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Second Milestone Report on Test Plan TP 08-02, "Iron, Lead, Sulfide, and EDTA Solubilities"

Je-Hun Jang[1], Yong-Liang Xiong[1], Sungtae Kim[2], and Martin B. Nemer[2,]

[1] Repository Performance Dept. 6212
[2] Performance Assessment & Decision Analysis Dept. 6211
Sandia National Laboratories
Defense Waste Management Programs
Carlsbad, NM 88220

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Author:	Je-Hun Jang, 6212	3/22/2012 Date
Author:	Yong-Liang Xiong, 6212	03/22/2012 Date
Author:	Sungtae Kim, 6211	3/22/2012 Date
Author:	For Martin B. Nemer, 1512	3/22/2012 Date
Technical Reviewer:	Gregory T. Roselle, 6212	3/26/2012 Date
QA Reviewer:	Shelly R. Nielsen, 6210	3-22-12 Date
Management Reviewer:	for CDL Christi D. Leigh, 6212	3/28/2012 Date

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Abbreviation or Acronym	Definition
[X]	concentration of component X
A	pH correction factor
ACS	American Chemical Society
AP	Analysis Plan
aq	aqueous (phase identifier)
BD	Below Detection
Cit^{-3}	citrate anion, conjugate base of citric acid, $C_6H_5O_7^{-3}$
$CaCit^-$	calcium citrate aqueous complex anion
Cl^-	chloride anion
CO_3^{2-}	carbonate anion
DI	de-ionized
DDI	deoxygenated de-ionized
DRC	Document Review and Comment, form number NP 6-1-1
$EDTA^{-4}$	ethylenediaminetetraacetate anion, $C_{10}H_{12}N_2O_8^{-4}$
ES&H	Environmental Safety and Health
Fe^{2+}	ferrous iron aqueous cation
Fe(II)	total ferrous iron
Fe(III)	total ferric iron
$FeCit^-$	ferrous iron citrate aqueous complex anion
$FeOH^+$	ferrous iron hydroxide aqueous complex cation
$Fe(OH)_3^-$	ferrous iron trihydroxide aqueous complex anion
$FeEDTA^{-2}$	ferrous iron EDTA aqueous complex anion
FeOx(aq)	ferrous iron oxalate aqueous complex
Fe_T	total iron, i.e., Fe(II) + Fe(III)
FeS	iron sulfide

g	gram, or gas (phase identifier)
H_2	hydrogen molecule
HCO_3^-	bicarbonate anion
$HEDTA^{3-}$	hydrogen EDTA aqueous complex anion
HS^-	hydrogen sulfide anion
HCl	hydrochloric acid
H_2S	hydrogen sulfide
IC	Ion Chromatography
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectroscopy
ICP-MS	Inductively Coupled Plasma Mass Spectroscopy
m	molal (mol/kg)
M	molar (mol/L)
Mg^{2+}	magnesium aqueous cation
Na^+	sodium aqueous cation
NA	Not Analyzed
Ox^{-2}	oxalate anion, $C_2O_4^{-2}$, conjugate base of oxalic acid
Pb_T	total lead
PbOx(aq)	lead oxalate aqueous complex
$PbEDTA^{2-}$	lead EDTA aqueous complex anion
$PbCl^+$	lead chloride aqueous complex cation
$PbCit^-$	lead citrate aqueous complex anion
pH	negative logarithm of hydrogen ion activity
PI	Principle Investigator
QA	Quality Assurance
s	solid (phase identifier)
SNL	Sandia National Laboratories
SNL/DWMP	Sandia National Laboratories Defense Waste Management Programs
SP	Specific Procedure
SO_4^{2-}	sulfate anion
TP	Test Plan

WIPP	Waste Isolation Pilot Plant
XRD	X-ray diffraction

1 INTRODUCTION

The purpose of this milestone report is to (1) summarize experimental data obtained to date under Test Plan TP 08-02, "Iron, Lead, Sulfide, and EDTA Solubilities" (Ismail et al., 2008), and (2) determine future activities needed to complete the work scope defined in Test Plan TP 08-02 by tabulating the results to date. Test Plan TP 08-02 supports the Waste Isolation Pilot Plant's (WIPP's) geochemical model used to estimate the solubilities of major actinide species present in the repository. The data provided in this report addresses the solubility of WIPP-relevant non-actinide solids and the Pitzer ion-interaction parameters for the aqueous species associated with those solids. This report is a continuation from the previous one (Jang et al., 2011), and contains data to date.

In Test Plan TP 08-02, the systems containing Fe(II)- and Pb(II)-bearing 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.

Table 1-1 Ion-pairs identified for investigation in Test Plan TP 08-02[a].

1.	$FeOH^+$—SO_4^{2-}	15.	$PbCl^+$—CO_3^{2-}
2.	$FeOH^+$—CO_3^{2-}	16.	$PbCl^+$—SO_4^{2-}
3*.	$FeOH^+$—HS^-	17*.	$PbCl^+$—HS^-
4*.	Fe^{2+}—HS^-	18.	Na^+—$PbEDTA^{2-}$
5.	Na^+—$Fe(OH)_3^-$	19.	Mg^{2+}—$PbEDTA^{2-}$
6.	Mg^{2+}—$Fe(OH)_3^-$	20.	Na^+—$PbCit^-$
7.	FeOx(aq)—Na^+	21.	Mg^{2+}—$PbCit^-$
8.	FeOx(aq)—Mg^{2+}	22.	PbOx(aq)—Na^+
9.	FeOx(aq)—Cl^-	23.	PbOx(aq)—Mg^{2+}
10.	Na^+—$FeEDTA^{2-}$	24.	PbOx(aq)—Cl^-
11.	Mg^{2+}—$FeEDTA^{2-}$	25*.	Na^+—HS^-
12.	Na^+—$FeCit^-$	26*.	Mg^{2+}—HS^-
13.	Mg^{2+}—$FeCit^-$	27*.	Cl^-—HS^-
14.	$PbCl^+$—HCO_3^-		

[a] Based on Table 2 of TP 08-02 (Ismail et al., 2008)

Table 1-1 identifies twenty-seven systems for investigation, which are currently underway, except those marked with asterisks (See section 2.6). Many of the experiments have

been running for periods exceeding one year. Once a system has come to equilibrium, based on the stability of measured concentration(s) of selected aqueous component(s) over time, final measurements of the aqueous component(s) of interest can be made and the thermodynamic and Pitzer parameters of interest can be derived.

Five additional systems have been identified for investigation based on the results from the initial test phase. These systems are listed in Table 1-2, and were selected due to their WIPP-relevance and lack of data in the literature.

Table 1-2 Ion-pairs and/or triplets added for investigation in the second phase of Test Plan TP 08-02.

28.	$FeOx(aq)—Na^{+}—Mg^{2+}$	31.	$Cl^{-}—HEDTA^{3-}$
29.	$Na^{+}—CaCit^{-}$	32.	$Mg^{2+}—HEDTA^{3-}$
30.	$Mg^{2+}—CaCit^{-}$		

2 MATERIALS AND METHODS

Solubility-controlling solids of interest were either chemicals that are certified as ACS reagent grade or better, or synthesized and characterized in the laboratory using XRD when ACS reagents are not available. Solutions were prepared using appropriate reagent grade commercial salts.

2.1 Anoxic Conditions

Experiments involving Fe(II) were strictly performed inside anoxic gloveboxes. Samples containing dissolved Fe(II) were preserved in dilute HCl inside the gloveboxes prior to further handling under normal air to limit the oxidation rate of Fe(II).

2.2 Measurement of Dissolved Fe(II) and Dissolved Total Fe

Ferrozine assay was used to measure the concentration of dissolved Fe(II) ($[Fe(II)]_{diss}$) and dissolved total Fe concentrations ($[Fe_T]_{diss} = [Fe(II)]_{diss} + [Fe(III)]_{diss}$). Details on ferrozine assay are in WIPP-Solubility-4 Supplemental Binder-1, WIPP-Solubility-11 Supplemental Binder-1, and p.77 of WIPP-Solubility-9. UV-Visible spectrophotomer was used to read the absorbance at 562 nm as per current revision of SP 12-25. ICP-AES was sometimes used to measure $[Fe_T]_{diss}$, when it was desirable (See section 2.4 for cation analysis using ICP-AES).

2.3 Anion Measurements

IC was used for anion analysis per SP 12-22. For some organic anions, carbon coulometer was used per SP 12-2 to check the accuracy of IC results.

2.4 Cation Measurements

ICP-AES was used to measure the concentrations of cations, including $[Fe_T]_{diss}$ and $[Pb_T]_{diss}$ per current revision of SP 12-9.

2.5 pH Measurements

Solution pH was measured using commercial combination electrodes and meters per current revision of SP 12-14.

2.6 Experiments involving H_2S

Because of Environmental Safety and Health (ES&H) concerns regarding the use of chemical compounds that could be potential sources of hydrogen sulfide gas (H_2S), investigation of the systems requiring the use of HS^- was delayed (Items 3, 4, 17, and 25-27 in Table 1-1). The ES&H requirements for safe handling of hydrogen sulfide were fulfilled, and those solubility experiments involving the hydrogen sulfide ion (HS^-) in conjunction with Fe(II) and Pb(II) are ready to begin.

An iron sulfide (FeS(s), mackinawite) has been prepared in the dedicated glovebox. The required duration for these experiments is uncertain. Because of the low solubility of sulfide-bearing minerals in general, the sulfide experiments may require substantially more time to reach equilibrium than many of the other experiments listed in Table 1-1. Careful monitoring of system component(s), such as, pH and concentration of selected metal(s), may be required to establish that equilibrium conditions exist. The use of an ICP-MS may be required to obtain lower detection limits to measure the dissolved concentrations of Fe and Pb.

3 RESULTS

Following sections describe the preparation of the experimental set-ups and results to date for ion-pairs listed in Table 1-1 and Table 1-2 in the order therein. Each section has two types of tables; one to describe the experimental set-ups and the other to tabulate results to date. When single table frame does not provide proper summary of experimental set-ups and/or results to date, multiple tables were used under same table identifier followed by "(continued)". Refer to Table 3-1 and Table 3-2 in section 3.1 for an example. For those experiments which were not initiated, a short description of the experiments and two empty tables were provided; one for description of experimental set-ups, the other for measurement of all components involved in the experimental set-ups. One or two of the listed components will be monitored over time to see if the system approaches a steady-state so that we can assume equilibrium. Though all components are listed, it is each PI's decision whether to proceed with all the measurements or to select a few relevant components. For example, to prepare NaCl solutions, the mass of NaCl is weighed, and the amount of DI water is determined either gravimetrically or volumetrically. This procedure determines the concentrations of sodium and chloride which are significantly more accurate than common laboratory instruments can do, such as ICP-AES or IC. It might be wiser to analyze a few, not every single, NaCl solution as check samples. However, due to the hygroscopic nature of commercial salt of magnesium ($MgCl_2 \cdot 6H_2O$), it is recommended that the PIs frequently check Mg^{+2} and Cl^- concentration in the solutions as the salt ages. If unforeseen parallel reactions are suspected that can remove any of Na^+, Mg^{+2}, or Cl^- from supporting solutions, it is highly recommended to check their concentrations on a regular basis.

3.1 Solubility of $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2(s)$ in mixed NaCl and Na_2SO_4 solutions (the "$FeOH^+$—SO_4^{2-}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Fe_2(OH)_3Cl(s)$ (iron hibbingite) and $Fe(OH)_2(s)$ (ferrous iron hydroxide) in mixed NaCl (sodium chloride) and Na_2SO_4 (sodium sulfate) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair "$FeOH^+$—SO_4^{2-}" (Item 1, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-1. The solid phases, $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2(s)$, were synthesized from $FeCl_2 \cdot 4H_2O$ (Fisher) and KOH (Fisher), and $FeCl_2 \cdot 4H_2O$ (Fisher) and NaOH (Fisher), respectively. Brines were prepared from DI water, NaCl (Fisher), and Na_2SO_4 (Fisher).

Over a period of several months, the solid phase in the first six experimental set-ups defined in Table 3-1 reduced water in the brine and formed green rust sulfate, causing pressure increases inside the experimental set-up reactors. The respective pressures were about 1 – 10 psi higher than normal atmosphere (1 atmosphere = 14.696 psi). Thus, new experimental set-ups (later six set-ups) were prepared with an $Fe(OH)_2$ solid phase and a brine containing NaCl in addition to Na_2SO_4. The new formulation seems to have prevented (or greatly reduced) the rate of water reduction.

The experimental set-ups are periodically monitored for pH and dissolved Fe(II) concentrations([Fe(II)]). About 3 years of aging have made the experimental set-up's pH levels change appreciably. Once stable pH readings are achieved, concentrations of other dissolved components (sodium, sulfate, and chloride) are to be determined. These will be used to estimate the Pitzer ion-interaction parameters for the ion pair "$FeOH^+$—SO_4^{2-}". Experimental results gathered to date are shown in Table 3-2.

Table 3-1 Preparation of experimental set-ups for the solubility of $Fe_2(OH)_3Cl(s)$ in Na_2SO_4 solutions, and for the solubility of $Fe(OH)_2(s)$ in mixed Na_2SO_4 and NaCl solutions (the "$FeOH^+$—SO_4^{2-}" experiment).

Set-up ID	$Fe_2(OH)_3Cl(s)$ (g)	$Fe(OH)_2$ (g)	Na_2SO_4 (m)	NaCl (m)	Reference
0.05m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	0.05	-	WIPP-Solubility-1, pg. 15-19, 96-97
0.38m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	0.38	-	
0.76m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	0.76	-	
1.14m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	1.19	-	
1.52m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	1.52	-	
1.9m-SO_4-$Fe(OH)_2$-(1,2)	0.7	-	1.9	-	
0.01m Na_2SO_4+0.15NaCl-GR	-	2.05	0.01	0.15	WIPP-Solubility-1, pg. 91
0.1m Na_2SO_4+0.15NaCl-GR	-	2.02	0.1	0.15	
0.5m Na_2SO_4+0.15NaCl-GR	-	2.04	0.5	0.15	
1m Na_2SO_4+0.15NaCl-GR	-	2.02	1	0.15	
1.5m Na_2SO_4+0.15NaCl-GR	-	2.02	1.5	0.15	
1.8m Na_2SO_4+0.15NaCl-GR	-	2.03	1.8	0.15	

Table 3-2 Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in Na_2SO_4 solutions (the "$FeOH^+$—SO_4^{2-}" experiment).

	pH[a]			$[Fe_T]$ (mol/L)[c]		$[Fe_T]$ (mol/L)[d]		[Fe(II)] (mol/L)[d]		$[SO_4^{2-}]$ (mol/L)[e]
Set-up ID	**(84 days)**	**(133 days)**	**(1149 days)**	**(90 days)**	**(133 days)**	**(135 days)**	**(206 days)**	**(135 days)**	**(206 days)**	**(311 days)**
0.05m-SO_4-$Fe(OH)_2$-1	8.126	-	7.753	6.27E-03	-	-	-	-	-	-
0.38m-SO_4-$Fe(OH)_2$-1	8.307	-	8.059	8.58E-03	-	-	-	-	-	-
0.76m-SO_4-$Fe(OH)_2$-1	8.361	-	8.173	8.90E-03	-	-	-	-	-	-
1.14m-SO_4-$Fe(OH)_2$-1	8.507	-	8.278	6.21E-03	-	-	-	-	-	-
1.52m-SO_4-$Fe(OH)_2$-1	8.400	-	8.123	8.31E-03	-	-	-	-	-	-
1.9m-SO_4-$Fe(OH)_2$-1	8.521	-	8.187[f]	5.36E-03	-	-	-	-	-	-
0.05m-SO_4-$Fe(OH)_2$-2	-	7.908	7.751	-	9.88E-03	7.60E-03	1.26E-02	2.64E-03	1.16E-02	4.05E-02
0.38m-SO_4-$Fe(OH)_2$-2	-	8.158	8.090	-	1.16E-02	6.43E-03	1.39E-02	9.30E-03	1.25E-02	3.99E-01
0.76m-SO_4-$Fe(OH)_2$-2	-	8.265	8.175	-	1.13E-02	1.01E-02	1.40E-02	9.12E-03	1.34E-02	8.02E-01
1.14m-SO_4-$Fe(OH)_2$-2	-	8.357	8.150	-	9.61E-03	8.15E-03	1.21E-02	1.62E-03	1.10E-02	1.82E+00
1.52m-SO_4-$Fe(OH)_2$-2	-	8.372[b]	8.043[f]	-	1.18E-02	1.09E-02	1.47E-02	9.61E-03	1.39E-02	1.79E+00
1.9m-SO_4-$Fe(OH)_2$-2	-	8.471[b]	7.886[f]	-	1.02E-02	9.06E-03	1.47E-02	5.92E-03	1.46E-02	2.05E+00
Reference	WIPP-Solubility-1, pg. 66	WIPP-Solubility-4, pg. 38, 40	WIPP-Solubility-18, pg. 49	WIPP-Solubility-1, pg. 71-72	WIPP-Solubility-4, pg. 34-46	WIPP-Solubility-4, pg. 34-38, 45-46, 75-77	WIPP-Solubility-6, pg. 14-15	WIPP-Solubility-4, pg. 34-38, 45-46, 75-77	WIPP-Solubility-6, pg. 14-15	WIPP-Solubility-6, pg. 62-64

[a] Measured with pH electrode and meter, [b]134 days, [f]1150 days, [c] Measured using ICP-AES; WIPP-Solubility-1.

[d] Measured using the Ferrozine method, [e] Measured using IC.

Table 3-2(continued) Measured data for the solubility of $Fe(OH)_2(s)$ in mixed Na_2SO_4 and NaCl solutions (the "$FeOH^+$—SO_4^{2-}" experiment).

Set-up ID	pH[a]			$[Fe_T]$ (mol/L)[b]		[Fe(II)] (mol/L)[b]	
	(55 days)	(86 days)	(880 days)	(55 days)	(85 days)	(55 days)	(85 days)
0.01m Na_2SO_4+0.15NaCl-GR	8.110	7.943	7.938	1.67E-03	1.86E-03	1.57E-03	1.81E-03
0.1m Na_2SO_4+0.15NaCl-GR	8.354	8.369	8.287	1.30E-03	1.53E-03	1.18E-03	1.41E-03
0.5m Na_2SO_4+0.15NaCl-GR	8.603	8.634	8.483	1.17E-03	1.28E-03	9.80E-04	1.22E-03
1m Na_2SO_4+0.15NaCl-GR	8.730	8.767	8.528	9.45E-04	1.05E-03	9.17E-04	1.01E-03
1.5m Na_2SO_4+0.15NaCl-GR	8.810	8.834	8.639	7.36E-04	1.08E-03	7.14E-04	9.99E-04
1.8m Na_2SO_4+0.15NaCl-GR	8.773	8.817	8.650	6.99E-04	7.77E-04	6.72E-04	7.84E-04
Reference	WIPP-Solubility-6, pg. 50	WIPP-Solubility-6, pg. 66	WIPP-Solubility-18, pg. 35	WIPP-Solubility-6, pg. 51-55	WIPP-Solubility-6, pg. 70	WIPP-Solubility-6, pg. 51-55	WIPP-Solubility-6, pg. 70

[a] Measured with pH electrode and meter.

[b] Measured using the Ferrozine method.

3.2 Solubility of $FeCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$FeOH^+$—CO_3^{2-}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $FeCO_3$(s) (siderite) in mixed Na_2CO_3 (sodium carbonate) and NaCl (sodium chloride) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair "$FeOH^+$—CO_3^{2-}" (Item 2, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid $FeCO_3$(s) are shown below in Table 3-3. The solid phase, $FeCO_3$(s), was synthesized using two recipes: (1) mixing $FeCl_2 \cdot 4H_2O$ (Fisher), Na_2CO_3 (Fisher), NaOH (Fisher) and DI water and heating the mixture at 80 °C, and (2) mixing $FeCl_2 \cdot 4H_2O$ (Fisher), $NaHCO_3$ (Fisher) and DI water. $FeCO_3$(s) from the former recipe was used in setting up FeCO3-XCO3-1 (X = 0.01, 0.1, 0.5, 1.0, 1.5, 2.0) reactors. $FeCO_3$(s) from the latter recipe was used in setting up $FeCO_3$-XCO_3-(3,4,5,6) (X = 0.01, 0.1, 0.5, 1.0, 1.5, 2.0) reactors. Brines were prepared from DI water, NaCl (Fisher), and Na_2CO_3 (Fisher).

The solid phase in some of the $FeCO_3$-XCO_3-(3,4,5,6) experimental set-ups has been covered with green rust-like layer. Based on a prediction of CO_2 (g) generation, pressure inside all $FeCO_3$-XCO_3-(4,5,6) experimental set-up reactors was measured. The respective pressure was about 0.2 – 0.4 psi higher than the normal atmosphere (14.696 psi).

The experimental set-ups will be continuously monitored for pH and Fe concentration among those listed in Table 3-4. Once stable pH readings are achieved, concentrations of components will be analyzed to derive the Pitzer ion-interaction parameters for the ion pair "$FeOH^+$—CO_3^{2-}".

Table 3-3 Preparation of experimental set-ups for the solubility of $FeCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$FeOH^+$— CO_3^{2-}" experiment).

Set-up ID	$FeCO_3$(s) (g)	NaCl (m)	Na_2CO_3 (m)	Reference
$FeCO_3$-0.01CO_3-1	0.5#	0.15	0.01	CAR W-09-05, and notebooks cited therein*
$FeCO_3$-0.1CO_3-1	0.5#	0.15	0.1	
$FeCO_3$-0.5CO_3-1	0.5#	0.15	0.5	
$FeCO_3$-1.0CO_3-1	0.5#	0.15	1.0	
$FeCO_3$-1.5CO_3-1	0.5#	0.15	1.5	
$FeCO_3$-2.0CO_3-1	0.5#	0.15	2.0	
$FeCO_3$-0.01CO_3-3	0.47	1.5	0.01	WIPP-Solubility-18, p.37-39, 57-58
$FeCO_3$-0.1CO_3-3	0.49	1.5	0.1	
$FeCO_3$-0.5CO_3-3	0.5	1.5	0.5	
$FeCO_3$-1.0CO_3-3	0.46	1.5	1.0	
$FeCO_3$-1.5CO_3-3	0.48	1.5	1.5	
$FeCO_3$-2.0CO_3-3	0.5	1.5	2.0	
$FeCO_3$-0.01CO_3-4	0.53	1.5	0.01	WIPP-Solubility-18, p.37-39, 57-58
$FeCO_3$-0.1CO_3-4	0.52	1.5	0.1	
$FeCO_3$-0.5CO_3-4	0.49	1.5	0.5	
$FeCO_3$-1.0CO_3-4	0.48	1.5	1.0	
$FeCO_3$-1.5CO_3-4	0.49	1.5	1.5	
$FeCO_3$-2.0CO_3-4	0.46	1.5	2.0	
$FeCO_3$-0.01CO_3-5	0.52	0.15	0.01	WIPP-Solubility-18, p.66
$FeCO_3$-0.1CO_3-5	0.47	0.15	0.1	
$FeCO_3$-0.5CO_3-5	0.51	0.15	0.5	
$FeCO_3$-1.0CO_3-5	0.48	0.15	1.0	
$FeCO_3$-1.5CO_3-5	0.49	0.15	1.5	
$FeCO_3$-2.0CO_3-5	0.53	0.15	2.0	
$FeCO_3$-0.01CO_3-6	0.5	0.15	0.01	WIPP-Solubility-18, p.66
$FeCO_3$-0.1CO_3-6	0.48	0.15	0.1	
$FeCO_3$-0.5CO_3-6	0.48	0.15	0.5	
$FeCO_3$-1.0CO_3-6	0.47	0.15	1.0	
$FeCO_3$-1.5CO_3-6	0.48	0.15	1.5	
$FeCO_3$-2.0CO_3-6	0.51	0.15	2.0	

Approximately 0.5g based on visual appearance. Exact solid mass is not critical in solubility experiments.

