Analysis Date 02/24/2011	WIPP-Borate-1, Pgs 34-37; WIPP-Borate-1 Supplemental Binder 1, ICP-AES Analysis Date 11/22/2010

[a] Measured with pH electrode and pH meter; [b] measured with ICP-AES

3.4.9 $NaB(OH)_4(aq)$—Mg^{2+}, Na^+ Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion triplet "$NaB(OH)_4(aq)$—Mg^{2+}, Na^+" (Item 9, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-14. The solid phase, $Na_2B_4O_7•10H_2O$, was purchased from Fisher Scientific. Brines were prepared from DI water, NaCl (Fisher) and $MgCl_2•6H_2O$ (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved B concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as magnesium, sodium and chloride) are to be determined. Experimental results gathered to date are shown in Table 3-15.

Table 3-14 Preparation of experimental set-ups for investigation of $NaB(OH)_4(aq)$—Mg^{2+}, Na^+ Interactions.

Set-up ID	$Na_2B_4O_7 \cdot 10H_2O$ (g)	NaCl (m)	$MgCl_2$ (m)	Reference
$Na_2B_4O_7$-$MgCl_2$-A-1	5.0048	5.0	0.500	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-B-1	5.0018	3.5	0.800	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-C-1	5.0088	3.0	1.25	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-D-1	5.0082	2.0	1.50	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-E-1	5.0055	1.5	1.75	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-F-1	5.0083	0.50	2.00	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-A-2	5.0091	5.0	0.500	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-B-2	5.0029	3.5	0.800	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-C-2	5.0037	3.0	1.25	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-D-2	5.0017	2.0	1.50	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-E-2	5.0063	1.5	1.75	WIPP-Borate-1, Page 6
$Na_2B_4O_7$-$MgCl_2$-F-2	5.0057	0.50	2.00	WIPP-Borate-1, Page 6

Table 3-15 Measured data for the solubility of $Na_2B_4O_7 \cdot 10H_2O$ in NaCl + $MgCl_2$ solutions (the "$NaB(OH)_4(aq)$—Mg^{2+}, Na^+" experiment).

Set-up ID	pH [a] (273 days)	Na, m [b] (273 days)	Boron, m [c] (273 days)
$Na_2B_4O_7$-$MgCl_2$-A-1	7.69	5.17E-00	3.31E-01
$Na_2B_4O_7$-$MgCl_2$-B-1	7.62	3.76E-00	5.10E-01
$Na_2B_4O_7$-$MgCl_2$-C-1	7.29	3.27E-00	5.42E-01
$Na_2B_4O_7$-$MgCl_2$-D-1	7.18	2.28E-00	5.51E-01
$Na_2B_4O_7$-$MgCl_2$-E-1	7.02	1.77E-00	5.34E-01
$Na_2B_4O_7$-$MgCl_2$-F-1	6.88	7.67E-01	5.33E-01
$Na_2B_4O_7$-$MgCl_2$-A-2	7.72	5.17E-00	3.41E-01
$Na_2B_4O_7$-$MgCl_2$-B-2	7.61	3.75E-00	5.00E-01
$Na_2B_4O_7$-$MgCl_2$-C-2	7.29	3.27E-00	5.39E-01
$Na_2B_4O_7$-$MgCl_2$-D-2	6.65	2.14E-00	2.81E-01
$Na_2B_4O_7$-$MgCl_2$-E-2	6.71	1.67E-00	3.36E-01
$Na_2B_4O_7$-$MgCl_2$-F-2	6.47	6.51E-01	3.03E-01
Reference	WIPP-Borate-1, Page 80	WIPP-Borate-1, Pg 82; WIPP-Borate-2, Pg 38; WIPP-Borate-2 Supplemental Binder 1, ICP-AES Analysis Date 04/07/2011	WIPP-Borate-1, Pg 82; WIPP-Borate-2, Pg 44; WIPP-Borate-2 Supplemental Binder 1, ICP-AES Analysis Date 04/05/2011

[a] Measured with pH electrode and pH meter; [b] calculated from initial NaCl concentrations and charge-balance on B, which is determined with ICP-AES, and the formula for calculation is

$m_{Na} = m_{NaCl} + 2 \times \frac{m_{TotalBoron}}{4}$; [c] measured with ICP-AES

3.4.10 PbB_4O_7(aq)—Na^+, Cl^- Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for the ion pair "PbB_4O_7(aq)—Na^+, Cl^-" (Item 10, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-16. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, NaCl (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sodium, and borate) are to be determined.