* Those pages are p.31 and p.97 of WIPP-Solubility-1 for $FeCO_3$(s) preparation and XRD, p.21-22 of WIPP-Solubility-3 for solution preparation. On p.70-77 of WIPP-Solubility-4, one of the PIs mentioned Fe(II) measurement for the samples above by the Ferrozine method, but data are not traceable in the associated binder therein (WIPP-Solubility-4 supplemental binder-1 tab 11/11/08).

Table 3-4 Measured data for the solubility of $FeCO_3(s)$ in mixed Na_2CO_3 and NaCl solutions (the "$FeOH^+$—CO_3^{2-}" experiment).

	pH[a]			$[Fe_T]$ (mol/L)[d]	
Set-up ID	**(44 days)**	**(92 days)**	**(42 days)**	**(43 days)**	**(94 days)**
$FeCO_3$-0.01CO_3-3	9.718[b]	-	-	-	8.06E-07
$FeCO_3$-0.1CO_3-3	10.521	-	-	-	1.97E-06
$FeCO_3$-0.5CO_3-3	11.003	-	-	-	2.63E-05
$FeCO_3$-1.0CO_3-3	11.169	-	-	-	9.63E-05
$FeCO_3$-1.5CO_3-3	11.252	-	-	-	2.02E-04
$FeCO_3$-2.0CO_3-3	11.145	-	-	-	3.69E-04
$FeCO_3$-0.01CO_3-4	-	9.690	-	-	3.58E-07
$FeCO_3$-0.1CO_3-4	-	10.539	-	-	1.79E-07
$FeCO_3$-0.5CO_3-4	-	11.033	-	-	1.90E-05
$FeCO_3$-1.0CO_3-4	-	11.204	-	-	8.95E-05
$FeCO_3$-1.5CO_3-4	-	11.021	-	-	1.85E-04
$FeCO_3$-2.0CO_3-4	-	10.930	-	-	3.33E-04
$FeCO_3$-0.01CO_3-5	-	-	10.150[c]	6.27E-07	-
$FeCO_3$-0.1CO_3-5	-	-	10.921[c]	3.58E-06	-
$FeCO_3$-0.5CO_3-5	-	-	11.248[c]	2.33E-05	-
$FeCO_3$-1.0CO_3-5	-	-	11.331	8.06E-05	-
$FeCO_3$-1.5CO_3-5	-	-	11.369	2.30E-04	-
$FeCO_3$-2.0CO_3-5	-	-	11.366	4.34E-04	-
$FeCO_3$-0.01CO_3-6	-	-	10.128	7.16E-07	-
$FeCO_3$-0.1CO_3-6	-	-	10.872	1.79E-06	-
$FeCO_3$-0.5CO_3-6	-	-	11.169	2.36E-05	-
$FeCO_3$-1.0CO_3-6	-	-	11.279	9.20E-05	-
$FeCO_3$-1.5CO_3-6	-	-	11.322	2.37E-04	-
$FeCO_3$-2.0CO_3-6	-	-	11.338	4.57E-04	-
Reference	WIPP-Solubility-18, pg. 59, 68	WIPP-Solubility-18, pg. 74	WIPP-Solubility-18, pg. 74	WIPP-Solubility-18, pg. 76-80	WIPP-Solubility-18, pg. 79-81

[a] Measured with pH electrode and meter, [b]8 days, [c]41 days.

[d] Measured using ICP.

3.3 Solubility of FeS(s) in mixed NaHS and Na_2S solutions (the "$FeOH^+$—HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of FeS(s) (mackinawite) in mixed NaHS (sodium bisulfide) and Na_2S (sodium sulfide) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "$FeOH^+$—HS^-" (Item 3, Table 1-1). The solid phase is under preparation in an anoxic glovebox dedicated for sulfide experiments. Experimental set-ups will be listed in Table 3-5, and they will be periodically monitored for one or more component(s) among those listed in Table 3-6. Once stable readings are achieved for the selected component(s), concentrations of other components will be determined.

Table 3-5 Preparation of experimental set-ups for the solubility of FeS(s) in mixed NaHS and Na_2S solutions (the "$FeOH^+$—HS^-" experiment).

Set-up ID	Iron sulfide (g)	NaHS (m)	Na_2S (m)	Reference
No Data to Date				

Table 3-6 Measured data for the solubility of FeS(s) in mixed NaHS and Na_2S solutions (the "$FeOH^+$—HS^-" experiment).

Set-up ID	$[Fe(II)]_{diss}$	$[S^{2-}_T]_{diss}$	$[Na(I)]_{diss}$	pH
Reference	No Data to Date			

3.4 Solubility of FeS(s) in Na_2S solutions (the "Fe^{2+}—HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of FeS(s) (mackinawite) in Na_2S (sodium sulfide) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Fe^{2+}—HS^-" (Item 4, Table 1-1). Experimental set-ups will be listed in Table 3-7, and they will be periodically monitored for one or more component(s) among those listed in Table 3-8. Once stable readings are achieved for the selected component(s), concentrations of other components will be determined.

Table 3-7 Preparation of experimental set-ups for the solubility of FeS(s) in NaCl solutions (the "Fe^{2+}—HS^-" experiment).

Set-up ID	Iron sulfide (g)	Na_2S (m)	Reference
No Data to Date			

Table 3-8 Measured data for the solubility of FeS(s) in NaCl solutions (the "Fe^{2+}—HS^-" experiment).

Set-up ID	[Fe(II)]	[S(-II)]	[Na(I)]	pH
Reference	No Data to Date			

3.5 Solubility of $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

The objectives of this set of experiments are to (1) determine the solubility of $Fe_2(OH)_3Cl(s)$ (iron hibbingite), $FeCl_2 \cdot 4H_2O$(ferrous chloride tetrahydrate) and $Fe(OH)_2(s)$ (ferrous iron hydroxide) in NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Na^+—$Fe(OH)_3^-$" (Item 5, Table 1-1).

The experimental set-ups are shown in Table 3-9. The solid phases, $Fe_2(OH)_3Cl$ (s) and $Fe(OH)_2$ (s), were synthesized from $FeCl_2 \cdot 4H_2O$ (Fisher) and KOH (Fisher), and $FeCl_2 \cdot 4H_2O$ (Fisher) and NaOH (Fisher). Brines were prepared from DI water, NaCl (Fisher), and NaOH (Fisher).

These experimental set-ups have been periodically monitored for pH and dissolved Fe(II) concentrations ([Fe(II)]). Over 3 years aging has made pH of the experimental set-ups decrease. However, 5m-Cl-Fe(OH)2-O-(1,2) set-up reactors exhibit that their pH are steady around 8.965. Once stable pH readings are achieved for other experimental set-ups, concentrations of other dissolved components (sodium and chloride) are to be determined to estimate the Pitzer ion-interaction parameters for the ion pair "Na^+—$Fe(OH)_3^-$". Experimental results gathered to date are shown in Table 3-10.

Table 3-9 Preparation of experimental set-ups for the solubility of $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2(s)$ in approximately 50 ml of NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	$Fe_2(OH)_3Cl(s)$ (g)	$FeCl_2 \cdot 4H_2O(s)$ (g)	NaCl (m)	NaOH (m)	References
0.1m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	0.1	-	WIPP-Solubility-1 pg.15-17
1m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	1	-	
2m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	2	-	
3m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	3	-	
4m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	4	-	
5m-Cl-$Fe(OH)_2$-(1,2)	0.7	-	5	-	
1m-Cl-$Fe(OH)_2$-O-1	-	0.7207	1	1.0[a]	WIPP-Solubility-1 pg.82-86
1m-Cl-$Fe(OH)_2$-O-2	-	0.5104	1	1.0[b]	
5m-Cl-$Fe(OH)_2$-O-1	-	0.5629	5	1.0[c]	
5m-Cl-$Fe(OH)_2$-O-2	-	0.5486	5	1.0[d]	

[a] 1m NaOH was added too much, and pH reached nearly 11

[b] 1m NaOH was added until pH reached 10.6

[c] 1m NaOH was added until pH reached 9.3

[d] 1m NaOH was added until pH reached 10.7

Set-up ID	$Fe(OH)_2(s)$ (m)	NaCl (m)	NaOH (m)	References
SQDLTN+0	0.2176	0.0363	-	WIPP-Solubility-5, pg.73
SQDLTN+1	0.2176	0.152	-	
SQDLTN+2	0.2176	0.504	-	
SQDLTN+3	0.2176	1.22	-	
SQDLTN+4	0.2176	3.03	-	
SQDLTN+5	0.2176	5.97	-	

Table 3-9 (continued) Preparation of experimental set-ups for the solubility of $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	$FeCl_2 \cdot 4H_2O(s)$ (g)	Na^+ (mol/L)	Cl^- (mol/L)	References
KSPFe(OH)$_2$-1	n.d. [#]	0.2045	0.2065	WIPP-Solubility-5 pg. 30
KSPFe(OH)$_2$-2	n.d. [#]	0.2045	0.2065	
KSPFe(OH)$_2$-3	n.d. [#]	0.2045	0.2065	
KSPFe(OH)$_2$-4	n.d. [#]	0.2045	0.2065	
KSPLIFe(OH)$_2$-1	n.d. [#]	0.00203	0.00195	WIPP-Solubility-5 pg. 46-47
KSPLIFe(OH)$_2$-2	n.d. [#]	0.00203	0.00195	
KSPLIFe(OH)$_2$-3	n.d. [#]	0.00203	0.00195	
KSPLIFe(OH)$_2$-4	n.d. [#]	0.00203	0.00195	
KSPLIFe(OH)$_2$-5	n.d. [#]	0.00203	0.00195	
KSPLIFe(OH)$_2$-6	n.d. [#]	0.00203	0.00195	
Set-up ID	**Fe(II) (m)**	**Na^+ (m)**	**Cl^- (m)**	**References**
FeNaClA-1	0.3021	1.2131	1.2137	WIPP-Solubility-5 pg. 65
FeNaClA-2	0.2993	3.025	3.0256	
FeNaClA-3	0.3029	5.9693	5.9691	
SQDLTN-0	0.2519	0.5040	0.5038	WIPP-Solubility-5 pg. 65
SQDLTN-1	0.2418	0.1512	0.1511	WIPP-Solubility-5 pg. 66
SQDLTN-2	0.2176	0.03629	0.03626	WIPP-Solubility-5 pg. 69

[#] Not Determined. Mass of solid is not critical in solubility experiments.

Table 3-10 Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+— $Fe(OH)_3^-$" experiment).

Set-up ID	pH[a]								
	(139 days)	(235 days)	(273 days)	(382 days)	(383 days)	(389 days)	(428 days)	(1110 days)	(1202 days)
0.1m-Cl-$Fe(OH)_2$-1	-	-	-	8.244	8.297[b]	8.234	8.286	7.842	7.829
1m-Cl-$Fe(OH)_2$-1	-	-	-	8.606	8.546[b]	8.536	8.548	8.476	8.447
2m-Cl-$Fe(OH)_2$-1	-	-	-	8.594	8.551[b]	8.511	8.506	8.329	8.276[f]
3m-Cl-$Fe(OH)_2$-1	-	-	-	8.548	8.427	8.429	8.431[c]	8.314	8.268[f]
4m-Cl-$Fe(OH)_2$-1	-	-	-	8.484	8.393	8.373	8.349[c]	8.296[e]	8.227[f]
5m-Cl-$Fe(OH)_2$-1	-	-	-	8.284	8.205	8.173	8.155[d]	8.022[e]	7.913[f]
0.1m-Cl-$Fe(OH)_2$-2	8.397	-	8.261	-	-	-	8.207	7.810	7.829
1m-Cl-$Fe(OH)_2$-2	8.507	-	8.550	-	-	-	8.534	8.385	8.442
2m-Cl-$Fe(OH)_2$-2	8.519	-	8.539	-	-	-	8.510	8.353	8.307[f]
3m-Cl-$Fe(OH)_2$-2	8.456	-	8.428	-	-	-	8.339[c]	8.258	8.217[f]
4m-Cl-$Fe(OH)_2$-2	8.385	-	8.337	-	-	-	8.289[c]	8.185[e]	8.084[f]
5m-Cl-$Fe(OH)_2$-2	8.311	8.190	8.222	-	-	8.161	8.168[d]	8.121[e]	8.032[f]
Reference	WIPP-Solubility-4, pg. 38-42	WIPP-Solubility-4, pg. 89-92	WIPP-Solubility-6, pg. 24-26	WIPP-Solubility-8, pg. 15-16	WIPP-Solubility-8, pg. 24-25	WIPP-Solubility-8, pg. 26-27	WIPP-Solubility-8, pg. 28-31	WIPP-Solubility-18, pg. 26-27	WIPP-Solubility-18, pg. 60-61

[a] Measured with pH electrode and meter, [b]386 days, [c]432 days, [d]435 days, [e]1111 days, [f]1203 days.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	[Fe_T] (mol/L)[a] (138 days)	[Fe_T] (mol/L)[b] (274 days)	[Fe_T] (mol/L)[b] (371 days)	[Fe_T] (mol/L)[b] (438 days)	[Fe(II)] (mol/L)[b] (277 days)	[Fe(II)] (mol/L)[b] (371 days)	[Fe(II)] (mol/L)[b] (438 days)	[Cl^-] (mol/L)[c] (273 days)	[Cl^-] (mol/L)[c] (382 days)
0.1m-Cl-$Fe(OH)_2$-1	-	-	1.50E-03	1.56E-03	-	1.48E-03	1.42E-03	-	1.06E-01
1m-Cl-$Fe(OH)_2$-1	-	-	2.57E-04	2.48E-04	-	2.43E-04	2.52E-04	-	9.79E-01
2m-Cl-$Fe(OH)_2$-1	-	-	1.63E-04	1.64E-04	-	1.50E-04	1.60E-04	-	1.93E+00
3m-Cl-$Fe(OH)_2$-1	-	-	1.55E-04	1.13E-04	-	1.40E-04	1.15E-04	-	2.73E+00
4m-Cl-$Fe(OH)_2$-1	-	-	8.13E-05	9.29E-05	-	6.35E-05	7.19E-05	-	3.24E+00
5m-Cl-$Fe(OH)_2$-1	-	-	9.03E-05	9.95E-05	-	8.04E-05	1.03E-04	-	3.96E+00
0.1m-Cl-$Fe(OH)_2$-2	7.85E-04	1.38E-03	-	1.95E-03	1.32E-03	-	1.89E-03	1.01E-01[d]	-
1m-Cl-$Fe(OH)_2$-2	2.74E-04	2.11E-04	-	2.48E-04	2.63E-04	-	2.48E-04	8.89E-01	-
2m-Cl-$Fe(OH)_2$-2	1.48E-04	4.02E-05	-	1.63E-04	1.44E-04	-	1.62E-04	1.71E+00	-
3m-Cl-$Fe(OH)_2$-2	1.16E-04	6.80E-05	-	1.38E-04	1.09E-04	-	1.32E-04	2.59E+00	-
4m-Cl-$Fe(OH)_2$-2	9.04E-05	1.16E-05	-	1.08E-04	8.16E-05	-	1.02E-04	3.46E+00	-
5m-Cl-$Fe(OH)_2$-2	7.74E-05	1.30E-05	-	8.60E-05	7.06E-05	-	8.18E-05	4.37E+00	-
Reference	WIPP-Solubility-4, pg. 34-47	WIPP-Solubility-6, pg. 29	WIPP-Solubility-6, pg. 87-90	WIPP-Solubility-8, pg. 32-38	WIPP-Solubility-6, pg. 30-32	WIPP-Solubility-6, pg. 87-90	WIPP-Solubility-8, pg. 32-38	WIPP-Solubility-6, pg. 24-28 and 33-34	WIPP-Solubility-8, pg. 17, 39, 47

[a] Measured using ICP-AES.

[b] Measured using the Ferrozine method.

[c] Measured using the IC, [d]277 days.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	pH[a] (23 days)	(40 days)	(78 days)	(191 days)	(243 days)	(590 days)	(931 days)	(1048 days)
1m-Cl-$Fe(OH)_2$-O-1	8.626	-	10.628	10.585	10.457[b]	-	10.064	9.971
1m-Cl-$Fe(OH)_2$-O-2	8.531	8.673	8.607	8.581	8.533	-	8.459	8.501
5m-Cl-$Fe(OH)_2$-O-1	8.910	8.890	8.939	8.965	8.955	8.904	9.019	8.98
5m-Cl-$Fe(OH)_2$-O-2	8.297	8.798	8.919	8.928	8.970	8.942	9.017	8.931
Reference	WIPP-Solubility-4, pg. 86-87	WIPP-Solubility-4, pg. 89-91	WIPP-Solubility-6, pg. 24-26	WIPP-Solubility-8, pg. 25	WIPP-Solubility-8, pg. 30-31	WIPP-Solubility-11, pg. 24	WIPP-Solubility-18, pg. 28	WIPP-Solubility-18, pg. 69

[a] Measured with pH electrode and meter, [b] 240 days.

Set-up ID	[Fe(II)][a] (mol/L) (75 days)	(243 days)	(590 days)	[Fe_T][a] (mol/L) (75 days)	(176 days)	(243 days)	(590 days)	[Cl^-][b] (mol/L) (82 days)	(187 days)
1m-Cl-$Fe(OH)_2$-O-1	-	-	-	-	-	-	-	-	-
1m-Cl-$Fe(OH)_2$-O-2	1.30E-04	2.15E-04	-	1.33E-04	-	2.38E-04	-	-	0.94
5m-Cl-$Fe(OH)_2$-O-1	7.81E-06	-	2.69E-07	8.57E-06	5.92E-06	6.28E-06	5.35E-06	3.84	3.97
5m-Cl-$Fe(OH)_2$-O-2	6.71E-06	-	-	7.43E-06	6.94E-06	7.42E-06	8.55E-06	3.9	4.46
Reference	WIPP-Solubility-6, pg. 18-24	WIPP-Solubility-8, pg. 32-33, 54-55	WIPP-Solubility-11, pg. 30-31	WIPP-Solubility-6, pg. 18-24	WIPP-Solubility-11, pg. 31	WIPP-Solubility-8, pg. 32-33, 54-55	WIPP-Solubility-11, pg. 30-31	WIPP-Solubility-6, pg. 33-34	WIPP-Solubility-8, pg. 17, 39, 47

[a] Measured using the Ferrozine method.

[b] Measured using IC.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	pH*								$[Fe(II)]_{diss}$ (mol/L)			[Cl(-I)][a] (m)	[Cl(-I)][b] (mol/L)
	(1 days)	(10 days)	(21 days)	(28 days)	(57 days)	(94 days)	(112 days)	(168 days)	(28 days)	(94 days)	(112 days)	(28, 94, 112 days)	(112 days)
SQDLTN+0	8.105	8.039	7.973	8.004	8.076	8.017	8.021	8.011	1.48E-03	1.59E-03	1.60E-03	0.0363	3.40E-02
SQDLTN+1	8.144	7.929	8.031	8.096	8.109	8.101	8.09	7.982	1.17E-03	1.28E-03	1.28E-03	0.152	1.29E-01
SQDLTN+2	8.181	8.017	8.084	8.121	8.09	8.172	8.15	8.178	1.02E-03	1.14E-03	1.15E-03	0.504	4.28E-01
SQDLTN+3	8.195	8.008	8.112	8.151	8.101	8.207	8.188	8.232	8.59E-04	9.13E-04	9.15E-04	1.22	1.09E+00
SQDLTN+4	8.11	7.862	8.036	8.077	7.956	8.145	8.137	8.278	6.26E-04	6.39E-04	6.10E-04	3.03	2.54E+00
SQDLTN+5	7.943	7.949	8.043	8.153	8.725	8.83	8.841	8.957	1.19E-04	6.14E-06	3.90E-06	5.97	4.93E+00
Reference	WIPP-Solubility-5, p.73, 95								WIPP-Solubility-5, p.94	WIPP-Solubility-7, p.56	WIPP-Solubility-7, p.70	WIPP-Solubility-5, p.73	WIPP-Solubility-7, p.72

* Measured with pH electrode and meter; [a] gravimetric determination, [b] Measured using IC.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

	pH*									
Set-up ID	**(0 days)**	**(14 days)**	**(28 days)**	**(32 days)**	**(49 days)**	**(71 days)**	**(85 days)**	**(92 days)**	**(173 days)**	**(1068 days)**
KSPFe(OH)$_2$-1	7.653	7.641	7.532	7.531	7.529	7.386	7.574	7.288	7.591	7.498
KSPFe(OH)$_2$-2	7.949	7.963	7.887	7.895	7.862	7.693	7.732	7.578	7.949	7.889
KSPFe(OH)$_2$-3	8.447	8.287	8.238	8.199	8.204	7.915	7.981	7.846	8.255	8.165
KSPFe(OH)$_2$-4	9.046	8.550	8.485	8.522	8.469	8.203	8.222	8.178	8.512	8.325#
Reference	WIPP-Solubility-5, p.31	WIPP-Solubility-5, p.40	WIPP-Solubility-5, p.43	WIPP-Solubility-5, p.46	WIPP-Solubility-5, p.54	WIPP-Solubility-5, p.70	WIPP-Solubility-5, p.80	WIPP-Solubility-5, p.80	WIPP-Solubility-5, p.80	WIPP-Solubility-25, pg. 42, 44

* Measured with pH electrode and meter, #1069 days.

	$[Fe(II)]_{diss}$ (mol/L)[a]		[Cl(-I)][b] (mol/L)	$[Na(I)]_{diss}$, (mol/L)[c]
Set-up ID	**(92 days)**	**(173 days)**	**(173 days)**	**(1070 days)**
KSPFe(OH)$_2$-1	1.26E-02	1.27E-02	2.40E-01	2.00E-01
KSPFe(OH)$_2$-2	2.86E-03	2.92E-03	2.17E-01	1.93E-01
KSPFe(OH)$_2$-3	6.88E-04	6.98E-04	2.08E-01	1.90E-01
KSPFe(OH)$_2$-4	2.21E-04	2.31E-04	2.15E-01	1.96E-01
Reference	WIPP-Solubility-5, p.86	WIPP-Solubility-7, p.60	WIPP-Solubility-7, p.66	WIPP-Solubility-25, pg. 54

[a]Measured using the Ferrozine Method, [b]Measured using the IC, [c]Measured using the ICP-AES.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

Set-up ID	pH*						$[Fe(II)]_{diss}$ (mol/L)[a]		[Cl(-I)] (mol/L)[b]	$[Na(I)]_{diss}$, (mol/L)[c]
	(0 days)	(39 days)	(53 days)	(63 days)	(142 days)	(1037 days)	(63 days)	(142 days)	(142 days)	(1038 days)
KSPLIFe(OH)$_2$-1	7.497	7.476	7.467	7.448	7.521	7.446	2.23E-02	2.17E-02	4.84E-02	1.80E-03
KSPLIFe(OH)$_2$-2	7.909	7.880	7.881	7.859	7.930	7.853	2.63E-03	2.72E-03	8.01E-03	1.76E-03
KSPLIFe(OH)$_2$-3	8.346	8.276	8.265	8.251	8.326	8.222	4.38E-04	9.71E-04	8.40E-03	6.26E-03
KSPLIFe(OH)$_2$-4	9.209	9.076	9.008	9.007	9.038	8.653	1.29E-05	1.57E-05	2.88E-03	1.90E-03
KSPLIFe(OH)$_2$-5	9.759	9.598	9.538	9.528	9.582	8.699	2.06E-06	1.37E-06	2.90E-03	1.97E-03
KSPLIFe(OH)$_2$-6	10.209	10.101	10.062	10.037	10.137	9.029	3.18E-07	1.39E-07	2.94E-03	2.05E-03
Reference	WIPP-Solubility-5, p.47	WIPP-Solubility-5, p.70	WIPP-Solubility-5, p.80	WIPP-Solubility-5, p.80	WIPP-Solubility-5, p.80	WIPP-Solubility-25, pg. 44	WIPP-Solubility-5, p.89	WIPP-Solubility-7, p.61	WIPP-Solubility-7, p.66	WIPP-Solubility-25, pg.56-57

* Measured with pH electrode and meter.

[a]Measured using the Ferrozine Method, [b]Measured using the IC, [c]Measured using the ICP-AES.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

	pH*									
Set-up ID	**(1 days)**	**(2 days)**	**(7 days)**	**(16 days)**	**(27 days)**	**(34 days)**	**(63 days)**	**(103 days)**	**(119 days)**	**(1008 days)**
FeNaClA-1	10.172	8.79	8.147	8.034	8.048	8.090	8.137	8.122	8.033	8.071
FeNaClA-2	10.842	10.477	8.363	8.268	8.217	8.269	8.248	8.257	8.216	8.565
FeNaClA-3	10.492	10.296	8.488	8.458	8.468	8.453	8.552	8.478	8.492	8.758
Reference	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.95	WIPP-Solubility-5, p.95	WIPP-Solubility-5, p.95	WIPP-Solubility-25, pg. 55

* Measured with pH electrode and meter.

	pH*									
Set-up ID	**(0 days)**	**(1 days)**	**(5 days)**	**(7 days)**	**(16 days)**	**(27 days)**	**(34 days)**	**(63 days)**	**(103 days)**	**(119 days)**
SQDLTN-0	-	10.567	9.081[a]	8.230	8.161	8.141	8.175	8.207	8.197	8.210
SQDLTN-1	8.024	7.705	8.011[b]	-	7.954[c]	7.921[d]	7.968[e]	7.996[i]	7.949[k]	8.001[m]
SQDLTN-2	8.169	-	8.092	-	8.042[f]	8.006[g]	8.018[h]	8.078[j]	7.994[L]	8.035[n]
Reference	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.68	WIPP-Solubility-5, p.95	WIPP-Solubility-5, p.95	WIPP-Solubility-5, p.95

*Measured with pH electrode and meter, [a] 2 days, [b] 6 days, [c] 15 days, [d] 26 days, [e] 33 days, [f] 14 days, [g] 25 days, [h] 32 days, [i] 62 days, [j] 61 days, [k] 102 days, [L] 101 days, [m] 118 days, [n] 117 days.

Table 3-10 (continued) Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Na^+—$Fe(OH)_3^-$" experiment).

	$[Fe(II)]_{diss}$ (mol/L)[a]			[Cl(-I)] (mol/L)[b]
Set-up ID	**(34 days)**	**(103 days)**	**(120 days)**	**(120 days)**
FeNaClA-1	1.17E-03	1.29E-03	1.27E-03	1.17E+00
FeNaClA-2	2.77E-04	3.50E-04	3.53E-04	2.64E+00
FeNaClA-3	3.23E-05	3.73E-05	3.77E-05	5.03E+00
SQDLTN-0	8.25E-04	1.00E-03	9.95E-04	4.77E-01
SQDLTN-1	2.07E-03[e]	2.28E-03[k]	0.00228[p]	1.40E-01[p]
SQDLTN-2	1.44E-03[h]	1.58E-03[L]	0.00159[m]	3.41E-02[m]
Reference	WIPP-Solubility-5, p.94	WIPP-Solubility-7, p.59	WIPP-Solubility-7, p.70	WIPP-Solubility-7, p.72

*Measured with pH electrode and meter, [e] 33 days, [h] 32 days, [k] 102 days, [L] 101 days, [m] 118 days, [p] 119 days.

[a]Measured using the Ferrozine Method, [b]Measured using the IC.

3.6 Solubility of $Fe_2(OH)_3Cl(s)$ and $Fe(OH)_2$ in $MgCl_2$ solutions (the "Mg^{2+}—$Fe(OH)^{3-}$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Fe_2(OH)_3Cl(s)$ (iron hibbingite) and $Fe(OH)_2(s)$ (iron hydroxide) in $MgCl_2$ (magnesium chloride) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair "Mg^{2+}—$Fe(OH)_3^-$" (Item 6, Table 1-1). Preparation and available data are in tables below.

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-11. The solid phase, $Fe_2(OH)_3Cl$ and $Fe(OH)_2(s)$, was synthesized from $FeCl_2 \cdot 4H_2O$ (Fisher), and NaOH (Fisher). Brines were prepared from DI water and $CaCl_2$ (Fisher). Because a high pH is needed to obtain a strong interaction between Mg^{2+} and $Fe(OH)_3^-$, we decided to use Ca^{2+} as an analogue in some experiments. The solid phase, $Ca(OH)_2$ (Fisher), was added to each experimental set-up to maintain a high pH.

The experimental set-ups have been monitored for pH or dissolved Fe(II) concentrations ([Fe(II)]). About 3 years aging has made the experimental set-ups nearly in stable state. Monitoring will continue, and once stable pH readings and values of [Fe(II)] are achieved, concentrations of other dissolved components ([Ca(II)], [Cl(-I)]) are to be determined to estimate the Pitzer ion-interaction parameters for the ion pair "Mg^{2+}—$Fe(OH)_3^-$". Experimental results gathered to date are shown in Table 3-12.

Table 3-11 Preparation of experimental set-ups for the solubility of $Fe(OH)_2(s)$ in $CaCl_2$ solutions, where Ca^{2+} is analogue for Mg^{2+} (the "Mg^{2+}—$Fe(OH)^{3-}$" experiment).

Set-up ID*	$Fe(OH)_2(s)$ (g)	$CaCl_2$ (m)	Ca(OH)2(s) (g)	Reference
$Fe(OH)_3$/Cl -0.01A	1	0.01	n.d.#	WIPP-Solubility-1, pg. 37-44
$Fe(OH)_3$/Cl -0.1A	1	0.1	n.d.#	
$Fe(OH)_3$/Cl -1A	1	1	n.d.#	
$Fe(OH)_3$/Cl -1.5A	1	1.5	n.d.#	
$Fe(OH)_3$/Cl -2A	1	2	n.d.#	
$Fe(OH)_3$/Cl -2.5A	1	2.5	n.d.#	

* These set-ups were prepared over a period of time spanning from 6/5/2008 to 8/11/2008. The last date of preparation was considered completion date of preparation to determine the number of days of equilibration in the table below.

Not Determined. Added in excess (~0.3gram). Refer to email from Martin Nemer on 3/3/11 (Jang and Nielsen, 2011) for the solid mass. Exact mass of $Ca(OH)_2$ is not critical in this experiment, and no record in the above reference.

Set-up ID	$Fe(OH)_2(s)$	$MgCl_2$ (m)	Reference
$Fe(OH)_3$/Mg;0.01a	n.d.#	0.01	WIPP-Solubility-7 pg. 33
$Fe(OH)_3$/Mg;0.1a	n.d.#	0.1	
$Fe(OH)_3$/Mg;1a	n.d.#	1	
$Fe(OH)_3$/Mg;1.5	n.d.#	1.5	
$Fe(OH)_3$/Mg;2	n.d.#	2	
$Fe(OH)_3$/Mg;2.5	n.d.#	2.5	

Not Determined.

Table 3-12 Measured data for the solubility of $Fe_2(OH)_3Cl(s)$ in NaCl solutions (the "Mg^{2+}—$Fe(OH)_3^-$" experiment)

	pH[a]			Fe_T (mol/L)[d]
Set-up ID	**(483 days)**	**(1085 days)**	**(1192 days)**	**(343 days)**
$Fe(OH)_3$/Cl -0.01A	7.754[a1]	7.620[a2]	7.649	6.53E-03
$Fe(OH)_3$/Cl -0.1A	12.074	12.042	12.056	1.50E-05[d1]
$Fe(OH)_3$/Cl -1A	11.599	11.573	11.582	1.32E-05[d1]
$Fe(OH)_3$/Cl -1.5A	-	11.40	11.404	1.52E-05[d1]
$Fe(OH)_3$/Cl -2A	10.682	11.167	11.189	2.11E-05[d1]
$Fe(OH)_3$/Cl -2.5A	10.985	10.940	10.969	3.41E-03
Reference	WIPP-Solubility-8, pg. 56, 57, and 59	WIPP-Solubility-18, pg. 36	WIPP-Solubility-18, pg. 70	WIPP-Solubility-1, pg. 75-76

[a] Measured with pH meter and electrode, [a1] 485 days, [a2] 1078 days.
[d] Measured using ICP-AES ; [d1]Results below ICP-AES calibration curve.

	pH*			
Set-up ID	**(1 days)**	**(52 days)**	**(105 days)**	**(940 days)**
$Fe(OH)_3$/Mg;0.01a	8.416	8.389	8.342	8.095
$Fe(OH)_3$/Mg;0.1a	8.559	8.436	8.404	8.319
$Fe(OH)_3$/Mg;1a	8.155	8.082	8.062	8.172
$Fe(OH)_3$/Mg;1.5	7.932	7.910	7.913	7.980
$Fe(OH)_3$/Mg;2	7.784	7.801	7.913	7.534
$Fe(OH)_3$/Mg;2.5	7.513	7.674	7.732	7.376
Reference	WIPP-Solubility-7 pg. 33	WIPP-Solubility-7 pg. 33	WIPP-Solubility-7 pg. 33	WIPP-Solubility-25, pg. 55

* Measured with pH electrode and meter.

3.7 Solubility of $FeC_2O_4 \cdot 2H_2O$(s) in NaCl solutions (the "FeOx(aq)—Na^+" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $FeC_2O_4 \cdot 2H_2O$(s) (ferrous oxalate dihydrate) in NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "FeOx(aq)—Na^+" (Item 7, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-13. Ferrous oxalate dihydrate ($FeC_2O_4 \cdot 2H_2O$) was purchased from Alfa Aesar (Cat A13479) and sodium chloride (NaCl) from Fisher. A known mass of $FeC_2O_4 \cdot 2H_2O$ was added to 50 mL of NaCl solutions of incremental concentrations (Table 3-13). In series -3 and -4 listed below, the ferrous oxalate dihydrate was first washed with sodium hydroxide to remove excess oxalic acid from the starting material.

The experimental set-ups are periodically monitored for pH and dissolved Fe(II) concentrations($[Fe(II)]_{diss}$). Once stable pH readings are achieved, concentrations of other dissolved components (sodium, oxalate, and chloride) are to be determined. Experimental results gathered to date are shown in Table 3-14.

Table 3-13 Preparation of experimental set-ups for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in NaCl solutions (the "FeOx(aq)—Na^+" experiment).

Set-up ID	$FeC_2O_4 \cdot 2H_2O$(s) (g)	NaCl	Reference
0.1-FeOx-3	1.2[a]	0.1 M	WIPP-Solubility-4, pg. 24-25
1M-FeOx-3	1.2[a]	1.0 M	
2M-FeOx-3	1.2[a]	2.0 M	
3M-FeOx-3	1.2[a]	3.0 M	
4M-FeOx-3	1.2[a]	4.0 M	
5M-FeOx-3*	1.2[a]	5.0 m	
0.1-FeOx-4	1.2[a]	0.1 M	
1M-FeOx-4	1.2[a]	1.0 M	
2M-FeOx-4	1.2[a]	2.0 M	
3M-FeOx-4	1.2[a]	3.0 M	
4M-FeOx-4	1.2[a]	4.0 M	
5M-FeOx-4*	1.2[a]	5.0 m	
FeOx-0.1A	2	0.1 m[#]	WIPP-Solubility-1, p. 44, 80
FeOx-1A	2	1.0 m[#]	
FeOx-2A	2	2.0 m[#]	
FeOx-3A	2	3.0 m[#]	
FeOx-4A	2	4.0 m[#]	
FeOx-5A	2	5.0 m[#]	
FeOx-0.1B	2	0.1 m[#]	
FeOx-1B	2	1.0 m[#]	
FeOx-2B	2	2.0 m[#]	
FeOx-3B	2	3.0 m[#]	
FeOx-4B	2	4.0 m[#]	
FeOx-5B	2	5.0 m[#]	

* Unlike their IDs, these samples were made in 5m NaCl solution.

[a] No record in reference of WIPP-Solubility-4, p.24-25. Martin Nemer approximately estimated.

[#] Preparation of NaCl solution was described in p.11 of WIPP-Solubility-2.

Table 3-14 Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in NaCl solutions (the "FeOx(aq)—Na^+" experiment)

	pH[a]									
Set-up ID	**(65 day)**	**(71 days)**	**(78 days)**	**(92 days)**	**(114 days)**	**(141 days)**	**(160 days)**	**(241 days)**	**(244 days)**	**(366 days)**
0.1-FeOx-3	5.231	5.264	5.13	5.045	5.225	5.104	5.096	5.188	-	-
1M-FeOx-3	5.498	5.481	5.381	5.318	5.445	5.282	5.228	5.321	-	-
2M-FeOx-3	5.232	5.223	5.032	5.213	5.21	5.065	5.029	5.171	-	-
3M-FeOx-3	5.159	5.15	5.139	5.123	5.114	5.006	4.858	5.036	-	-
4M-FeOx-3	5.131	5.113	5.083	5.066	5.095	4.98	4.985	4.977	-	-
5M-FeOx-3*	6.347	6.493	6.384	6.263	6.493	5.879	5.883	5.587	-	-
0.1-FeOx-4	-	-	-	-	-	5.15	5.098	-	5.144	5.199
1M-FeOx-4	-	-	-	-	-	5.226	5.204	-	5.263	5.327
2M-FeOx-4	-	-	-	-	-	5.063	5.036	-	5.098	5.177
3M-FeOx-4	-	-	-	-	-	5.011	4.955	-	5.005	5.112
4M-FeOx-4	-	-	-	-	-	4.989	4.947	-	4.904	4.878
5M-FeOx-4*	-	-	-	-	-	5.933	6.031	-	5.629	5.259
Reference	WIPP-Solubility-5, p.12	WIPP-Solubility-5, p.16	WIPP-Solubility-5, p.24	WIPP-Solubility-5, p.38	WIPP-Solubility-5, p.43	WIPP-Solubility-5, p.57	WIPP-Solubility-5, p.70	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72

* Unlike their IDs, these samples were made in 5m NaCl solution.

[a] Measured with Accumet pH electrode and VWR sympHony pH meter.

Table 3-14 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in NaCl solutions (the "FeOx(aq)—Na^+" experiment)

	$[Fe(II)]_{diss}$, (mol/L)[a]						
Set-up ID	**(65 days)**	**(71 days)**	**(78 days)**	**(92 days)**	**(115 days)**	**(244 days)**	**(367 days)**
0.1-FeOx-3	3.11E-04	3.46E-04	3.27E-04	3.31E-04	3.30E-04	3.11E-04	-
1M-FeOx-3	6.32E-04	6.21E-04	6.37E-04	6.19E-04	6.28E-04	6.26E-04	-
2M-FeOx-3	7.90E-04	7.50E-04	7.67E-04	7.33E-04	7.48E-04	7.49E-04	-
3M-FeOx-3	8.11E-04	7.70E-04	7.73E-04	7.56E-04	7.63E-04	7.56E-04	-
4M-FeOx-3	8.43E-04	7.81E-04	7.88E-04	7.76E-04	7.74E-04	7.54E-04	-
5M-FeOx-3*	7.75E-04	7.72E-04	7.70E-04	7.49E-04	7.54E-04	7.35E-04	-
0.1-FeOx-4	-	-	-	-	-	3.13E-04	3.25E-04
1M-FeOx-4	-	-	-	-	-	6.21E-04	5.98E-04
2M-FeOx-4	-	-	-	-	-	7.43E-04	7.33E-04
3M-FeOx-4	-	-	-	-	-	7.70E-04	7.63E-04
4M-FeOx-4	-	-	-	-	-	7.48E-04	7.46E-04
5M-FeOx-4*	-	-	-	-	-	7.20E-04	7.05E-04
Reference	WIPP-Solubility-5, p.13	WIPP-Solubility-5, p.17	WIPP-Solubility-5, p.25	WIPP-Solubility-5, p.39	WIPP-Solubility-5, p.45	WIPP-Solubility-7, p.50	WIPP-Solubility-7, p.78

[a] Measured using the Ferrozine method

* Unlike their IDs, these samples were made in 5m NaCl solution.

Table 3-14 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in NaCl solutions (the "FeOx(aq)—Na^+" experiment)

	Fe_T (mol/L)[b]	pH[a]		$[Fe(II)]_{diss}$, (mol/L)[c]
Set-up ID	**(43 days)**	**(511 days)**	**(1114 days)**	**(951 days)**
FeOx-0.1A	2.14E-04	3.975	3.998[a2]	1.44E-04
FeOx-0.1B	-	4.030	4.031[a2]	1.45E-04
FeOx-1A	7.53E-04	3.354	3.639	2.69E-04
FeOx-1B	-	3.421	3.764	2.86E-04
FeOx-2A	9.26E-04	3.011	3.314	3.61E-04
FeOx-2B	-	2.903	3.212	3.63E-04
FeOx-3A	1.32E-03	2.274	2.531	5.30E-04
FeOx-3B	-	2.246[a1]	2.489	5.35E-04
FeOx-4A	1.42E-03	1.923	2.140	7.19E-04
FeOx-4B	-	1.923[a1]	2.105	8.11E-04
FeOx-5A	1.62E-03	1.680	1.853	9.28E-04
FeOx-5B	-	1.668[a1]	1.826	1.01E-03
Reference	WIPP-Solubility-1, pg. 75-76	WIPP-Solubility-8, pg. 70-71	WIPP-Solubility-20 pg. 64	WIPP-Solubility-15, p.64

[a] Measured with pH electrode and meter, [a1] 510 days, [a2] 1112 days.

[b]Measured using the ICP-AES.

[c]Measured using the Ferrozine Method.

3.8 Solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $FeC_2O_4 \cdot 2H_2O$(s) (ferrous oxalate dihydrate) in $MgCl_2$ (magnesium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "FeOx(aq)—Mg^{+2}" (Item 8, Table 1-1).

The experimental set-ups including initial brine molalities and mass of solid materials are shown below in Table 3-15. $FeC_2O_4 \cdot 2H_2O$(s) was purchased from Alfa Aesar (puratronic, 99.999 % metal basis), and magnesium chloride hexahydrate ($MgCl_2 \cdot 6H_2O$) was purchased from Fisher. $FeC_2O_4 \cdot 2H_2O$(s) was added to $MgCl_2 \cdot 6H_2O$ solutions of incremental concentrations, ranging from 0.01 to 2.5 m $MgCl_2$. Since solubility should be independent of the solid mass and liquid volume as long as the solid phase persists until equilibrium is reached, the mass of $FeC_2O_4 \cdot 2H_2O$ and the volume of the $MgCl_2$ solutions were not measured for 30 of the experimental set-ups (FeOxMg-(1~6)-(1~5), Table 3-15 below). However, as these set-ups progressed toward equilibrium, some phenomena were observed that might be explained by the solid-to-liquid ratio (i.e., color change in solid phase). Thus, 8 additional set-ups (FeOxMg-Ratio-(no identifier or DI)-(1~4), Table 3-15 below) were prepared to test the hypothesis regarding the effect of the solid-to-liquid ratio.

The concentration of dissolved ferrous iron ($[Fe(II)]_{diss}$) and the pH are monitored over time to see if the experimental set-ups are approaching equilibrium. After observing stable pH and/or Fe(II) concentrations, dissolved concentrations for the other components in the system (magnesium, oxalate, chloride) are to be measured. Measured values to date for this investigation are documented in Table 3-16.

Table 3-15 Experimental set-ups for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

Set-up ID	$MgCl_2$ (m)	$FeC_2O_4 \cdot 2H_2O$(s) (g)	Volume of solution (mL)	Reference
FeOxMg-1-(1,2,3)	0.01	n.d.*	n.d.	WIPP-Solubility-5, p.4
FeOxMg-2-(1,2,3)	0.1	n.d.	n.d.	
FeOxMg-3-(1,2,3)	0.48	n.d.	n.d.	
FeOxMg-4-(1,2,3)	0.93	n.d.	n.d.	
FeOxMg-5-(1,2,3)	1.3	n.d.	n.d.	
FeOxMg-6-(1,2,3)	2.0	n.d.	n.d.	
FeOxMg-1-(4,5)	0.01	n.d.	n.d.	WIPP-Solubility-5, p.71
FeOxMg-2-(4,5)	0.1	n.d.	n.d.	
FeOxMg-3-(4,5)	0.49	n.d.	n.d.	
FeOxMg-4-(4,5)	0.92	n.d.	n.d.	
FeOxMg-5-(4,5)	1.3	n.d.	n.d.	
FeOxMg-6-(4,5)	2.0	n.d.	n.d.	
FeOxMg-Ratio-0	2.5	0	30	WIPP-Solubility-9, p.23
FeOxMg-Ratio-1	2.5	0.1205	56.4#	
FeOxMg-Ratio-2	2.5	1.0864	48.7#	
FeOxMg-Ratio-3	2.5	4.8462	41.2#	
FeOxMg-Ratio-4	2.5	10.2721	36.2#	
FeOxMg-Ratio-DI-1	0	0.1005	47.0#	WIPP-Solubility-9, p.36
FeOxMg-Ratio-DI-2	0	0.4593	48.2#	
FeOxMg-Ratio-DI-3	0	2.4009	43.7#	
FeOxMg-Ratio-DI-4	0	10.0479	41.7#	

Either 2.5 m $MgCl_2$ or DDI water.