Table 3-16 Preparation of experimental set-ups for investigation of $PbB_4O_7(aq)$—Na^+, Cl^- Interactions.

Set-up ID	PbO (g)	NaCl (m)	H_3BO_3(m)	Reference
PbB_4(AQ)-0.01Na-1	2.0007	0.010	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-0.1Na-1	2.0001	0.10	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-1.0Na-1	2.0004	1.0	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-2.0Na-1	2.0001	2.1	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-3.0Na-1	2.0005	3.2	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-4.0Na-1	2.0002	4.4	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-5.0Na-1	2.0000	5.0	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-0.01Na-2	2.0005	0.010	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-0.1Na-2	2.0009	0.10	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-1.0Na-2	2.0012	1.0	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-2.0Na-2	2.0002	2.1	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-3.0Na-2	2.0000	3.2	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-4.0Na-2	2.0012	4.4	0.30	WIPP-Borate-1, Page 15
PbB_4(AQ)-5.0Na-2	2.0010	5.0	0.30	WIPP-Borate-1, Page 15

3.4.11 $PbB_4O_7(aq)$—Mg^{2+}, Cl^- Interactions

The objective of this set of experiments is determine the Pitzer ion-interaction parameters for ion pair "$PbB_4O_7(aq)$—Mg^{2+}, Cl^-" (Item 11, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-17. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, $MgCl_2 \cdot 6H_2O$ (Fisher), and H_3BO_3 (Fisher).

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as magnesium, and borate) are to be determined.

Table 3-17 Preparation of experimental set-ups for investigation of $PbB_4O_7(aq)$—Mg^{2+}, Cl^- Interactions.

Set-up ID	PbO (g)	$MgCl_2$ (m)	H_3BO_3(m)	Reference
PbB_4(AQ)-0.01Mg-1	2.0004	0.010	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-0.1Mg-1	2.0006	0.10	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-1.0Mg-1	2.0001	1.0	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-1.5Mg-1	2.0001	1.5	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-2.0Mg-1	2.0002	2.0	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-2.5Mg-1	2.0000	2.5	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-0.01Mg-2	2.0006	0.010	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-0.1Mg-2	2.0006	0.10	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-1.0Mg-2	2.0000	1.0	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-1.5Mg-2	2.0000	1.5	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-2.0Mg-2	2.0009	2.0	0.30	WIPP-Borate-1, Page 16
PbB_4(AQ)-2.5Mg-2	2.0000	2.5	0.30	WIPP-Borate-1, Page 16

3.4.12 $PbB_4O_7(aq)$—Mg^{2+}, Na^+ Interactions

The objective of this set of experiments is to determine the Pitzer ion-interaction parameters for ion pair $PbB_4O_7(aq)$—Mg^{2+}, Na^+ (Item 12, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-18. The solid phase, PbO, was purchased from MP Biomedicals. Brines were prepared from DI water, NaCl (Fisher), $MgCl_2 \cdot 6H_2O$ (Fisher), and H_3BO_3 (Fisher). In the initial set-up, H_3BO_3 was not added. After two samplings, H_3BO_3 was added. The objective of this strategy is to compare lead concentrations in the presence of H_3BO_3 with those in the absence of H_3BO_3, at similar ionic strengths.

The experimental set-ups are periodically monitored for pH and dissolved Pb concentrations. Once stable pH readings are achieved, concentrations of other dissolved components (such as sodium, magnesium, and borate) are to be determined.

Table 3-18 Preparation of experimental set-ups for investigation of $PbB_4O_7(aq)$—Mg^{2+}, Na^+ Interactions.

Set-up ID	PbO (g)	NaCl (m)	$MgCl_2$ (m)	H_3BO_3 (m)	Reference
$PbB_4(AQ)$-$MgCl_2$-A-1	2.0000	5.0	0.500	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-B-1	2.0001	3.5	0.800	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-C-1	2.0009	3.0	1.25	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-D-1	2.0000	2.0	1.50	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-E-1	2.0000	1.5	1.75	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-F-1	2.0007	0.50	2.00	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-A-2	2.0012	5.0	0.500	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-B-2	2.0008	3.5	0.800	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-C-2	2.0000	3.0	1.25	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-D-2	2.0008	2.0	1.50	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-E-2	2.0007	1.5	1.75	0.3	WIPP-Borate-1, Page 19
$PbB_4(AQ)$-$MgCl_2$-F-2	2.0011	0.50	2.00	0.3	WIPP-Borate-1, Page 19

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