* Not determined.

Set-up ID	$Mg(OH)_2$ (g)	$FeCl_2 \cdot 4H2O$ (g)	$H_2C_2O_4 \cdot 2H_2O$ (g)	$MgCl_2 \cdot 6H_2O$ (g)	DDI water (mL)	Reference
OS-FeOxMg-0.05-1	0.154	0.4995	0.3341	-	50	WIPP-Solubility-7 pg. 52 and 53
OS-FeOxMg-0.5-1	1.4591	4.9783	3.1551	-	50	
OS-FeOxMg-1.0-1	1.4851	4.9711	3.2153	3.0698	40	
OS-FeOxMg-2.5-1	1.4551	4.9735	3.1678	15.2673	40	

Table 3-16 Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	pH[a]											
Set-up ID	**(7 days)**	**(13 days)**	**(21 days)**	**(34 days)**	**(57 days)**	**(83 days)**	**(104 days)**	**(156 days)**	**(171 days)**	**(287 days)**	**(542 days)**	**(979 days)**
FeOxMg-1-1	5.692	5.654	5.305	5.347	5.692	5.725	5.567	5.748	5.652	6.104	6.218	6.322
FeOxMg-2-1	5.272	5.282	5.305	5.11	5.302	5.402	5.345	5.356	5.319	5.73	5.946	6.034
FeOxMg-3-1	5.159	5.174	4.973	5.003	5.288	5.148	5.196	5.183	5.363	5.679	5.802	5.856
FeOxMg-4-1	5.146	5.114	4.916	4.948	5.275	5.048	5.036	4.998	5.221	5.414	5.501	5.487*
FeOxMg-5-1	5.012	5.052	4.793	4.804	5.222	4.961	4.853	4.797	5.159	5.346	5.423	5.437*
FeOxMg-6-1	4.585	4.571	4.565	4.364	4.807	4.385	3.677	4.117	4.236	4.509	4.805	4.650*
Reference	WIPP-Solubility-5, p.10	WIPP-Solubility-5, p.14	WIPP-Solubility-5, p.22	WIPP-Solubility-5, p.34	WIPP-Solubility-5, p.41	WIPP-Solubility-5, p.55	WIPP-Solubility-5, p.70	WIPP-Solubility-5, p.96				WIPP-Solubility-20, p.56

[a] Measured with pH electrode and meter, *981 days.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

Set-up ID	pH[a]									
	(83 days)	(104 days)	(156 days)	(177 days)	(181 days)	(295 days)	(307 days)	(534 days)	(545 days)	(979 days)
FeOxMg-1-2	5.71	5.697	5.663	5.716	-	6.126	-	-	6.213	6.675
FeOxMg-2-2	5.416	5.374	5.458	5.54	-	5.913	-	-	6.021	6.343
FeOxMg-3-2	5.244	5.204	5.282	5.392	-	5.731	-	-	5.808	5.975
FeOxMg-4-2	4.968	4.896	5.181	5.429	-	5.794	-	-	5.798	6.118[#]
FeOxMg-5-2	4.864	4.794	4.75	4.942	-	4.961	-	-	5.421	5.306[#]
FeOxMg-6-2	3.825[*]	3.782	4.153	4.069	-	4.31	-	-	4.680	4.624[#]
FeOxMg-1-3	4.567	4.562	4.589	-	4.636	-	4.663	4.695	-	4.754
FeOxMg-2-3	4.411	4.338	4.346	-	4.38	-	4.402	4.397	-	4.365
FeOxMg-3-3	4.163	4.111	4.134	-	4.158	-	4.190	4.192	-	4.101
FeOxMg-4-3	3.997[*]	3.952	3.941	-	4.005	-	4.04	4.042	-	3.927[#]
FeOxMg-5-3	3.938[*]	3.864	3.911	-	3.958	-	3.994	4.006	-	3.921[#]
FeOxMg-6-3	3.674[*]	3.553	3.649	-	3.767	-	3.827	3.864	-	3.787[#]
Reference	WIPP-Solubility-5, p.55, 56	WIPP-Solubility-5, p.70	WIPP-Solubility-5, p.96							WIPP-Solubility-20, p.56

[a] Measured with pH electrode and meter, [*]84 days, [#]981 days.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	pH[a]							
Set-up ID	**(6 days)**	**(51 days)**	**(79 days)**	**(203 days)**	**(204 days)**	**(443 days)**	**(444 days)**	**(877 days)**
FeOxMg-1-4	4.799	4.628	4.679	4.684	-	4.722	-	4.922
FeOxMg-2-4	4.646	4.477	4.516	4.543	-	4.595	-	4.775
FeOxMg-3-4	4.409	4.279	4.344	4.406	-	4.473	-	4.700
FeOxMg-4-4	4.114	3.992	4.048	4.103	-	4.166	-	4.297
FeOxMg-5-4	3.837	3.683	3.743	3.792	-	3.807	-	3.755*
FeOxMg-6-4	3.579	3.463	3.556	3.6	-	3.664	-	3.641*
FeOxMg-1-5	4.854	4.614	4.686	-	4.649	-	4.633	4.606
FeOxMg-2-5	4.706	4.508	4.548	-	4.532	-	4.491	4.498
FeOxMg-3-5	4.424	4.273	4.302	-	4.288	-	4.255	4.188
FeOxMg-4-5	4.153	4.03	4.06	-	4.063	-	4.041	3.952
FeOxMg-5-5	3.951	3.797	3.863	-	3.864	-	3.841	3.667*
FeOxMg-6-5	3.557	3.48	3.571	-	3.581	-	3.593	3.405*
Reference	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-5, p.72	WIPP-Solubility-20, p.56

[a] Measured with pH electrode and meter, *882 days.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	pH[a]							
Set-up ID	**(7 days)**	**(10 days)**	**(11 days)**	**(42 days)**	**(42 days)**	**(105 days)**	**(596 days)**	**(644 days)**
FeOxMg-Ratio-0	-	-	-	5.894	-	6.032	-	6.167
FeOxMg-Ratio-1	-	-	-	5.671	-	5.548	-	5.721
FeOxMg-Ratio-2	-	-	-	3.705	-	3.570	-	3.606
FeOxMg-Ratio-3	-	-	-	2.688	-	2.635	-	2.488
FeOxMg-Ratio-4	-	-	-	2.435	-	2.396	-	2.248
FeOxMg-Ratio-DI-1	5.898	-	-	-	6.202	-	7.193	-
FeOxMg-Ratio-DI-2	5.224	-	-	-	5.125	-	6.266	-
FeOxMg-Ratio-DI-3	4.886	-	-	-	4.609	-	4.633	-
FeOxMg-Ratio-DI-4	4.498	-	-	-	4.197	-	4.073	-
OS-FeOxMg-0.05-1	-	-	2.479	-	-	-	-	-
OS-FeOxMg-0.5-1	-	-	1.334*	-	-	-	-	-
OS-FeOxMg-1.0-1	-	1.033*	-	-	-	-	-	-
OS-FeOxMg-2.5-1	-	0.531*	-	-	-	-	-	-
Reference	WIPP-Solubility-9, p.37	WIPP-Solubility-7, p.53	WIPP-Solubility-7, p.53	WIPP-Solubility-9, p.32	WIPP-Solubility-9, p.37	WIPP-Solubility-9, p.32	WIPP-Solubility-20, pg. 83	WIPP-Solubility-20, pg. 83

[a] Measured with pH electrode and meter, * Outside of calibration range.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

Set-up ID	$Fe[(II)]_{diss}$, (mol/L)[a]										
	(7 days)	(13 days)	(21 days)	(34 days)	(57 days)	(171 days)	(177 days)	(288 days)	(295 days)	(541 days)	(981 days)
FeOxMg-1-1	5.03E-04	5.17E-04	5.20E-04	4.99E-04	5.17E-04	5.08E-04	-	5.10E-04	-	5.12E-04	5.37E-04
FeOxMg-2-1	1.48E-03	1.47E-03	1.47E-03	1.51E-03	1.49E-03	1.54E-03	-	1.51E-03	-	1.57E-03	1.72E-03
FeOxMg-3-1	2.76E-03	3.50E-03	3.50E-03	3.58E-03	3.68E-03	3.81E-03	-	3.98E-03	-	4.47E-03	5.14E-03
FeOxMg-4-1	2.62E-03	4.15E-03	4.78E-03	5.14E-03	5.39E-03	6.69E-03	-	7.62E-03	-	8.82E-03	9.78E-03
FeOxMg-5-1	2.68E-03	4.53E-03	5.30E-03	6.02E-03	6.67E-03	8.70E-03	-	8.65E-03	-	9.09E-03	9.28E-03
FeOxMg-6-1	2.79E-03	5.14E-03	6.26E-03	7.42E-03	8.46E-03	8.95E-03	-	8.64E-03	-	8.91E-03	9.02E-03
FeOxMg-1-2	-	-	-	-	-	-	5.18E-04	-	5.01E-04	5.12E-04	5.31E-04
FeOxMg-2-2	-	-	-	-	-	-	1.53E-03	-	1.56E-03	1.55E-03	1.70E-03
FeOxMg-3-2	-	-	-	-	-	-	3.74E-03	-	4.00E-03	4.24E-03	4.88E-03
FeOxMg-4-2	-	-	-	-	-	-	6.40E-03	-	7.51E-03	8.44E-03	9.00E-03
FeOxMg-5-2	-	-	-	-	-	-	8.41E-03	-	8.72E-03	8.79E-03	8.93E-03
FeOxMg-6-2	-	-	-	-	-	-	8.99E-03	-	9.33E-03	8.92E-03	8.98E-03
Reference	WIPP-Solubility-5, p.11	WIPP-Solubility-5, p.15	WIPP-Solubility-5, p.23	WIPP-Solubility-5, p.35	WIPP-Solubility-5, p.42	WIPP-Solubility-7, p.37	WIPP-Solubility-7, p.44	WIPP-Solubility-7, p.76		WIPP-Solubility-9, p.70	WIPP-Solubility-20, pg. 82

[a] Measured using the Ferrozine method.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	$Fe[(II)]_{diss}$, (mol/L)[a]									
Set-up ID	**(79 days)**	**(80 days)**	**(181 days)**	**(203 days)**	**(204 days)**	**(307 days)**	**(455 days)**	**(535 days)**	**(882 days)**	**(981 days)**
FeOxMg-1-3	-	-	5.09E-04	-	-	5.08E-04	-	5.07E-04	-	5.40E-04
FeOxMg-2-3	-	-	1.55E-03	-	-	1.57E-03	-	1.60E-03	-	1.73E-03
FeOxMg-3-3	-	-	4.18E-03	-	-	4.42E-03	-	4.93E-03	-	5.67E-03
FeOxMg-4-3	-	-	7.55E-03	-	-	8.49E-03	-	1.01E-02	-	1.18E-02
FeOxMg-5-3	-	-	9.15E-03	-	-	9.95E-03	-	1.00E-02	-	1.00E-02
FeOxMg-6-3	-	-	9.80E-03	-	-	9.65E-03	-	9.92E-03	-	9.91E-03
FeOxMg-1-4	5.27E-04	-	-	5.25E-04	-	-	5.23E-04	-	5.57E-04	-
FeOxMg-2-4	1.60E-03	-	-	1.61E-03	-	-	1.68E-03	-	1.83E-03	-
FeOxMg-3-4	4.63E-03	-	-	5.20E-03	-	-	6.05E-03	-	6.94E-03	-
FeOxMg-4-4	8.00E-03	-	-	1.01E-02	-	-	1.15E-02	-	1.34E-02	-
FeOxMg-5-4	1.23E-02	-	-	1.41E-02	-	-	1.76E-02	-	2.04E-02	-
FeOxMg-6-4	1.79E-02	-	-	2.24E-02	-	-	2.62E-02	-	2.96E-02	-
FeOxMg-1-5	-	5.11E-04	-	-	5.04E-04	-	5.22E-04	-	5.87E-04	-
FeOxMg-2-5	-	1.57E-03	-	-	1.58E-03	-	1.61E-03	-	1.78E-03	-
FeOxMg-3-5	-	4.54E-03	-	-	5.16E-03	-	5.85E-03	-	6.83E-03	-
FeOxMg-4-5	-	7.93E-03	-	-	9.37E-03	-	1.11E-02	-	1.29E-02	-
FeOxMg-5-5	-	1.12E-02	-	-	1.41E-02	-	1.68E-02	-	1.88E-02	-
FeOxMg-6-5	-	1.78E-02	-	-	2.23E-02	-	2.55E-02	-	2.90E-02	-
Reference	WIPP-Solubility-7, p.45	WIPP-Solubility-7, p.46	WIPP-Solubility-7, p.45	WIPP-Solubility-7, p.77	WIPP-Solubility-7, p.78	WIPP-Solubility-7, p.77	WIPP-Solubility-9, p.77	WIPP-Solubility-9, p.64	WIPP-Solubility-20, pg. 82	

[a] Measured using the Ferrozine method.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

Set-up ID	$[FeT]_{diss}$ (mol/L)[a] (882 days)	$[FeT]_{diss}$ (mol/L)[a] (981 days)
FeOxMg-1-3	-	5.28E-04
FeOxMg-2-3	-	1.81E-03
FeOxMg-3-3	-	6.56E-03
FeOxMg-4-3	-	1.35E-02
FeOxMg-5-3	-	1.14E-02
FeOxMg-6-3	-	1.16E-02
FeOxMg-1-4	5.39E-04	-
FeOxMg-2-4	1.93E-03	-
FeOxMg-3-4	7.95E-03	-
FeOxMg-4-4	1.39E-02	-
FeOxMg-5-4	2.25E-02	-
FeOxMg-6-4	3.24E-02	-
FeOxMg-1-5	5.42E-04	-
FeOxMg-2-5	1.90E-03	-
FeOxMg-3-5	7.88E-03	-
FeOxMg-4-5	1.36E-02	-
FeOxMg-5-5	2.19E-02	-
FeOxMg-6-5	3.14E-02	-
Reference	WIPP-Solubility-20, p.56	WIPP-Solubility-20, p.56

[a]Measured by ICP-AES.

Set-up ID	$[FeT]_{diss}$ (mol/L)[a] (981 days)
FeOxMg-1-1	5.36E-04
FeOxMg-2-1	1.72E-03
FeOxMg-3-1	5.92E-03
FeOxMg-4-1	1.15E-02
FeOxMg-5-1	1.08E-02
FeOxMg-6-1	1.08E-02
FeOxMg-1-2	5.29E-04
FeOxMg-2-2	1.71E-03
FeOxMg-3-2	5.76E-03
FeOxMg-4-2	1.04E-02
FeOxMg-5-2	1.03E-02
FeOxMg-6-2	1.07E-02
Reference	WIPP-Solubility-20, p.56

[a]Measured by ICP-AES.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	$[Cl(-I)]_{diss}$, (mol/L)[a]		$[Mg(II)]_{diss}$, (mol/L)[b]		
Set-up ID	**(535 days)**	**(541 days)**	**(535 days)**	**(541 days)**	**(981 days)**
FeOxMg-1-1	-	2.19E-02	-	1.02E-02	1.03E-02
FeOxMg-2-1	-	1.98E-01	-	9.99E-02	1.00E-01
FeOxMg-3-1	-	8.94E-01	-	5.03E-01	4.52E-01
FeOxMg-4-1	-	1.74E+00	-	9.56E-01	8.82E-01
FeOxMg-5-1	-	2.42E+00	-	1.30E+00	1.28E+00
FeOxMg-6-1	-	3.55E+00	-	1.77E+00	1.86E+00
FeOxMg-1-2	-	2.12E-02	-	1.01E-02	1.02E-02
FeOxMg-2-2	-	2.13E-01	-	1.00E-01	9.84E-02
FeOxMg-3-2	-	8.84E-01	-	4.98E-01	4.64E-01
FeOxMg-4-2	-	1.72E+00	-	9.39E-01	8.79E-01
FeOxMg-5-2	-	2.46E+00	-	1.30E+00	1.25E+00
FeOxMg-6-2	-	3.70E+00	-	1.76E+00	1.83E+00
FeOxMg-1-3	1.83E-02	-	1.26E-02	-	1.03E-02
FeOxMg-2-3	1.89E-01	-	1.29E-01	-	1.03E-01
FeOxMg-3-3	8.77E-01	-	5.45E-01	-	4.72E-01
FeOxMg-4-3	1.69E+00	-	1.06E+00	-	8.68E-01
FeOxMg-5-3	2.42E+00	-	1.38E+00	-	1.29E+00
FeOxMg-6-3	3.46E+00	-	1.87E+00	-	1.86E+00
Reference	WIPP-Solubility-9, p.66	WIPP-Solubility-9, p.98	WIPP-Solubility-9, p.65	WIPP-Solubility-9, p.71	WIPP-Solubility-20, p.56

[a] Measured by IC; [b] Measured by ICP-AES.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

Set-up ID	$[Mg(II)]_{diss}$, (mol/L)[b] (455 days)	$[Mg(II)]_{diss}$, (mol/L)[b] (882 days)
FeOxMg-1-4	9.94E-03	9.57E-03
FeOxMg-2-4	1.01E-01	9.76E-02
FeOxMg-3-4	4.56E-01	4.44E-01
FeOxMg-4-4	9.00E-01	8.41E-01
FeOxMg-5-4	1.28E+00	1.22E+00
FeOxMg-6-4	1.86E+00	1.75E+00
FeOxMg-1-5	1.02E-02	9.50E-03
FeOxMg-2-5	1.03E-01	9.70E-02
FeOxMg-3-5	4.52E-01	4.51E-01
FeOxMg-4-5	8.88E-01	8.60E-01
FeOxMg-5-5	1.28E+00	1.23E+00
FeOxMg-6-5	1.83E+00	1.75E+00
Reference	WIPP-Solubility-15, p.67	WIPP-Solubility-20, p.56

[a] Measured by IC; [b] Measured by ICP-AES.

Table 3-16 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in $MgCl_2$ solutions (the "FeOx(aq)—Mg^{2+}" experiment).

	$[Fe(II)]_{diss}$, (mol/L)[a]		$[FeT]_{diss}$ (mol/L)[b]
Set-up ID	**(80 days)**	**(597 days)**	**(597 days)**
FeOxMg-Ratio-DI-1	1.82E-04	2.11E-04	2.01E-04
FeOxMg-Ratio-DI-2	1.86E-04	2.13E-04	2.01E-04
FeOxMg-Ratio-DI-3	2.09E-04	2.36E-04	2.27E-04
FeOxMg-Ratio-DI-4	3.30E-04	4.16E-04	4.67E-04
Reference	WIPP-Solubility-9, p.59	WIPP-Solubility-20, pg. 81	WIPP-Solubility-20, p.83

[a] Measured using the Ferrozine method, [b]Measured by ICP-AES.

	$[Cl(-I)]_{diss}$, (mol/L)[a]	$[Mg(II)]_{diss}$, (mol/L)[b]		$[Fe(II)]_{diss}$, (mol/L)[c]		$[FeT]_{diss}$ (mol/L)[d]
Set-up ID	**(103 days)**	**(103 days)**	**(645 days)**	**(103 days)**	**(645 days)**	**(645 days)**
FeOxMg-Ratio-0	4.53E+00	2.24E+00	2.30E+00	1.02E-05	2.04E-05	0.00E+00
FeOxMg-Ratio-1	4.47E+00	2.29E+00	2.28E+00	1.09E-02	1.11E-02	1.09E-02
FeOxMg-Ratio-2	4.28E+00	2.23E+00	2.25E+00	3.20E-02	4.84E-02	4.70E-02
FeOxMg-Ratio-3	4.47E+00	2.22E+00	2.25E+00	4.69E-02	6.49E-02	6.24E-02
FeOxMg-Ratio-4	4.45E+00	2.17E+00	2.20E+00	5.34E-02	7.27E-02	6.91E-02
Reference	WIPP-Solubility-9, p.99	WIPP-Solubility-9, p.67	WIPP-Solubility-20, pg. 83	WIPP-Solubility-9, p.60	WIPP-Solubility-20, pg. 81	WIPP-Solubility-20, p.83

[a] Measured by IC; [b] Measured by ICP-AES, [c]Measured using the Ferrozine Method, [d]Measured using the ICP-AES.

3.9 Solubility of $FeC_2O_4 \cdot 2H_2O$(s) in NaCl solutions; Solubility of $FeC_2O_4 \cdot 2H_2O$(s) in $MgCl_2$ solutions (the "FeOx(aq)—Cl^-" experiment)

The objective of this section is to determine the Pitzer ion-interaction parameters for the ion pair "FeOx(aq)-Cl^-" (Item 9, Table 1-1). The experimental results from sections 3.7 and 3.8 will be combined to determine the parameters for the ion pair "FeOx(aq)-Cl^-". Refer to sections 3.7 and 3.8 for the data.

3.10 Solubility of $Fe(OH)_2$(s) in mixed $Na_2C_{10}H_{14}O_8N_2 \cdot 2H_2O$ ($Na_2H_2EDTA \cdot 2H_2O$) and NaCl solutions (the "Na^+—$FeEDTA^{2-}$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Fe(OH)_2$(s) (ferrous iron hydroxide) in $Na_2H_2EDTA \cdot 2H_2O$ (disodium dihydrogen EDTA dihydrate) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair "Na^+—$FeEDTA^{2-}$" (Item 10, Table 1-1).

The experimental set-ups are listed in Table 3-17. Solid was synthesized by mixing 13.353 g NaOH (Fisher) and 33.1869 g $FeCl_2 \cdot 4H_2O$ (Fisher). The experimental set-ups have been periodically monitored for pH and dissolved total Fe concentrations ($[Fe_T]_{diss}$). Once stable pH readings are achieved, concentrations of other dissolved components (sodium, EDTA, and chloride) are to be determined. Experimental results gathered to date are shown in Table 3-18.

Table 3-17 Preparation of experimental set-ups for the solubility of $Fe(OH)_2(s)$ in Na_2H_2EDTA solutions (the "Na^+—$FeEDTA^{2-}$" experiment).

Set-up ID	$Fe(OH)_2(s)$ (g)	NaCl (m)	Reference
$Fe(OH)_2$-Na_4EDTA-0.01A	0.9	0.01	WIPP-Solubility-1, pg. 51-55
$Fe(OH)_2$-Na_4EDTA-0.1A	0.9	0.1	
$Fe(OH)_2$-Na_4EDTA-1A	0.9	1	
$Fe(OH)_2$-Na_4EDTA-2A	0.9	2	
$Fe(OH)_2$-Na_4EDTA-3A	0.9	3	
$Fe(OH)_2$-Na_4EDTA-4A	0.9	4	
$Fe(OH)_2$-Na_4EDTA-5A	0.9	5	
$Fe(OH)_2$-Na_4EDTA-0.01B	0.9	0.01	
$Fe(OH)_2$-Na_4EDTA-0.1B	0.9	0.1	
$Fe(OH)_2$-Na_4EDTA-1B	0.9	1	
$Fe(OH)_2$-Na_4EDTA-2B	0.9	2	
$Fe(OH)_2$-Na_4EDTA-3B	0.9	3	
$Fe(OH)_2$-Na_4EDTA-4B	0.9	4	
$Fe(OH)_2$-Na_4EDTA-5B	0.9	5	

Table 3-18 Measured data for the solubility of $Fe(OH)_2(s)$ in Na_2H_2EDTA solutions (the "Na^+—$FeEDTA^{2-}$" experiment).

Set-up ID	pH[a] (464 days)	pH[a] (1000 days)	pH[a] (1001 days)
$Fe(OH)_2$-Na_4EDTA-0.01A	7.820	7.820	-
$Fe(OH)_2$-Na_4EDTA-0.1A	7.986	7.948	-
$Fe(OH)_2$-Na_4EDTA-1A	8.343	8.265	-
$Fe(OH)_2$-Na_4EDTA-2A	8.655	8.593	-
$Fe(OH)_2$-Na_4EDTA-3A	8.836	-	8.729
$Fe(OH)_2$-Na_4EDTA-4A	8.817	-	8.766
$Fe(OH)_2$-Na_4EDTA-5A	8.998	-	8.930
$Fe(OH)_2$-Na_4EDTA-0.01B	-	7.847	-
$Fe(OH)_2$-Na_4EDTA-0.1B	7.953	7.921	-
$Fe(OH)_2$-Na_4EDTA-1B	8.370	8.341	-
$Fe(OH)_2$-Na_4EDTA-2B	8.503	8.481	-
$Fe(OH)_2$-Na_4EDTA-3B	8.772	-	8.730
$Fe(OH)_2$-Na_4EDTA-4B	8.904	-	8.849
$Fe(OH)_2$-Na_4EDTA-5B	9.001	-	8.928
Reference	WIPP-Solubility-8, p.59, 61	WIPP-Solubility-15, p.97	WIPP-Solubility-15, p.97

[a] Measured with pH electrode and meter

Table 3-18 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in Na_2H_2EDTA solutions (the "Na^+—$FeEDTA^{2-}$" experiment).

	$[Fe_T]$ (mol/L)[a]		
Set-up ID	**(58 days)**	**(519 days)**	**(1001 days)**
$Fe(OH)_2$-Na_4EDTA-0.01A	4.71E-02	5.43E-02	5.31E-02
$Fe(OH)_2$-Na_4EDTA-0.1A	4.28E-02	5.13E-02	4.73E-02
$Fe(OH)_2$-Na_4EDTA-1A	3.82E-02	4.45E-02	3.81E-02
$Fe(OH)_2$-Na_4EDTA-2A	3.75E-02	4.70E-02	3.76E-02
$Fe(OH)_2$-Na_4EDTA-3A	3.62E-02	4.84E-02	3.69E-02
$Fe(OH)_2$-Na_4EDTA-4A	3.69E-02	4.79E-02	3.31E-02
$Fe(OH)_2$-Na_4EDTA-5A	3.66E-02	4.84E-02	3.40E-02*
$Fe(OH)_2$-Na_4EDTA-0.01B	-	-	5.01E-02
$Fe(OH)_2$-Na_4EDTA-0.1B	-	5.15E-02	4.83E-02
$Fe(OH)_2$-Na_4EDTA-1B	-	4.47E-02	3.90E-02
$Fe(OH)_2$-Na_4EDTA-2B	-	4.63E-02	3.74E-02
$Fe(OH)_2$-Na_4EDTA-3B	-	4.80E-02	3.64E-02
$Fe(OH)_2$-Na_4EDTA-4B	-	4.77E-02	3.48E-02
$Fe(OH)_2$-Na_4EDTA-5B	-	4.90E-02	3.33E-02
Reference	WIPP-Solubility-4, p.26-31	WIPP-Solubility-8, p.92-95, WIPP-Solubility-10 p. 9	WIPP-Solubility-20, p.26

[a]Measured by ICP-AES, *1002 days.

Table 3-18 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in Na_2H_2EDTA solutions (the "Na^+—$FeEDTA^{2-}$" experiment).

Set-up ID	$[Fe(II)]_{diss}$, (mol/L)[a] (1001 days)	$[EDTA^{-4}]$, (mol/L)[b] (1001 days)	$[Na(I)]_{diss}$, (mol/L)[c] (1001 days)
$Fe(OH)_2$-Na_4EDTA-0.01A	2.88E-02	4.09E-02	9.48E-02
$Fe(OH)_2$-Na_4EDTA-0.1A	2.48E-02	3.92E-02	1.59E-01
$Fe(OH)_2$-Na_4EDTA-1A	2.01E-02	4.04E-02	8.09E-01
$Fe(OH)_2$-Na_4EDTA-2A	1.96E-02	4.02E-02	1.58E+00
$Fe(OH)_2$-Na_4EDTA-3A	1.98E-02	4.12E-02	2.37E+00
$Fe(OH)_2$-Na_4EDTA-4A	1.93E-02	3.96E-02	2.78E+00
$Fe(OH)_2$-Na_4EDTA-5A	1.98E-02*	4.02E-02*	3.40E+00*
$Fe(OH)_2$-Na_4EDTA-0.01B	2.69E-02	3.97E-02	9.31E-02
$Fe(OH)_2$-Na_4EDTA-0.1B	2.42E-02	3.98E-02	1.62E-01
$Fe(OH)_2$-Na_4EDTA-1B	1.92E-02	3.93E-02	8.26E-01
$Fe(OH)_2$-Na_4EDTA-2B	1.94E-02	3.95E-02	1.61E+00
$Fe(OH)_2$-Na_4EDTA-3B	1.97E-02	3.99E-02	2.23E+00
$Fe(OH)_2$-Na_4EDTA-4B	1.96E-02	3.96E-02	3.01E+00
$Fe(OH)_2$-Na_4EDTA-5B	1.93E-02	4.03E-02	3.25E+00
Reference	WIPP-Solubility-15, p.99	WIPP-Solubility-20, p.50	WIPP-Solubility-20, p.26

[a] Measured using the Ferrozine method, [b]Measured using the Total Carbon Coulometer, [c]Measured using ICP-AES, *1002 days.

3.11 Solubility of $Fe(OH)_2(s)$ in $C_{10}H_{12}MgN_2Na_2O_8 \cdot 4H_2O$ ($MgNa_2EDTA \cdot 4H_2O$) solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

The objectives of this set of experiments are to (1) determine the solubility of $Fe(OH)_2(s)$ (ferrous iron hydroxide) in $MgNa_2EDTA \cdot 4H_2O$ (magnesium disodium EDTA tetrahydrate) solutions, and (2) determine the Pitzer ion-interaction parameters for ion pair "Mg^{2+}—$FeEDTA^{2-}$" (Item 11, Table 1-1).

Ferrous iron hydroxide, $Fe(OH)_2(s)$, was synthesized; 0.256 mol of $FeCl_2 \cdot 4H_2O$ (Fisher) was dissolved and mixed with 98 mL of 5.211 M NaOH (Fisher) (WIPP-Solubility-5, page 52). XRD is given in WIPP-Solubility-5, page 77. $Fe(OH)_2(s)$ was added to magnesium disodium EDTA (J.T. Baker) solutions of incremental concentrations, ranging from 0.0107 to 0.769 m magnesium disodium EDTA (See Table 3-19). Since solubility is independent of the solid mass and experimental set-up volume as long as solid remains upon equilibration, the mass of $Fe(OH)_2(s)$ and the volume of $MgNa_2EDTA$ solutions were not determined for all experimental set-ups. The experimental set-ups were periodically monitored for pH. Once stable pH readings were observed, the concentrations of other dissolved components (dissolved total Fe, magnesium, sodium, and EDTA) were or are to be determined. Experimental results gathered to date are shown in Table 3-20.

Table 3-19 Preparation of experimental set-ups for the solubility of $Fe(OH)_2(s)$* in $MgNa_2EDTA \cdot 4H_2O$ solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

Set-up ID	$MgNa_2EDTA$ (m)	$FeCl_2 \cdot 4H_20$ (g)	NaOH (g)	MgNa2EDTA·4H2O (g)	Volume of H_2O (mL)	Reference
$FeMgNa_2EDTA$-1-(1,2,3)	0.0107	-	-	-	-	WIPP-Solubility-7, p.41
$FeMgNa_2EDTA$-2-(1,2,3)	0.108	-	-	-	-	
$FeMgNa_2EDTA$-3-(1,2,3)	0.216	-	-	-	-	
$FeMgNa_2EDTA$-4-(1,2,3)	0.396	-	-	-	-	
$FeMgNa_2EDTA$-5-(1,2,3)	0.597	-	-	-	-	
$FeMgNa_2EDTA$-6-(1,2,3)	0.769	-	-	-	-	
OS-$FeMgNa_2EDTA$-2-1	-	4.2059	1.6360	0.2556	48.4	WIPP-Solubility-9, p.57
OS-$FeMgNa_2EDTA$-3-1	-	4.0987	1.6514	2.1287	47.3	
OS-$FeMgNa_2EDTA$-4-1	-	4.0553	1.6574	4.4052	45.8	
OS-$FeMgNa_2EDTA$-5-1	-	4.0007	1.6027	11.3196	46.4	WIPP-Solubility-9, p.56
OS-$FeMgNa_2EDTA$-6-1	-	4.5155	1.6799	17.8048	46.2	WIPP-Solubility-9, p.53

* Mass of solid not determined. See second paragraph above for reason.

Table 3-20 Measured data for the solubility of $Fe(OH)_2(s)$ in $MgNa_2EDTA \cdot 4H_2O$ solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

	pH*								
Set-up ID	**(1 day)**	**(32 days)**	**(35 days)**	**(93 days)**	**(94 days)**	**(206 days)**	**(212 days)**	**(830 days)**	**(833 days)**
$FeMgNa_2EDTA$-1-1	10.597	10.528	-	10.381	-	10.359	-	10.193	-
$FeMgNa_2EDTA$-1-2	10.583	10.549	-	10.397	-	10.382	-	10.184	-
$FeMgNa_2EDTA$-1-3	10.593	10.546	-	10.407	-	10.388	-	10.152	-
$FeMgNa_2EDTA$-2-1	10.705	10.613	-	10.516	-	10.472	-	10.331	-
$FeMgNa_2EDTA$-2-2	10.705	10.647	-	10.539	-	10.491	-	10.333	-
$FeMgNa_2EDTA$-2-3	10.717	10.635	-	10.527	-	10.473	-	10.294	-
$FeMgNa_2EDTA$-3-1	10.680	-	10.676	10.527	-	-	10.507	10.348	-
$FeMgNa_2EDTA$-3-2	10.719	-	10.688	10.534	-	-	10.510	-	10.430
$FeMgNa_2EDTA$-3-3	10.705	-	10.699	10.539	-	-	10.533	-	10.418
$FeMgNa_2EDTA$-4-1	10.673	-	10.685	10.530	-	-	10.524	-	10.396
$FeMgNa_2EDTA$-4-2	10.649	-	10.701	10.550	-	-	10.545	-	10.404
$FeMgNa_2EDTA$-4-3	10.603	-	10.694	10.539	-	-	10.529	-	10.368
$FeMgNa_2EDTA$-5-1	10.640	-	10.715	-	10.552	-	10.560	-	10.524
$FeMgNa_2EDTA$-5-2	10.513	-	10.708	-	10.551	-	10.553	-	10.521
$FeMgNa_2EDTA$-5-3	10.544	-	10.702	-	10.549	-	10.540	-	10.500
$FeMgNa_2EDTA$-6-1	10.362	-	10.678	-	10.565	-	10.562	-	10.519
$FeMgNa_2EDTA$-6-2	10.495	-	10.708	-	10.560	-	10.555	-	10.438[a]
$FeMgNa_2EDTA$-6-3	10.397	-	10.702	-	10.567	-	10.564	-	10.419[a]
Reference	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-7, p.42	WIPP-Solubility-20, pg. 84	WIPP-Solubility-20, pg. 84

* Measured with pH electrode and meter, [a]834 days.

Table 3-20 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in $MgNa_2EDTA{\cdot}4H_2O$ solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

	$[Fe_T]_{diss}$ (mol/L)*			$[Mg(II)]_{diss}$ (mol/L)*			$[Na(I)]_{diss}$ (mol/L)*		
Set-up ID	**(237 days)**	**(295 days)**	**(842 days)**	**(237 days)**	**(295 days)**	**(842 days)**	**(237 days)**	**(295 days)**	**(842 days)**
$FeMgNa_2EDTA$-1-1	-	1.08E-02	1.02E-02	-	1.51E-04	6.21E-04	-	1.79E-02	2.15E-02
$FeMgNa_2EDTA$-1-2	-	1.07E-02	1.03E-02	-	1.39E-04	6.00E-04	-	1.74E-02	2.16E-02
$FeMgNa_2EDTA$-1-3	-	1.08E-02	1.03E-02	-	1.12E-04	5.89E-04	-	1.66E-02	2.12E-02
$FeMgNa_2EDTA$-2-1	-	7.61E-02	7.49E-02	-	5.90E-02	3.30E-02	-	1.80E-01	2.17E-01
$FeMgNa_2EDTA$-2-2	-	6.01E-02	5.81E-02	-	8.72E-02	4.87E-02	-	1.82E-01	2.11E-01
$FeMgNa_2EDTA$-2-3	-	7.49E-02	7.08E-02	-	6.62E-02	3.64E-02	-	1.80E-01	2.13E-01
$FeMgNa_2EDTA$-3-1	8.36E-02	-	7.02E-02	2.63E-01	-	1.36E-01	4.52E-01	-	4.11E-01
$FeMgNa_2EDTA$-3-2	7.90E-02	-	6.90E-02	2.55E-01	-	1.38E-01	4.23E-01	-	4.11E-01
$FeMgNa_2EDTA$-3-3	6.65E-02	-	5.54E-02	2.85E-01	-	1.52E-01	4.43E-01	-	4.11E-01
$FeMgNa_2EDTA$-4-1	9.98E-02	-	8.10E-02	4.86E-01	-	2.88E-01	8.72E-01	-	7.31E-01
$FeMgNa_2EDTA$-4-2	7.60E-02	-	6.30E-02	5.08E-01	-	3.14E-01	8.01E-01	-	7.33E-01
$FeMgNa_2EDTA$-4-3	8.67E-02	-	7.19E-02	5.02E-01	-	3.04E-01	8.20E-01	-	7.46E-01
$FeMgNa_2EDTA$-5-1	-	6.30E-02	6.16E-02	-	7.90E-01	4.94E-01	-	1.03E+00	1.09E+00
$FeMgNa_2EDTA$-5-2	-	6.47E-02	6.35E-02	-	7.78E-01	4.90E-01	-	9.99E-01	1.08E+00
$FeMgNa_2EDTA$-5-3	-	7.72E-02	7.39E-02	-	7.70E-01	4.64E-01	-	1.02E+00	1.05E+00
$FeMgNa_2EDTA$-6-1	-	6.92E-02	6.50E-02	-	9.79E-01	6.19E-01	-	1.32E+00	1.36E+00
$FeMgNa_2EDTA$-6-2	-	7.27E-02	6.78E-02	-	9.79E-01	6.11E-01	-	1.33E+00	1.36E+00
$FeMgNa_2EDTA$-6-3	-	6.32E-02	6.05E-02	-	9.71E-01	6.18E-01	-	1.27E+00	1.35E+00
Reference	WIPP-Solubility-9, pg.34	WIPP-Solubility-9, p.41-43	WIPP-Solubility-20, pg. 84	WIPP-Solubility-9, p.40	WIPP-Solubility-9, p.41-43	WIPP-Solubility-20, pg. 84	WIPP-Solubility-9, p.45	WIPP-Solubility-9, p.52	WIPP-Solubility-20, pg. 84

*Measured using the ICP-AES.

Table 3-20 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in $MgNa_2EDTA{\cdot}4H_2O$ solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

Set-up ID	[EDTA^{-4}], mol/L[a]		
	(247 days)	(295 days)	(842 days)
$FeMgNa_2EDTA$-1-1	-	9.95E-03	9.55E-03
$FeMgNa_2EDTA$-1-2	-	9.63E-03	9.67E-03
$FeMgNa_2EDTA$-1-3	-	9.87E-03	9.90E-03
$FeMgNa_2EDTA$-2-1	-	9.95E-02	1.01E-01
$FeMgNa_2EDTA$-2-2	-	9.71E-02	9.63E-02
$FeMgNa_2EDTA$-2-3	-	9.72E-02	1.04E-01
$FeMgNa_2EDTA$-3-1	3.11E-01	-	2.07E-01
$FeMgNa_2EDTA$-3-2	3.98E-01	-	2.02E-01
$FeMgNa_2EDTA$-3-3	3.54E-01	-	2.00E-01
$FeMgNa_2EDTA$-4-1	5.89E-01	-	3.62E-01
$FeMgNa_2EDTA$-4-2	5.49E-01	-	3.63E-01
$FeMgNa_2EDTA$-4-3	5.62E-01	-	3.29E-01
$FeMgNa_2EDTA$-5-1	-	5.74E-01	5.33E-01
$FeMgNa_2EDTA$-5-2	-	5.66E-01	4.91E-01
$FeMgNa_2EDTA$-5-3	-	5.67E-01	5.21E-01
$FeMgNa_2EDTA$-6-1	-	7.09E-01	6.82E-01
$FeMgNa_2EDTA$-6-2	-	7.03E-01	6.94E-01
$FeMgNa_2EDTA$-6-3	-	7.04E-01	7.07E-01
Reference	WIPP-Solubility-20, pg.49	WIPP-Solubility-20, pg.49	WIPP-Solubility-20, pg.84

[a]Measured using the Total Carbon Coulometer.

Table 3-20 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in $MgNa_2EDTA{\cdot}4H_2O$ solutions (the "Mg^{2+}—$FeEDTA^{2-}$" experiment).

Set-up ID	pH[a] (463 day)	[FeT]diss (mol/L)[b1] (468 day)	[Mg(II)]diss (mol/L)[b1] (468 day)	[Na(I)]diss (mol/L)[b1] (468 day)	[EDTA-4], (mol/L)[c1] (468 day)
OS-FeMgNa_2EDTA-2-1	8.259	1.19E-02	1.12E-02	8.13E-01	1.11E-02
OS-FeMgNa_2EDTA-3-1	9.358	9.96E-02	1.86E-02	9.96E-01	9.46E-02
OS-FeMgNa_2EDTA-4-1	9.492[a1]	2.07E-01	1.64E-02	1.22E+00	2.10E-01
OS-FeMgNa_2EDTA-5-1	9.782[b]	3.83E-01[d]	6.88E-02[d]	1.61E+00[d]	4.29E-01[d]
OS-FeMgNa_2EDTA-6-1	9.654[c]	4.06E-01[e]	3.53E-01[e]	2.22E+00[e]	7.21E-01[e]
Reference	WIPP-Solubility-20, pg. 65	WIPP-Solubility-20, pg. 85	WIPP-Solubility-20, pg. 85	WIPP-Solubility-20, pg. 85	WIPP-Solubility-20, pg. 85

[a] Measured with pH electrode and meter, [a1]464days, [b]469 days, [c]470 days.

[b1]Measured using the ICP-AES, [d] 473 days, [e] 474 days, [c1]Measured using the Total Carbon Coulometer.

3.12 Solubility of $Fe(OH)_2(s)$ in $Na_3C_6H_5O_7 \cdot 2H_2O$ ($Na_3Citrate \cdot 2H_2O$) solutions (the "Na^+—$FeCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Fe(OH)_2(s)$ (ferrous iron hydroxide) in $Na_3Citrate \cdot 2H_2O$ (trisodium citrate dihydrate) solutions, and (2) determine the Pitzer ion-interaction parameters for ion pair, "Na^+—$FeCit^-$(aq)" (Item 12, Table 1-1).

Ferrous iron hydroxide, $Fe(OH)_2(s)$, was synthesized; 0.256 mol of $FeCl_2 \cdot 4H_2O$ (Fisher) was dissolved and mixed with 98 mL of 5.2 M NaOH (Fisher) (WIPP-Solubility-5, page 52). XRD is given in WIPP-Solubility-5, page 77. $Fe(OH)_2(s)$ was added to trisodium citrate dihydrate (Fisher) solutions of incremental concentrations, ranging from 0.01 to 1.87 m of trisodium citrate (Table 3-21). Since solubility is independent of the solid mass and experimental set-up volume as long as solid remains upon equilibration, the mass of $Fe(OH)_2(s)$ and the volume of trisodium citrate solutions were not determined for all experimental set-ups.

The experimental set-ups were periodically monitored for pH and dissolved ferrous iron concentration. Once stable readings of pH and dissolved ferrous iron concentrations are achieved, the concentrations of other dissolved components (sodium, citrate) were to be measured. Experimental results gathered to date are shown in Table 3-22.

Table 3-21 Preparation of experimental set-ups for the solubility of $Fe(OH)_2(s)$* in $Na_3C_6H_5O_7 \cdot 2H_2O$ solutions (the "Na^+—$FeCit^-$" experiment).

Set-up ID	$Na_3C_6H_5O_7$ (m)	Reference
FeCitNa-1-(1,2,3)	0.01	WIPP-Solubility-5, p.60-61
FeCitNa-2-(1,2,3)	0.0991	
FeCitNa-3-(1,2,3)	0.493	
FeCitNa-4-(1,2,3)	0.968	
FeCitNa-5-(1,2,3)	1.43	
FeCitNa-6-(1,2,3)	1.87	

* Mass of solid not determined. See second paragraph above for reason.

Table 3-22 Measured data for the solubility of $Fe(OH)_2(s)$ in $Na_3C_6H_5O_7 \cdot 2H_2O$ solutions (the "Na^+—$FeCit^-$" experiment).

Set-up ID	pH*							
	(1 day)	(8 days)	(26 days)	(68 days)	(97 days)	(223 days)	(936 days)	(938 days)
FeCitNa-1-1	10.300	10.505	10.519	10.561	10.544	10.564	10.459	-
FeCitNa-1-2	10.327	10.512	10.519	10.552	10.540	10.553	10.468	-
FeCitNa-1-3	10.273	10.509	10.516	10.552	10.553	10.562	10.494	-
FeCitNa-2-1	10.774	11.213	11.401	11.442	11.451	11.461	11.406	-
FeCitNa-2-2	10.566	11.119	11.346	11.409	11.421	11.444	11.432	-
FeCitNa-2-3	10.829	11.247	11.401	11.451	11.455	11.461	11.434	-
FeCitNa-3-1	10.694	11.394	11.648	11.762	11.801[a]	11.892[c]	-	11.792
FeCitNa-3-2	10.799	11.432	11.674	11.783	11.819[a]	11.892[c]	-	11.746
FeCitNa-3-3	10.873	11.506	11.755	11.858	11.886[a]	11.940[c]	-	11.760
FeCitNa-4-1	10.669	11.532	11.838	11.961	12.011[a]	12.121[c]	-	11.902
FeCitNa-4-2	9.474	11.345	11.667	11.796	11.842[a]	11.950[c]	-	11.694
FeCitNa-4-3	10.879	11.610	11.888	12.023	12.065[a]	12.151[c]	-	11.852
FeCitNa-5-1	9.176	11.438	11.869	11.985	12.004[b]	12.156[d]	-	11.795
FeCitNa-5-2	10.497	11.660	12.006	12.128	12.153[b]	12.286[d]	-	11.885
FeCitNa-5-3	8.833	11.477	11.847	11.983	12.027[b]	12.168[d]	-	11.815
FeCitNa-6-1	8.938	11.615	12.004	12.136	12.163[b]	12.319[d]	-	11.922
FeCitNa-6-2	8.658	11.622	11.993	12.143	12.169[b]	12.354[d]	-	11.845
FeCitNa-6-3	8.859	11.691	12.046	12.194	12.220[b]	12.373[d]	-	11.885
Reference	WIPP-Solubility-5, p.61	WIPP-Solubility-5, p.67	WIPP-Solubility-5, p.67	WIPP-Solubility-5, p.67	WIPP-Solubility-5, p.67	WIPP-Solubility-5, p.67	WIPP-Solubility-20 pg. 79	WIPP-Solubility-20 pg. 79

* Measured with pH electrode and meter; [a] 104 days; [b] 105 days; [c] 230 days; [d] 236 days.

Table 3-22 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in $Na_3C_6H_5O_7 \cdot 2H_2O$ solutions (the "Na^+—$FeCit^-$" experiment).

Set-up ID	$[Fe(II)]_{diss}$, (mol/L)[a]						
	(97 day)	(104 days)	(105 days)	(223 days)	(231 days)	(237 days)	(939 days)
FeCitNa-1-1	6.25E-04	-	-	6.58E-04	-	-	8.08E-04
FeCitNa-1-2	6.97E-04	-	-	7.33E-04	-	-	8.92E-04
FeCitNa-1-3	5.94E-04	-	-	6.13E-04	-	-	7.34E-04
FeCitNa-2-1	4.26E-03	-	-	4.36E-03	-	-	4.51E-03
FeCitNa-2-2	3.99E-03	-	-	4.15E-03	-	-	4.33E-03
FeCitNa-2-3	4.27E-03	-	-	4.39E-03	-	-	4.49E-03
FeCitNa-3-1	-	1.06E-02	-	-	1.22E-02	-	1.39E-02
FeCitNa-3-2	-	1.08E-02	-	-	1.24E-02	-	1.38E-02
FeCitNa-3-3	-	1.24E-02	-	-	1.37E-02	-	1.48E-02
FeCitNa-4-1	-	1.53E-02	-	-	1.80E-02	-	2.08E-02
FeCitNa-4-2	-	1.07E-02	-	-	1.25E-02	-	1.43E-02
FeCitNa-4-3	-	1.71E-02	-	-	1.94E-02	-	2.18E-02
FeCitNa-5-1	-	-	1.45E-02	-	-	1.69E-02	2.01E-02
FeCitNa-5-2	-	-	1.92E-02	-	-	2.29E-02	2.61E-02
FeCitNa-5-3	-	-	1.45E-02	-	-	1.76E-02	2.09E-02
FeCitNa-6-1	-	-	1.72E-02	-	-	2.01E-02	2.26E-02
FeCitNa-6-2	-	-	1.91E-02	-	-	2.04E-02	2.41E-02
FeCitNa-6-3	-	-	2.08E-02	-	-	2.19E-02	2.67E-02
Reference	WIPP-Solubility-7, p.51	WIPP-Solubility-7, p.54	WIPP-Solubility-7, p.55	WIPP-Solubility-7, p.79	WIPP-Solubility-7, p.79	WIPP-Solubility-7, p.80	WIPP-Solubility-20, pg. 80

[a]Measured using the Ferrozine method.

Table 3-22 (continued) Measured data for the solubility of $Fe(OH)_2(s)$ in $Na_3C_6H_5O_7 \cdot 2H_2O$ solutions (the "Na^+—$FeCit^-$" experiment).

	$[Citrate^{-3}]_{T,\,diss}$, (mol/L)[a]		$[Fe_T]$, (mol/L)[b]	$[Na(I)]_{diss}$, (mol/L)[b]
Set-up ID	**(611 day)**	**(939 day)**	**(939 day)**	**(939 day)**
FeCitNa-1-1	1.09E-02	1.00E-02	7.86E-04	3.07E-02
FeCitNa-1-2	1.07E-02	9.98E-03	8.91E-04	3.09E-02
FeCitNa-1-3	1.07E-02	1.01E-02	7.35E-04	3.10E-02
FeCitNa-2-1	1.09E-01	9.78E-02	4.39E-03	3.01E-01
FeCitNa-2-2	1.07E-01	1.01E-01	4.25E-03	2.98E-01
FeCitNa-2-3	1.08E-01	9.97E-02	4.35E-03	2.95E-01
FeCitNa-3-1	5.14E-01	4.81E-01	1.36E-02	1.39E+00
FeCitNa-3-2	5.21E-01	4.83E-01	1.37E-02	1.42E+00
FeCitNa-3-3	5.15E-01	4.82E-01	1.45E-02	1.41E+00
FeCitNa-4-1	9.75E-01	9.11E-01	2.07E-02	2.69E+00
FeCitNa-4-2	9.58E-01	9.21E-01	1.43E-02	2.80E+00
FeCitNa-4-3	9.78E-01	9.07E-01	2.17E-02	2.74E+00
FeCitNa-5-1	1.39E+00	1.30E+00	1.98E-02	3.81E+00
FeCitNa-5-2	1.37E+00	1.29E+00	2.57E-02	3.78E+00
FeCitNa-5-3	1.39E+00	1.30E+00	2.08E-02	3.82E+00
FeCitNa-6-1	1.74E+00	1.62E+00	2.22E-02	4.83E+00
FeCitNa-6-2	1.74E+00	1.65E+00	2.38E-02	4.77E+00
FeCitNa-6-3	1.74E+00	1.61E+00	2.62E-02	4.80E+00
Reference	WIPP-Solubility-15, p.29	WIPP-Solubility-20, pg. 79	WIPP-Solubility-20, pg. 79	WIPP-Solubility-20, pg. 79

[a]Measured using the IC, [b]Measured using the ICP-AES.

3.13 Solubility of $Fe(OH)_2(s)$ in mixed $C_6H_6MgO_7 \cdot xH_2O$ (MgHCitrate·xH_2O) and NaCl solutions (the "Mg^{2+}—$FeCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Fe(OH)_2(s)$ (ferrous iron hydroxide) in mixed MgHCitrate·xH_2O (magnesium hydrogen citrate hydrate) and NaCl (sodium chloride) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Mg^{2+}—$FeCit^-$" (Item 13, Table 1-1).

The experimental set-ups are listed in Table 3-23, and they have been periodically monitored for one or more component(s) among those listed in Table 3-24. Once stable readings are achieved for the selected component(s), concentrations of other components are to be determined.

Table 3-23 Preparation of experimental set-ups for the solubility of $Fe(OH)_2(s)$ in mixed MgHCitrate and NaCl solutions (the "Mg^{2+}—$FeCit^-$" experiment).

Set-up ID	42 mL NaCl (m)	2M $Fe(OH)_2$ (mL)*	1.03M MgCitrate (mL)	Reference
MgFeCit-1-1	0.1	3	5	WIPP-Solubility-15 p. 82-83, 91
MgFeCit-1-2	0.1	3	5	
MgFeCit-1-3	0.1	3	5	
MgFeCit-1-4	0.1	3	5	
MgFeCit-2-1	1.0	3	5	
MgFeCit-2-2	1.0	3	5	
MgFeCit-2-3	1.0	3	5	
MgFeCit-3-1	2.0	3	5	
MgFeCit-3-2	2.0	3	5	
MgFeCit-3-3	2.0	3	5	
MgFeCit-4-1	3.0	3	5	
MgFeCit-4-2	3.0	3	5	
MgFeCit-4-3	3.0	3	5	
MgFeCit-5-1	4.0	3	5	
MgFeCit-5-2	4.0	3	5	
MgFeCit-5-3	4.0	3	5	
MgFeCit-6-1	5.0	3	5	
MgFeCit-6-2	5.0	3	5	
MgFeCit-6-3	5.0	3	5	

*Mass of solid for the preparation above is: 2 mol $Fe(OH)_2$/L × 0.003 L × 90 gram/mol = 0.5 gram.

Table 3-24 Measured data for the solubility of $Fe(OH)_2(s)$ in mixed MgHCitrate and NaCl solutions (the "Mg^{2+}—$FeCit^-$" experiment).

Set-up ID	pH* (3 days)	(9 days)	(10 days)	(63 days)	(64 days)
MgFeCit-1-1	7.602	-	-	8.167	-
MgFeCit-1-2	7.600	-	-	8.201	-
MgFeCit-1-3	7.177	-	-	8.215	-
MgFeCit-1-4	6.953[a]	-	-	7.941[b]	-
MgFeCit-2-1	-	7.820	-	7.982	-
MgFeCit-2-2	-	7.773	-	7.979	-
MgFeCit-2-3	-	7.403	-	8.046	-
MgFeCit-3-1	-	7.844	-	7.859	-
MgFeCit-3-2	-	7.828	-	7.856	-
MgFeCit-3-3	-	7.827	-	7.936	-
MgFeCit-4-1	-	7.739	-	-	7.741
MgFeCit-4-2	-	7.737	-	-	7.747
MgFeCit-4-3	-	7.749	-	-	7.801
MgFeCit-5-1	-	-	7.637	-	7.667
MgFeCit-5-2	-	-	7.670	-	7.655
MgFeCit-5-3	-	-	7.666	-	7.702
MgFeCit-6-1	-	-	7.632	-	7.617
MgFeCit-6-2	-	-	7.632	-	7.617
MgFeCit-6-3	-	-	7.631	-	7.660
Reference	WIPP-Solubility-15, p.91	WIPP-Solubility-15, p.91	WIPP-Solubility-15, p.91	WIPP-Solubility-20, p.45	WIPP-Solubility-20, p.45

* Measured with pH electrode and meter, [a]1 day, [b]55 days.

Table 3-24(continued) Measured data for the solubility of $Fe(OH)_2(s)$ in mixed MgHCitrate and NaCl solutions (the "Mg^{2+}—$FeCit^{-}$" experiment).

Set-up ID	$[Citrate^{-3}]_{T,diss}$, (mol/L)[a] (65 days)	$[Citrate^{-3}]_{T,diss}$, (mol/L)[b] (65 days)	$[Fe(II)]_{diss}$, (mol/L)[c] (65 days)
MgFeCit-1-1	5.40E-02	5.29E-02	5.73E-02
MgFeCit-1-2	5.41E-02	-	5.75E-02
MgFeCit-1-3	5.26E-02	-	5.71E-02
MgFeCit-1-4	5.48E-02[a1]	-	5.66E-02[a1]
MgFeCit-2-1	5.35E-02	5.10E-02	5.60E-02
MgFeCit-2-2	5.45E-02	-	5.79E-02
MgFeCit-2-3	5.56E-02	-	5.69E-02
MgFeCit-3-1	5.41E-02	5.14E-02	5.70E-02
MgFeCit-3-2	5.34E-02	-	5.76E-02
MgFeCit-3-3	5.46E-02	-	5.81E-02
MgFeCit-4-1	5.37E-02	5.29E-02	5.70E-02
MgFeCit-4-2	5.42E-02	-	5.79E-02
MgFeCit-4-3	5.48E-02	-	5.67E-02
MgFeCit-5-1	5.36E-02	5.11E-02	5.53E-02
MgFeCit-5-2	5.58E-02	-	5.78E-02
MgFeCit-5-3	5.44E-02	-	5.79E-02
MgFeCit-6-1	5.10E-02	5.04E-02	5.57E-02
MgFeCit-6-2	5.19E-02	-	5.52E-02
MgFeCit-6-3	5.28E-02	-	5.57E-02
Reference	WIPP-Solubility-20, p.42	WIPP-Solubility-20, p.48	WIPP-Solubility-20, p.58, 60

[a]Measured using the IC, [a1]57 days.

[b]Measured using the Total Carbon Coulometer.

[c]Measured using the Ferrozine method.

Table 3-24(continued) Measured data for the solubility of $Fe(OH)_2(s)$ in mixed MgHCitrate and NaCl solutions (the "Mg^{2+}—$FeCit^-$" experiment).

Set-up ID	$[Fe_T]$, (mol/L)[a] (65 days)	$[Mg(II)]_{diss}$, (mol/L)[a] (65 days)	$[Na(I)]_{diss}$, (mol/L)[a] (65 days)
MgFeCit-1-1	5.85E-02	4.92E-02	8.53E-02
MgFeCit-1-2	5.83E-02	4.92E-02	8.44E-02
MgFeCit-1-3	5.76E-02	4.86E-02	8.35E-02
MgFeCit-1-4	5.63E-02[al]	4.83E-02[al]	8.13E-02[al]
MgFeCit-2-1	5.46E-02	5.30E-02	7.83E-01
MgFeCit-2-2	5.69E-02	5.48E-02	8.00E-01
MgFeCit-2-3	5.60E-02	5.45E-02	8.26E-01
MgFeCit-3-1	5.39E-02	5.66E-02	1.57E+00
MgFeCit-3-2	5.43E-02	5.70E-02	1.57E+00
MgFeCit-3-3	5.44E-02	5.62E-02	1.54E+00
MgFeCit-4-1	5.32E-02	5.80E-02	2.30E+00
MgFeCit-4-2	5.34E-02	5.90E-02	2.30E+00
MgFeCit-4-3	5.28E-02	5.78E-02	2.29E+00
MgFeCit-5-1	5.05E-02	5.87E-02	2.88E+00
MgFeCit-5-2	4.89E-02	5.60E-02	2.78E+00
MgFeCit-5-3	5.14E-02	5.94E-02	2.99E+00
MgFeCit-6-1	4.89E-02	5.70E-02	3.50E+00
MgFeCit-6-2	4.92E-02	5.71E-02	3.44E+00
MgFeCit-6-3	4.90E-02	5.72E-02	3.51E+00
Reference	WIPP-Solubility-20, p.47	WIPP-Solubility-20, p.47	WIPP-Solubility-20, p.51

[a]Measured using the ICP-AES.
[al]57 days.

3.14 Solubility of $PbCO_3$(s) in mixed $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbCO_3$(s) (lead carbonate) in $NaHCO_3$ (sodium bicarbonate) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "$PbCl^+$—HCO_3^-" (Item 14, Table 1-1).

A known mass of $PbCO_3$ from Alfa Aesar was added to 100 mL of mixed $NaHCO_3$ and NaCl solutions as shown in Table 3-25 below.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, and carbonate) are also determined. Experimental results are shown in Table 3-26.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for experiments with high ionic strengths (e.g., $PbCO_3$-1.0/0.15-1, $PbCO_3$-1.0/0.15-2, $PbCO_3$-1.0/0.3-1, and $PbCO_3$-1.0/0.3-1) vary in a very narrow range from 8.80 to 9.05 after 1,020 days. The corresponding lead concentrations are also nearly constant. For example, for $PbCO_3$-1.0/0.15-1, lead concentrations range from 8.90E-05 molal to 1.09E-04 molal.

Table 3-25 Preparation of experimental set-ups for the solubility of $Pb(CO)_3$(s) in mixed $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment).

Set-up ID	$PbCO_3$(s) (g)	$NaHCO_3$ (m)	NaCl (m)	Reference
$PbCO_3$-0.01/0.15-1	2.0029	0.0086	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-0.01/0.15-2	1.9998	0.0086	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-0.05/0.15-1	2.0027	0.043	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-0.05/0.15-2	2.0037	0.043	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-0.5/0.15-1	2.0022	0.43	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-0.5/0.15-2	2.0013	0.43	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-1.0/0.15-1	2.0032	0.86	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-1.0/0.15-2	1.9995	0.86	0.15	WIPP-Solubility-3, p. 17
$PbCO_3$-1.0/0.3-1	2.0026	0.86	0.3	WIPP-Solubility-3, p. 17
$PbCO_3$-1.0/0.3-2	2.0029	0.86	0.3	WIPP-Solubility-3, p. 17

Table 3-26 Measured data for the solubility of $Pb(CO)_3(s)$ in mixed $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment). pH data measured with pH electrode and meter.

	pH				
Set-up ID	**741 Days**	**1020 Days**	**1069 Days**	**1119 Days**	**1167 Days**
$PbCO_3$-0.01/0.15-1	9.18	8.79	8.76	8.65	8.68
$PbCO_3$-0.01/0.15-2	9.45	9.25	9.23	9.32	9.22
$PbCO_3$-0.05/0.15-1	9.11	9.01	9.05	9.16	9.08
$PbCO_3$-0.05/0.15-2	9.10	9.16	9.17	9.26	9.18
$PbCO_3$-0.5/0.15-1	8.82	9.68	9.55	9.59	9.49
$PbCO_3$-0.5/0.15-2	8.92	9.08	9.09	9.16	9.09
$PbCO_3$-1.0/0.15-1	8.70	8.89	8.89	8.97	8.90
$PbCO_3$-1.0/0.15-2	8.63	8.80	8.82	8.91	8.85
$PbCO_3$-1.0/0.3-1	8.62	8.96	8.97	9.05	8.98
$PbCO_3$-1.0/0.3-2	8.60	8.80	8.80	8.89	8.83
Reference	WIPP-Solubility-12 pg. 10-11	WIPP-Solubility-12 pg. 66	WIPP-Solubility-12 pg. 97	WIPP-Solubility-21 pg.31	WIPP-Solubility-21 pg. 59

Table 3-26 (continued) Measured data for the solubility of $Pb(CO)_3(s)$ in $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment). Na data measured with ICP-AES.

	[Na(I)] (m)				
Set-up ID	**741 Days**	**1020 Days**	**1069 Days**	**1119 Days**	**1167 Days**
$PbCO_3$-0.01/0.15-1	1.60E-01	1.82E-01	1.81E-01	1.60E-01	1.75E-01
$PbCO_3$-0.01/0.15-2	1.57E-01	1.76E-01	1.73E-01	1.56E-01	1.70E-01
$PbCO_3$-0.05/0.15-1	1.95E-01	2.04E-01	1.94E-01	1.90E-01	1.98E-01
$PbCO_3$-0.05/0.15-2	1.91E-01	2.08E-01	1.95E-01	1.89E-01	2.00E-01
$PbCO_3$-0.5/0.15-1	5.50E-01	5.55E-01	5.09E-01	4.98E-01	5.28E-01
$PbCO_3$-0.5/0.15-2	5.15E-01	5.36E-01	5.27E-01	5.13E-01	5.44E-01
$PbCO_3$-1.0/0.15-1	9.12E-01	9.05E-01	9.19E-01	9.04E-01	9.32E-01
$PbCO_3$-1.0/0.15-2	9.32E-01	8.94E-01	9.12E-01	9.11E-01	9.28E-01
$PbCO_3$-1.0/0.3-1	9.00E-01	1.05E+00	1.03E+00	1.05E+00	1.09E+00
$PbCO_3$-1.0/0.3-2	1.07E+00	1.05E+00	1.05E+00	1.07E+00	1.07E+00
Reference	WIPP-Solubility-22 Pg. 93	WIPP-Solubility-16 Pg. 87,88	WIPP-Solubility-13 pg.97	WIPP-Solubility-22 Pg. 93	WIPP-Solubility-24 Pg. 91-92

Table 3-26 (continued) Measured data for the solubility of $Pb(CO)_3(s)$ in mixed $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment). Pb data measured with ICP-AES.

	[Pb(II)] (m)				
Set-up ID	**741 Days**	**1020 Days**	**1069 Days**	**1119 Days**	**1167 Days**
$PbCO_3$-0.01/0.15-1	1.12E-06	5.83E-07	1.59E-06	5.96E-07	3.49E-06
$PbCO_3$-0.01/0.15-2	7.10E-07	3.92E-06	2.23E-06	1.31E-06	1.42E-06
$PbCO_3$-0.05/0.15-1	2.94E-06	4.96E-06	5.14E-06	3.69E-06	4.02E-06
$PbCO_3$-0.05/0.15-2	2.94E-06	4.73E-06	5.03E-06	4.35E-06	4.44E-06
$PbCO_3$-0.5/0.15-1	2.58E-05	9.64E-05	7.14E-05	6.57E-05	6.24E-05
$PbCO_3$-0.5/0.15-2	2.69E-05	4.48E-05	4.65E-05	5.04E-05	5.04E-05
$PbCO_3$-1.0/0.15-1	5.83E-05	8.90E-05	9.94E-05	1.05E-04	1.09E-04
$PbCO_3$-1.0/0.15-2	6.04E-05	8.11E-05	9.28E-05	9.72E-05	9.89E-05
$PbCO_3$-1.0/0.3-1	6.67E-05	1.25E-04	1.27E-04	1.38E-04	1.13E-04
$PbCO_3$-1.0/0.3-2	7.12E-05	9.14E-05	1.06E-04	1.07E-04	1.43E-04
Reference	WIPP-Solubility-14 pg. 43	WIPP-Solubility-16 pg. 72-76	WIPP-Solubility-22 pg. 14,15	WIPP-Solubility-22 pg. 78	WIPP-Solubility-24 Pg. 80

Table 3-26 (continued) Measured data for the solubility of $Pb(CO)_3(s)$ in mixed $NaHCO_3$ and NaCl solutions (the "$PbCl^+$—HCO_3^-" experiment). CO_3^{2-} data measured with Carbon Coulometer.

	$[CO_3^{2-}]T$
Set-up ID	**741 Days**
$PbCO_3$-0.01/0.15-1	8.95E-03
$PbCO_3$-0.01/0.15-2	8.56E-03
$PbCO_3$-0.05/0.15-1	3.66E-02
$PbCO_3$-0.05/0.15-2	3.73E-02
$PbCO_3$-0.5/0.15-1	3.58E-01
$PbCO_3$-0.5/0.15-2	3.64E-01
$PbCO_3$-1.0/0.15-1	6.82E-01
$PbCO_3$-1.0/0.15-2	7.01E-01
$PbCO_3$-1.0/0.3-1	6.92E-01
$PbCO_3$-1.0/0.3-2	6.65E-01
Reference	WIPP-Solubililty-10 Pg. 80,87 & WIPP-Solubility-17 Pg. 70 & WIPP-Solubility-12 Pg.28

3.15 Solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbCO_3$(s) (lead carbonate) in Na_2CO_3 (sodium carbonate) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "$PbCl^+$—CO_3^{2-}" (Item 15, Table 1-1).

A known mass of $PbCO_3$ from Alfa Aesar was added to 100 mL of mixed Na_2CO_3 and NaCl solutions as shown in Table 3-27 below. The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, and carbonate) are also determined. Experimental results are shown in Table 3-28.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant. As an example, the pH readings for $PbCO_3$-0.01CO_3-1 are ~9.5. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-27 Preparation of experimental set-ups for the solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment).

Set-up ID	$PbCO_3$(s) (g)	Na_2CO_3 (m)	NaCl (m)	Reference
$PbCO_3$-0.01CO_3-1	2.0079	0.01	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-0.01CO_3-2	2.0077	0.01	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-0.1CO_3-1	2.0063	0.1	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-0.1CO_3-2	2.0074	0.1	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-0.5CO_3-1	2.0057	0.5	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-0.5CO_3-2	2.0003	0.5	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-1.0CO_3-1	2.0057	1	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-1.0CO_3-2	2.0043	1	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-1.5CO_3-1	2.0031	1.5	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-1.5CO_3-2	2.002	1.5	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-2.0CO_3-1	2.0066	2	0.15	WIPP-Solubility-3, p. 24
$PbCO_3$-2.0CO_3-2	2.0033	2	0.15	WIPP-Solubility-3, p. 24

Table 3-28 Measured data for the solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment). pH data measured with pH electrode and meter.

	pH				
Set-up ID	**832 Days**	**966 Days**	**1015 Days**	**1064 Days**	**1113 Days**
$PbCO_3$-0.01CO_3-1	9.50	9.54	9.54	9.53	9.53
$PbCO_3$-0.01CO_3-2	9.53	9.54	9.55	9.53	9.53
$PbCO_3$-0.1CO_3-1	10.17	10.14	10.14	10.11	10.12
$PbCO_3$-0.1CO_3-2	10.18	10.15	10.17	10.13	10.14
$PbCO_3$-0.5CO_3-1	10.88	10.78	10.79	10.72	10.75
$PbCO_3$-0.5CO_3-2	10.86	10.77	10.78	10.69	10.73
$PbCO_3$-1.0CO_3-1	11.14	10.99	11.02	10.91	10.93
$PbCO_3$-1.0CO_3-2	11.09	10.97	10.99	10.87	10.90
$PbCO_3$-1.5CO_3-1	11.25	11.09	11.11	11.00	11.02
$PbCO_3$-1.5CO_3-2	11.24	11.10	11.11	10.98	10.98
$PbCO_3$-2.0CO_3-1	11.36	11.20	11.22	11.07	11.09
$PbCO_3$-2.0CO_3-2	11.38	11.23	11.23	11.07	11.09
Reference	WIPP-Solubility-12 pg. 50-51	WIPP-Solubility-12 pg. 68	WIPP-Solubility-12 pg. 99	WIPP-Solubility-21 pg. 34	WIPP-Solubility-21 pg. 62

Table 3-28 (continued) Measured data for the solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment). Na data measured with ICP-AES.

	[Na(I)] (m)				
Set-up ID	**832 Days**	**966 Days**	**1015 Days**	**1064 Days**	**1113 Days**
$PbCO_3$-0.01CO_3-1	1.84E-01	1.84E-01	1.75E-01	1.68E-01	1.77E-01
$PbCO_3$-0.01CO_3-2	1.86E-01	1.88E-01	1.79E-01	1.64E-01	1.81E-01
$PbCO_3$-0.1CO_3-1	3.06E-01	3.06E-01	2.92E-01	2.83E-01	3.13E-01
$PbCO_3$-0.1CO_3-2	3.09E-01	3.06E-01	2.93E-01	2.95E-01	3.14E-01
$PbCO_3$-0.5CO_3-1	1.23E+00	1.00E+00	1.01E+00	1.08E+00	1.07E+00
$PbCO_3$-0.5CO_3-2	1.05E+00	1.03E+00	1.02E+00	1.08E+00	1.07E+00
$PbCO_3$-1.0CO_3-1	2.10E+00	1.97E+00	1.93E+00	2.18E+00	2.08E+00
$PbCO_3$-1.0CO_3-2	2.06E+00	2.00E+00	1.90E+00	2.13E+00	2.07E+00
$PbCO_3$-1.5CO_3-1	3.14E+00	3.02E+00	2.98E+00	2.95E+00	3.14E+00
$PbCO_3$-1.5CO_3-2	3.17E+00	3.01E+00	2.89E+00	2.91E+00	3.15E+00
$PbCO_3$-2.0CO_3-1	3.80E+00	3.70E+00	3.69E+00	3.89E+00	3.84E+00
$PbCO_3$-2.0CO_3-2	3.76E+00	3.79E+00	3.62E+00	3.33E+00	3.89E+00
Reference	WIPP-Solubility-16 Pg. 24	WIPP-Solubility-16 Pg. 87-88	WIPP-Solubility-22 pg. 8	WIPP-Solubility-22 Pg. 94	WIPP-Solubility-24 Pg. 91-92

Table 3-28 (continued) Measured data for the solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment). Pb data measured with ICP-AES.

	[Pb(II)] (m)				
Set-up ID	**832 Days**	**966 Days**	**1015 Days**	**1064 Days**	**1113 Days**
$PbCO_3$-0.01CO_3-1	3.17E-06	2.34E-06	2.88E-06	3.16E-06	2.53E-06
$PbCO_3$-0.01CO_3-2	3.13E-06	2.85E-06	3.48E-06	3.73E-06	3.00E-06
$PbCO_3$-0.1CO_3-1	1.78E-05	1.78E-05	1.84E-05	1.89E-05	1.75E-05
$PbCO_3$-0.1CO_3-2	1.72E-05	1.71E-05	4.45E-05	1.86E-05	1.75E-05
$PbCO_3$-0.5CO_3-1	7.30E-05	7.51E-05	7.95E-05	8.25E-05	7.74E-05
$PbCO_3$-0.5CO_3-2	7.11E-05	7.51E-05	7.05E-05	8.18E-05	7.84E-05
$PbCO_3$-1.0CO_3-1	1.62E-04	1.76E-04	1.84E-04	1.92E-04	1.83E-04
$PbCO_3$-1.0CO_3-2	1.66E-04	1.83E-04	1.81E-04	1.92E-04	1.95E-04
$PbCO_3$-1.5CO_3-1	2.91E-04	3.02E-04	3.14E-04	3.22E-04	3.24E-04
$PbCO_3$-1.5CO_3-2	2.86E-04	3.05E-04	3.14E-04	3.27E-04	3.23E-04
$PbCO_3$-2.0CO_3-1	NA	4.25E-04	4.51E-04	4.59E-04	4.37E-04
$PbCO_3$-2.0CO_3-2	NA	4.21E-04	4.43E-04	5.79E-04	4.49E-04
Reference	WIPP-Solubility-14 pg. 46-47 & WIPP-Solubility-17 Pg. 15	WIPP-Solubility-13 pg. 51	WIPP-Solubility-22 pg. 12	WIPP-Solubility-22 pg. 76	WIPP-Solubility-24 Pg. 74

Table 3-28 (continued) Measured data for the solubility of $PbCO_3$(s) in mixed Na_2CO_3 and NaCl solutions (the "$PbCl^+$—CO_3^{2-}" experiment). CO_3^{2-} data measured with Carbon Coulometer.

	$[CO_3^{2-}]T$ (m)	
Set-up ID	**832 Days**	**1113 Days**
$PbCO_3$-0.01CO_3-1	1.70E-02	1.53E-02
$PbCO_3$-0.01CO_3-2	1.63E-02	1.75E-02
$PbCO_3$-0.1CO_3-1	9.63E-02	9.56E-02
$PbCO_3$-0.1CO_3-2	9.62E-02	9.79E-02
$PbCO_3$-0.5CO_3-1	4.81E-01	5.24E-01
$PbCO_3$-0.5CO_3-2	4.83E-01	4.79E-01
$PbCO_3$-1.0CO_3-1	9.69E-01	9.33E-01
$PbCO_3$-1.0CO_3-2	9.53E-01	9.20E-01
$PbCO_3$-1.5CO_3-1	1.39E+00	1.37E+00
$PbCO_3$-1.5CO_3-2	1.34E+00	1.37E+00
$PbCO_3$-2.0CO_3-1	1.58E+00	1.80E+00
$PbCO_3$-2.0CO_3-2	1.78E+00	1.76E+00
Reference	WIPP-Solubility-17 pg. 19,20,22,23,25	WIPP-Solubility-17 pg. 51,53,58 & WIPP-Solubility-24 Pg.48

3.16 Solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbSO_4$(s) (lead sulfate) in mixed Na_2SO_4 (sodium sulfate) and NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "$PbCl^+$—SO_4^{2-}" (Item 16, Table 1-1).

A known mass of $PbSO_4$ from ACROS Organics was added to 100 mL of mixed Na_2SO_4 and NaCl solutions as shown in Table 3-29 below.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, and sulfate) are also determined. Experimental results gathered to date are shown in Table 3-30.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 743 days. As an example, the pH readings for $PbSO_4$-0.01-1 are between 2.7 and 2.8. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-29 Preparation of experimental set-ups for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment).

Set-up ID	$PbSO_4$(s) (g)	Na_2SO_4 (m)	NaCl (m)	Reference
$PbSO_4$-0.01-1	2.0038	0.01	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-0.01-2	2.002	0.01	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-0.1-1	2.0029	0.1	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-0.1-2	2.0078	0.1	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-0.5-1	2.0032	0.5	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-0.5-2	2.0064	0.5	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.0-1	2.0031	1	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.0-2	2.0048	1	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.5-1	2.0007	1.5	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.5-2	2.0056	1.5	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.8-1	2.0035	1.8	0.15	WIPP-Solubility-3, p. 20
$PbSO_4$-1.8-2	2.0032	1.8	0.15	WIPP-Solubility-3, p. 20

Table 3-30 Measured data for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	360 Days	743 Days	1010 Days	1059 Days	1107 Days	1158 Days
$PbSO_4$-0.01-1	2.78	2.45	2.73	2.75	2.70	2.75
$PbSO_4$-0.01-2	2.82	2.54	2.70	2.75	2.71	2.82
$PbSO_4$-0.1-1	3.11	3.09	3.09	3.12	3.04	3.28
$PbSO_4$-0.1-2	3.12	3.19	3.05	3.05	3.00	3.14
$PbSO_4$-0.5-1	3.37	3.52	3.44	3.41	3.45	3.42
$PbSO_4$-0.5-2	3.36	3.51	3.41	3.42	3.43	3.41
$PbSO_4$-1.0-1	3.49	3.49	3.52	3.53	3.33	3.56
$PbSO_4$-1.0-2	3.47	3.40	3.51	3.51	3.34	3.45
$PbSO_4$-1.5-1	3.57	3.36	3.60	3.58	3.53	3.62
$PbSO_4$-1.5-2	3.55	3.35	3.57	3.63	3.49	3.62
$PbSO_4$-1.8-1	3.52	3.49	3.52	3.58	3.47	3.68
$PbSO_4$-1.8-2	3.53	3.31	3.51	3.55	3.48	3.55
Reference	WIPP-Solubility-3 pg. 51-52	WIPP-Solubility-12 pg. 15-16	WIPP-Solubility-12 pg. 64	WIPP-Solubility-12 pg. 95	WIPP-Solubility-21 pg. 28-29	WIPP-Solubility-21 pg.58

Table 3-30 (continued) Measured data for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment). Na measured with ICP-AES.

	[Na(I)] (m)					
Set-up ID	**360 Days**	**743 Days**	**1010 Days**	**1059 Days**	**1107 Days**	**1158 Days**
$PbSO_4$-0.01-1	NA	1.66E-01	1.62E-01	1.68E-01	1.68E-01	1.70E-01
$PbSO_4$-0.01-2	NA	1.73E-01	1.60E-01	1.64E-01	1.68E-01	1.70E-01
$PbSO_4$-0.1-1	NA	3.34E-01	3.21E-01	3.38E-01	3.15E-01	3.35E-01
$PbSO_4$-0.1-2	NA	3.30E-01	3.18E-01	3.50E-01	3.01E-01	3.13E-01
$PbSO_4$-0.5-1	1.09E+00	1.09E+00	1.05E+00	1.06E+00	1.03E+00	1.10E+00
$PbSO_4$-0.5-2	1.10E+00	1.09E+00	1.06E+00	1.04E+00	9.79E-01	1.08E+00
$PbSO_4$-1.0-1	2.11E+00	2.14E+00	2.07E+00	2.06E+00	2.01E+00	2.20E+00
$PbSO_4$-1.0-2	2.07E+00	2.15E+00	2.05E+00	2.00E+00	2.01E+00	2.05E+00
$PbSO_4$-1.5-1	2.79E+00	2.98E+00	2.80E+00	3.05E+00	2.75E+00	3.11E+00
$PbSO_4$-1.5-2	2.74E+00	3.06E+00	2.88E+00	3.09E+00	2.66E+00	3.08E+00
$PbSO_4$-1.8-1	2.70E+00	2.28E+00	2.57E+00	2.83E+00	2.49E+00	3.27E+00
$PbSO_4$-1.8-2	2.70E+00	2.23E+00	2.56E+00	2.80E+00	2.70E+00	3.27E+00
Reference	WIPP-Solubility-24 Pg. 6	WIPP-Solubility-24 Pg. 6	WIPP-Solubility-13 Pg. 47-48	WIPP-Solubility-13 Pg. 99	WIPP-Solubility-22 Pg. 80	WIPP-Solubility-24 Pg. 86

Table 3-30 (continued) Measured data for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)					
Set-up ID	**360 Days**	**743 Days**	**1010 Days**	**1059 Days**	**1107 Days**	**1158 Days**
$PbSO_4$-0.01-1	6.35E-05	6.09E-05	6.62E-05	7.15E-05	6.37E-05	6.75E-05
$PbSO_4$-0.01-2	7.95E-05	6.16E-05	6.43E-05	7.26E-05	6.96E-05	6.76E-05
$PbSO_4$-0.1-1	8.23E-05	2.21E-05	2.28E-05	2.68E-05	2.56E-05	2.43E-05
$PbSO_4$-0.1-2	5.79E-05	2.28E-05	2.36E-05	2.04E-05	2.56E-05	2.47E-05
$PbSO_4$-0.5-1	2.92E-05	3.35E-05	3.35E-05	3.28E-05	3.51E-05	3.59E-05
$PbSO_4$-0.5-2	4.71E-05	3.09E-05	3.36E-05	4.10E-05	3.21E-05	3.56E-05
$PbSO_4$-1.0-1	8.33E-05	4.53E-05	5.32E-05	5.88E-05	5.42E-05	5.99E-05
$PbSO_4$-1.0-2	5.25E-05	4.59E-05	5.40E-05	5.08E-05	5.31E-05	5.45E-05
$PbSO_4$-1.5-1	6.91E-05	6.37E-05	7.30E-05	7.58E-05	7.07E-05	7.91E-05
$PbSO_4$-1.5-2	6.94E-05	6.46E-05	7.23E-05	7.65E-05	7.21E-05	7.53E-05
$PbSO_4$-1.8-1	6.62E-05	6.91E-05	6.65E-05	7.66E-05	8.21E-05	7.91E-05
$PbSO_4$-1.8-2	6.63E-05	7.43E-05	5.98E-05	7.63E-05	8.40E-05	8.43E-05
Reference	WIPP-Solubility-3 pg. 58,64	WIPP-Solubility-14 pg. 43,46,47	WIPP-Solubility-16 pg. 72-76	WIPP-Solubility-22 pg. 16-17	WIPP-Solubility-22 pg. 78	WIPPl-Solubility-24 Pg. 80

Table 3-30 (continued) Measured data for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment). Cl^- measured with IC.

	[Cl(-I)] (m)			
Set-up ID	**360 Days**	**743 Days**	**1010 Days**	**1059 Days**
$PbSO_4$-0.01-1	NA	1.63E-01	1.58E-01	NA
$PbSO_4$-0.01-2	NA	1.58E-01	1.58E-01	NA
$PbSO_4$-0.1-1	NA	1.51E-01	1.58E-01	1.32E-01
$PbSO_4$-0.1-2	NA	1.44E-01	1.54E-01	1.57E-01
$PbSO_4$-0.5-1	1.52E-01	1.90E-01	1.60E-01	2.18E-01
$PbSO_4$-0.5-2	1.54E-01	1.61E-01	1.54E-01	1.54E-01
$PbSO_4$-1.0-1	1.53E-01	1.88E-01	1.43E-01	1.48E-01
$PbSO_4$-1.0-2	1.53E-01	1.44E-01	1.44E-01	1.51E-01
$PbSO_4$-1.5-1	1.48E-01	1.43E-01	1.45E-01	1.47E-01
$PbSO_4$-1.5-2	1.40E-01	1.43E-01	1.55E-01	1.43E-01
$PbSO_4$-1.8-1	1.60E-01	1.76E-01	1.71E-01	1.61E-01
$PbSO_4$-1.8-2	1.60E-01	1.76E-01	1.66E-01	1.63E-01
Reference	WIPP-Solubililty-24 Pg. 31	WIPP-Solubility-16 Pg. 63 & WIPP-Solubility-17 Pg. 10-11	WIPP-Solubility-13 pg. 50	WIPP-Solubility-19 pg. 54,59

Table 3-30 (continued) Measured data for the solubility of $PbSO_4$(s) in mixed Na_2SO_4 and NaCl solutions (the "$PbCl^+$—SO_4^{2-}" experiment). SO_4^{2-} measured with IC.

	$[SO_4^{2-}]T$		
Set-up ID	**743 Days**	**1010 Days**	**1059 Days**
$PbSO_4$-0.01-1	1.18E-02	1.17E-02	2.11E-02
$PbSO_4$-0.01-2	1.14E-02	1.21E-02	1.39E-02
$PbSO_4$-0.1-1	1.13E-01	1.13E-01	1.08E-01
$PbSO_4$-0.1-2	1.81E-01	1.10E-01	1.30E-01
$PbSO_4$-0.5-1	6.18E-01	5.60E-01	1.01E+00
$PbSO_4$-0.5-2	4.90E-01	5.38E-01	7.57E-01
$PbSO_4$-1.0-1	1.38E+00	1.01E+00	1.69E+00
$PbSO_4$-1.0-2	1.16E+00	1.03E+00	1.54E+00
$PbSO_4$-1.5-1	1.40E+00	1.48E+00	1.90E+00
$PbSO_4$-1.5-2	1.86E+00	1.55E+00	2.64E+00
$PbSO_4$-1.8-1	1.00E+00	1.48E+00	1.84E+00
$PbSO_4$-1.8-2	9.99E-01	1.31E+00	1.55E+00
Reference	WIPP-Solubility-17 pg. 10,13	WIPP-Solubility-13 pg. 50	WIPP-Solubility-19 pg. 54

3.17 Solubility of PbS(s) in mixed NaHS and NaCl solutions (the "$PbCl^+$—HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbS(s) (lead sulfide) in NaHS (sodium bisulfide) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "$PbCl^+$—HS^-" (Item 17, Table 1-1).

This set of experiments has not been started yet. It is planned to use PbS as a starting material. The supporting solutions will be the mixtures of NaHS and NaCl. A known mass of PbS will be added to 100 mL of mixed NaHS and NaCl solutions as shown in Table 3-31 below.

The experimental set-ups will be periodically monitored for one or more component(s) among those listed in Table 3-32. Once stable readings are achieved for the selected component(s), concentrations of other components are to be determined.

Table 3-31 Preparation of experimental set-ups for the solubility PbS(s) in mixed NaHS and NaCl solutions (the "$PbCl^+$—HS^-" experiment).

Set-up ID	PbS(s) (g)	NaCl (m)	Reference
No Data to Date			

Table 3-32 Measured data for experiments the solubility PbS(s) in mixed NaHS and NaCl solutions (the "$PbCl^+$—HS^-" experiment).

Set-up ID	pH	[Pb(II)]	[S(-II)]	[Na(I)]	[Cl(-I)]
Reference	No Data to Date				

3.18 Solubility of PbO(s) in mixed NaCl and $C_{10}H_{12}Mg_2N_2O_8$ (Mg_2EDTA) solutions (the "Na^+—$PbEDTA^{2-}$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbO(s) (lead oxide) in mixed NaCl (sodium chloride) and Mg_2EDTA (dimagnesium EDTA) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Na^+—$PbEDTA^{2-}$" (Item 18, Table 1-1).

A known mass of PbO from MP Biomedicals was added to 100 mL of mixed NaCl and Mg_2EDTA solutions as shown in Table 3-33 below.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, magnesium, and EDTA) are also determined. Experimental results gathered to date are shown in Table 3-34.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 848 days. As an example, the pH readings for Mg_2EDTA-0.01-1 are 10.6. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-33 Preparation of experimental set-ups for the solubility of PbO(s) in mixed NaCl and Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment).

Set-up ID	PbO(s) (g)	NaCl (m)	Mg_2EDTA (m)	Reference
Mg_2EDTA-0.01-1	2.5251	0.01	0.2	WIPP-Solubility-3, p. 38
Mg_2EDTA-0.01-2	2.7556	0.01	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-0.1-1	2.6232	0.1	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-0.1-2	2.4638	0.1	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-1.0-1	2.4546	1	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-1.0-2	2.6651	1	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-2.0-1	2.785	2	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-2.0-2	2.6525	2	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-3.0-1	2.5003	3	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-3.0-2	2.4043	3	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-4.0-1	2.538	4	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-4.0-2	2.4662	4	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-5.0-1	2.6222	5	0.16	WIPP-Solubility-3, p. 38
Mg_2EDTA-5.0-2	2.5535	5	0.16	WIPP-Solubility-3, p. 38

Table 3-34 Measured data for the solubility of PbO(s) in mixed NaCl and Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment). pH data measured with pH electrode and meter.

	pH				
Set-up ID	**848 Days**	**905 Days**	**951 Days**	**1000 Days**	**1056 Days**
Mg_2EDTA-0.01-1	10.73	10.62	10.57	10.56	10.59
Mg_2EDTA-0.01-2	10.64	10.57	10.53	10.48	10.51
Mg_2EDTA-0.1-1	10.83	10.75	10.66	10.62	10.66
Mg_2EDTA-0.1-2	10.75	10.62	10.56	10.52	10.54
Mg_2EDTA-1.0-1	10.67	10.55	10.48	10.46	10.50
Mg_2EDTA-1.0-2	10.59	10.54	10.45	10.43	10.48
Mg_2EDTA-2.0-1	10.51	10.44	10.33	10.28	10.33
Mg_2EDTA-2.0-2	10.45	10.39	10.28	10.25	10.29
Mg_2EDTA-3.0-1	10.42	10.36	10.23	10.21	10.22
Mg_2EDTA-3.0-2	10.36	10.23	10.06	10.04	10.04
Mg_2EDTA-4.0-1	10.46	10.37	10.22	10.18	10.18
Mg_2EDTA-4.0-2	10.28	10.20	10.08	10.04	10.06
Mg_2EDTA-5.0-1	10.02	9.93	9.76	9.74	10.11
Mg_2EDTA-5.0-2	10.32	10.27	10.11	10.11	9.77
Reference	WIPP-Solubility-12 pg.61	WIPP-Solubility-12 pg. 94	WIPP-Solubility- 21 pg. 25-26	WIPP-Solubility-21 pg. 56	WIPP-Solubility-21 pg. 84

Table 3-34 (continued) Measured data for the solubility of PbO(s) in mixed NaCl and Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment). Na measured with ICP-AES.

	[Na(I)] (m)				
Set-up ID	**848 Days**	**905 Days**	**951 Days**	**1000 Days**	**1056 Days**
Mg_2EDTA-0.01-1	NA	8.67E-01	8.42E-01	8.89E-01	9.22E-01
Mg_2EDTA-0.01-2	4.23E-01	2.52E-01	2.38E-01	2.41E-01	2.50E-01
Mg_2EDTA-0.1-1	4.88E-01	3.21E-01	3.11E-01	3.06E-01	3.24E-01
Mg_2EDTA-0.1-2	4.98E-01	3.24E-01	2.97E-01	3.09E-01	3.20E-01
Mg_2EDTA-1.0-1	1.13E+00	1.04E+00	1.02E+00	1.08E+00	1.05E+00
Mg_2EDTA-1.0-2	1.15E+00	1.03E+00	9.93E-01	1.09E+00	1.04E+00
Mg_2EDTA-2.0-1	1.89E+00	1.94E+00	1.96E+00	1.97E+00	1.93E+00
Mg_2EDTA-2.0-2	1.91E+00	1.95E+00	1.91E+00	2.03E+00	1.94E+00
Mg_2EDTA-3.0-1	2.68E+00	2.80E+00	2.52E+00	2.44E+00	2.68E+00
Mg_2EDTA-3.0-2	2.69E+00	2.78E+00	2.49E+00	2.68E+00	2.69E+00
Mg_2EDTA-4.0-1	3.38E+00	3.34E+00	3.03E+00	3.43E+00	3.25E+00
Mg_2EDTA-4.0-2	3.49E+00	3.32E+00	3.53E+00	3.25E+00	3.43E+00
Mg_2EDTA-5.0-1	3.88E+00	3.83E+00	3.56E+00	3.65E+00	3.79E+00
Mg_2EDTA-5.0-2	3.95E+00	3.93E+00	3.86E+00	3.38E+00	3.95E+00
Reference	WIPP-Solubility-14 pg. 85	WIPP-Solubility-13 Pg. 100 & WIPP-Solubility-22 Pg. 7	WIPP-Solubility-22 Pg. 80	WIPP-Solubility-24 Pg. 93	WIPP-Solubility-26 pg. 13

Table 3-34 (continued) Measured data for the solubility of PbO(s) in mixed NaCl + Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)				
Set-up ID	**848 Days**	**905 Days**	**951 Days**	**1000 Days**	**1056 Days**
Mg_2EDTA-0.01-1	NA	8.13E-02	7.68E-02	8.10E-02	7.53E-02
Mg_2EDTA-0.01-2	1.07E-01	9.89E-02	1.14E-01	1.11E-01	1.11E-01
Mg_2EDTA-0.1-1	1.01E-01	1.02E-01	1.03E-01	1.02E-01	1.06E-01
Mg_2EDTA-0.1-2	9.71E-02	1.01E-01	9.36E-02	9.92E-02	1.01E-01
Mg_2EDTA-1.0-1	9.35E-02	1.00E-01	9.13E-02	9.27E-02	8.94E-02
Mg_2EDTA-1.0-2	1.03E-01	9.52E-02	9.79E-02	1.03E-01	9.89E-02
Mg_2EDTA-2.0-1	1.06E-01	1.13E-01	1.04E-01	1.04E-01	1.02E-01
Mg_2EDTA-2.0-2	1.01E-01	8.86E-02	1.01E-01	1.04E-01	9.94E-02
Mg_2EDTA-3.0-1	9.58E-02	1.00E-01	9.31E-02	9.17E-02	9.41E-02
Mg_2EDTA-3.0-2	9.20E-02	9.14E-02	8.83E-02	9.60E-02	9.19E-02
Mg_2EDTA-4.0-1	8.97E-02	9.82E-02	8.42E-02	9.54E-02	8.84E-02
Mg_2EDTA-4.0-2	9.21E-02	8.98E-02	9.28E-02	9.13E-02	9.32E-02
Mg_2EDTA-5.0-1	9.68E-02	9.78E-02	9.71E-02	9.61E-02	9.19E-02
Mg_2EDTA-5.0-2	9.72E-02	9.99E-02	9.23E-02	8.90E-02	9.80E-02
Reference	WIPP-Solubility-14 Pg. 83	WIPP-Solubility-13 pg. 95	WIPP-Solubility-22 Pg. 72-73	WIPP-Solubility-24 Pg. 61	WIPP-Solubility-26 Pg. 14

Table 3-34 (continued) Measured data for the solubility of PbO(s) in mixed NaCl + Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)			
Set-up ID	**848 Days**	**905 Days**	**951 Days**	**1000 Days**
Mg_2EDTA-0.01-1	NA	4.08E-01	3.55E-01	3.80E-01
Mg_2EDTA-0.01-2	1.31E-02	1.37E-02	1.24E-02	1.17E-02
Mg_2EDTA-0.1-1	2.06E-02	2.22E-02	1.90E-02	1.87E-02
Mg_2EDTA-0.1-2	2.80E-02	2.87E-02	2.40E-02	2.39E-02
Mg_2EDTA-1.0-1	3.29E-02	3.39E-02	2.90E-02	2.65E-02
Mg_2EDTA-1.0-2	2.38E-02	2.42E-02	2.06E-02	1.85E-02
Mg_2EDTA-2.0-1	1.88E-02	1.98E-02	1.71E-02	1.44E-02
Mg_2EDTA-2.0-2	2.23E-02	2.34E-02	1.99E-02	1.77E-02
Mg_2EDTA-3.0-1	3.29E-02	3.43E-02	2.89E-02	2.35E-02
Mg_2EDTA-3.0-2	3.95E-02	4.05E-02	3.47E-02	2.99E-02
Mg_2EDTA-4.0-1	3.26E-02	3.47E-02	2.82E-02	2.52E-02
Mg_2EDTA-4.0-2	3.50E-02	3.62E-02	3.25E-02	2.56E-02
Mg_2EDTA-5.0-1	2.72E-02	2.88E-02	2.47E-02	2.02E-02
Mg_2EDTA-5.0-2	3.27E-02	3.34E-02	2.93E-02	2.26E-02
Reference	WIPP-Solubility-14 Pg. 88	WIPP-Solubility-13 Pg. 91	WIPP-Solubility-22 pg. 62	WIPP-Solubility-24 Pg. 68-69

Table 3-34 (continued) Measured data for the solubility of PbO(s) in mixed NaCl + Mg_2EDTA solutions (the "Na^+—$PbEDTA^{2-}$" experiment). EDTA measured with IC.

	[$EDTA^{4-}$] (m)				
Set-up ID	**848 Days**	**905 Days**	**951 Days**	**1000 Days**	**1056 Days**
Mg_2EDTA-0.01-1	6.46E-01	6.60E-01	6.53E-01	6.40E-01	6.53E-01
Mg_2EDTA-0.01-2	1.83E-01	1.90E-01	1.92E-01	1.90E-01	1.91E-01
Mg_2EDTA-0.1-1	1.83E-01	1.93E-01	1.82E-01	1.89E-01	1.88E-01
Mg_2EDTA-0.1-2	1.14E-01	1.93E-01	2.26E-01	1.89E-01	1.90E-01
Mg_2EDTA-1.0-1	1.13E-01	1.89E-01	1.89E-01	1.88E-01	1.88E-01
Mg_2EDTA-1.0-2	1.13E-01	1.91E-01	1.88E-01	1.87E-01	1.85E-01
Mg_2EDTA-2.0-1	1.83E-01	1.89E-01	1.91E-01	1.90E-01	1.88E-01
Mg_2EDTA-2.0-2	1.82E-01	1.92E-01	1.90E-01	1.90E-01	1.88E-01
Mg_2EDTA-3.0-1	1.89E-01	1.93E-01	1.92E-01	1.87E-01	1.88E-01
Mg_2EDTA-3.0-2	1.86E-01	1.90E-01	1.93E-01	1.91E-01	1.88E-01
Mg_2EDTA-4.0-1	1.84E-01	1.88E-01	1.90E-01	1.87E-01	1.89E-01
Mg_2EDTA-4.0-2	1.82E-01	1.89E-01	1.90E-01	1.88E-01	1.86E-01
Mg_2EDTA-5.0-1	1.87E-01	1.87E-01	1.92E-01	1.89E-01	1.90E-01
Mg_2EDTA-5.0-2	1.81E-01	1.92E-01	1.93E-01	1.93E-01	1.89E-01
Reference	WIPP-Solubility-13 Pg. 28	WIPP-Solubility-26 Pg. 18-19	WIPP-Solubility-26 Pg. 18-19	WIPP-Solubility-26 Pg. 18-19	WIPP-Solubility-26 Pg. 18-19

3.19 Solubility of PbO(s) in mixed $MgCl_2$ and $Na_2C_{10}H_{14}O_8N_2 \cdot 2H_2O$ ($Na_2H_2EDTA \cdot 2H_2O$) solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbO(s) (lead oxide) in mixed $MgCl_2$ (magnesium chloride) and $Na_2H_2EDTA \cdot 2H_2O$ (disodium dihydrogen EDTA dihydrate) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Mg^{2+}—$PbEDTA^{2-}$" (Item 19, Table 1-1).

A known mass of PbO from MP Biomedicals was added to 100 mL of mixed $MgCl_2$ and Na_2H_2EDTA solutions as shown in Table 3-35 below.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, magnesium, and EDTA) are also determined. Experimental results gathered to date are shown in Table 3-36.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 407 days. As an example, the pH readings for PbO-0.01ED-1 are between 11.7 and 11.8. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-35 Preparation of experimental set-ups for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment).

Set-up ID	PbO(s) (g)	$MgCl_2$ (m)	Na_2H_2EDTA (m)	Reference
PbO-0.01ED-1	2.0054	0.008	0.042	WIPP-Solubility-3, p. 35
PbO-0.01ED-2	2.0004	0.008	0.042	WIPP-Solubility-3, p. 35
PbO-0.1ED-1	2.004	0.08	0.042	WIPP-Solubility-3, p. 35
PbO-0.1ED-2	2.0043	0.08	0.042	WIPP-Solubility-3, p. 35
PbO-1.0ED-1	2.0041	0.8	0.042	WIPP-Solubility-3, p. 35
PbO-1.0ED-2	2.0056	0.8	0.042	WIPP-Solubility-3, p. 35
PbO-1.5ED-1	2.0049	1.2	0.042	WIPP-Solubility-3, p. 35
PbO-1.5ED-2	2.0005	1.2	0.042	WIPP-Solubility-3, p. 35
PbO-2.0ED-1	2.0033	1.6	0.042	WIPP-Solubility-3, p. 35
PbO-2.0ED-2	2.0069	1.6	0.042	WIPP-Solubility-3, p. 35
PbO-2.5ED-1	2.0016	2.0	0.042	WIPP-Solubility-3, p. 35
PbO-2.5ED-1	2.0036	2.0	0.042	WIPP-Solubility-3, p. 35

Table 3-36 Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**328 Days**	**407 Days**	**937 Days**	**986 Days**	**1035 Days**	**1084 Days**
PbO-0.01 ED-1	11.73	11.70	11.75	11.69	11.80	11.73
PbO-0.01 ED-2	11.67	11.68	11.73	11.66	11.79	11.73
PbO-0.1 ED-1	9.60	9.58	9.58	9.50	9.59	9.55
PbO-0.1 ED-2	9.61	9.63	9.57	9.46	9.61	9.54
PbO-1.0 ED-1	8.92	8.86	8.87	8.83	8.88	8.83
PbO-1.0 ED-2	8.92	8.83	8.86	8.87	8.81	8.86
PbO-1.5 ED-1	8.69	8.58	8.65	8.64	8.64	8.64
PbO-1.5 ED-2	8.69	8.65	8.66	8.65	8.67	8.65
PbO-2.0 ED-1	8.47	8.34	8.40	8.43	8.34	8.40
PbO-2.0 ED-2	8.46	8.36	8.43	8.43	8.47	8.41
PbO-2.5 ED-1	8.24	8.11	8.08	8.09	8.17	8.06
PbO-2.5 ED-2	8.23	8.10	8.08	8.10	8.18	8.06
Reference	WIPP-Solubility-3 pg. 67-68	WIPP-Solubility-3 pg. 75,77,80	WIPP-Solubility-12 pg. 75	WIPP-Solubility-21 pg. 8	WIPP-Solubility-21 pg. 39	WIPP-Solubility-21 pg. 68

Table 3-36(continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment). Na measured with ICP-AES.

	[Na(I)] (m)					
Set-up ID	**328 Days**	**407 Days**	**937 Days**	**986 Days**	**1035 Days**	**1084 Days**
PbO-0.01 ED-1	8.57E-02	8.44E-02	8.37E-02	8.56E-02	8.46E-02	8.56E-02
PbO-0.01 ED-2	8.43E-02	8.34E-02	8.40E-02	8.41E-02	8.22E-02	8.36E-02
PbO-0.1 ED-1	8.80E-02	8.47E-02	8.70E-02	8.46E-02	8.58E-02	8.64E-02
PbO-0.1 ED-2	8.61E-02	8.33E-02	8.60E-02	8.66E-02	8.61E-02	8.72E-02
PbO-1.0 ED-1	9.32E-02	7.31E-02	9.35E-02	9.64E-02	1.01E-01	9.40E-02
PbO-1.0 ED-2	9.19E-02	7.22E-02	9.38E-02	9.85E-02	9.84E-02	9.57E-02
PbO-1.5 ED-1	9.54E-02	7.46E-02	9.60E-02	9.91E-02	9.91E-02	9.68E-02
PbO-1.5 ED-2	9.71E-02	7.57E-02	9.62E-02	1.00E-01	1.08E-01	9.70E-02
PbO-2.0 ED-1	1.01E-01	7.83E-02	9.65E-02	1.03E-01	1.03E-01	1.02E-01
PbO-2.0 ED-2	1.15E-01	8.01E-02	9.82E-02	1.01E-01	1.03E-01	9.96E-02
PbO-2.5 ED-1	9.85E-02	7.38E-02	9.92E-02	1.02E-01	1.05E-01	9.93E-02
PbO-2.5 ED-2	9.90E-02	8.11E-02	9.89E-02	1.04E-01	1.06E-01	1.02E-01
Reference	WIPP-solubility-24 Pg. 29-30	WIPP-solubility-24 Pg. 29-30	WIPP-Solubility-19 Pg. 20	WIPP-Solubility-22 Pg. 81	WIPP-Solubility-22 Pg. 81	WIPP-Solubility-24 Pg. 86

Table 3-36(continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)					
Set-up ID	**328 Days**	**407 Days**	**937 Days**	**986 Days**	**1035 Days**	**1084 Days**
PbO-0.01 ED-1	3.58E-02	3.61E-02	4.14E-02	4.01E-02	4.06E-02	4.01E-02
PbO-0.01 ED-2	3.52E-02	3.58E-02	3.92E-02	3.97E-02	4.14E-02	3.91E-02
PbO-0.1 ED-1	3.44E-02	3.36E-02	5.32E-02	3.89E-02	4.09E-02	3.96E-02
PbO-0.1 ED-2	3.39E-02	3.50E-02	3.91E-02	3.96E-02	3.97E-02	3.96E-02
PbO-1.0 ED-1	2.53E-02	3.19E-02	3.85E-02	3.83E-02	4.34E-02	3.89E-02
PbO-1.0 ED-2	2.34E-02	2.86E-02	3.77E-02	3.77E-02	4.12E-02	3.45E-02
PbO-1.5 ED-1	1.99E-02	3.19E-02	3.80E-02	3.82E-02	4.17E-02	3.85E-02
PbO-1.5 ED-2	1.93E-02	3.16E-02	3.98E-02	3.81E-02	4.18E-02	3.82E-02
PbO-2.0 ED-1	1.63E-02	3.04E-02	3.55E-02	3.79E-02	4.07E-02	3.89E-02
PbO-2.0 ED-2	1.73E-02	3.08E-02	4.23E-02	3.72E-02	4.02E-02	3.83E-02
PbO-2.5 ED-1	1.67E-02	2.80E-02	3.81E-02	3.86E-02	3.92E-02	3.83E-02
PbO-2.5 ED-2	1.62E-02	3.16E-02	3.79E-02	3.89E-02	3.89E-02	3.81E-02
Reference	WIPP-Solubility-3 pg. 70,72	WIPP-Solubility-3 pg. 80-81	WIPP-Solubility-13 pg. 69	WIPP-Solubility-22 Pg. 72-73	WIPP-Solubility-22 Pg. 72-73	WIPP-Solubility-24 Pg. 76

Table 3-36 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)					
Set-up ID	**328 Days**	**407 Days**	**937 Days**	**986 Days**	**1035 Days**	**1084 Days**
PbO-0.01 ED-1	1.43E-04	1.11E-04	BD	BD	BD	BD
PbO-0.01 ED-2	1.41E-04	1.07E-04	BD	BD	BD	BD
PbO-0.1 ED-1	7.20E-02	7.14E-02	7.26E-02	6.71E-02	6.84E-02	6.73E-02
PbO-0.1 ED-2	7.03E-02	7.00E-02	7.18E-02	6.76E-02	6.92E-02	6.80E-02
PbO-1.0 ED-1	7.31E-01	5.92E-01	7.69E-01	7.38E-01	7.64E-01	7.12E-01
PbO-1.0 ED-2	7.08E-01	5.55E-01	7.67E-01	7.34E-01	6.60E-01	6.27E-01
PbO-1.5 ED-1	1.10E+00	8.45E-01	1.11E+00	1.07E+00	1.02E+00	1.06E+00
PbO-1.5 ED-2	1.10E+00	8.67E-01	1.09E+00	1.07E+00	1.12E+00	1.03E+00
PbO-2.0 ED-1	1.49E+00	1.14E+00	1.43E+00	1.43E+00	1.44E+00	1.41E+00
PbO-2.0 ED-2	1.67E+00	1.19E+00	1.44E+00	1.41E+00	1.45E+00	1.44E+00
PbO-2.5 ED-1	1.81E+00	1.31E+00	1.79E+00	1.79E+00	1.82E+00	1.76E+00
PbO-2.5 ED-2	1.82E+00	1.42E+00	1.77E+00	1.76E+00	1.79E+00	1.76E+00
Reference	WIPP-Solubility-24 Pg. 12	WIPP-Solubility-24 Pg. 12	WIPP-Solubility-13 pg. 85-86	WIPP-solubility-22 Pg.63	WIPP-solubility-22 Pg.63	WIPP-Solubility-24 Pg. 68-69

BD: Below Detection

Table 3-36 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and Na_2H_2EDTA solutions (the "Mg^{2+}—$PbEDTA^{2-}$" experiment). EDTA measured with IC.

	[$EDTA^{4-}$] (m)					
Set-up ID	**328 Days**	**407 Days**	**937 Days**	**986 Days**	**1035 Days**	**1084 Days**
PbO-0.01 ED-1	6.26E-02	6.33E-02	6.10E-02	5.72E-02	5.83E-02	5.61E-02
PbO-0.01 ED-2	6.10E-02	6.15E-02	6.08E-02	5.75E-02	5.87E-02	6.01E-02
PbO-0.1 ED-1	6.29E-02	6.18E-02	6.05E-02	5.78E-02	5.78E-02	5.74E-02
PbO-0.1 ED-2	6.15E-02	6.19E-02	6.03E-02	5.79E-02	5.84E-02	5.78E-02
PbO-1.0 ED-1	6.29E-02	7.02E-02	6.16E-02	5.92E-02	5.73E-02	5.89E-02
PbO-1.0 ED-2	6.36E-02	6.33E-02	6.27E-02	5.86E-02	6.33E-02	5.88E-02
PbO-1.5 ED-1	6.43E-02	7.08E-02	6.17E-02	5.97E-02	5.89E-02	5.77E-02
PbO-1.5 ED-2	6.39E-02	7.21E-02	6.26E-02	5.96E-02	5.93E-02	5.90E-02
PbO-2.0 ED-1	6.38E-02	7.13E-02	6.27E-02	5.99E-02	5.99E-02	5.87E-02
PbO-2.0 ED-2	6.40E-02	7.31E-02	6.12E-02	5.98E-02	5.93E-02	5.84E-02
PbO-2.5 ED-1	NA	NA	6.58E-02	5.87E-02	5.84E-02	5.89E-02
PbO-2.5 ED-2	NA	NA	6.42E-02	5.99E-02	5.90E-02	5.94E-02
Reference	WIPP-Solubility-13 pg. 42,46	WIPP-Solubility-13 pg. 43	WIPP-Solubility-16 Pg. 94	WIPP-Solubility-26 Pg. 21	WIPP-Solubility-26 Pg. 21	WIPP-Solubility-26 Pg. 21

3.20 Solubility of PbO(s) in mixed NaCl and $C_6H_6MgO_7 \cdot xH_2O$ (MgHCitrate·xH_2O) solutions (the "Na^+—$PbCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbO(s) (lead oxide) in mixed NaCl (sodium chloride) and MgHCitrate·xH_2O (magnesium hydrogen citrate hydrate) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Na^+—$PbCit^-$" (Item 20, Table 1-1).

A known mass of PbO from MP Biomedicals was added to 100 mL of mixed NaCl and MgHCit solutions as shown in Table 3-37 below. The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, magnesium, chloride, and citrate) are also determined. Experimental results gathered to date are shown in Table 3-38.

The results obtained so far demonstrate that the steady state seems to be attained in terms of lead concentrations after 83 days. However, the steady state has not been attained in terms of pH readings. As it seems that lead concentrations are constant, solubility of PbO in this system is independent from pH.

Table 3-37 Preparation of experimental set-ups for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment).

Set-up ID	PbO(s) (g)	NaCl (m)	MgHCit (m)	Reference
PbO-0.01NaCl-1	2.0100	0.01	0.12	WIPP-Solubility-12 Pg. 63
PbO-0.1NaCl-1	2.0400	0.1	0.12	WIPP-Solubility-12 Pg. 63
PbO-1.0NaCl-1	2.6418	1	0.12	WIPP-Solubility-12 Pg. 63
PbO-2.0NaCl-1	2.5444	2	0.12	WIPP-Solubility-12 Pg. 63
PbO-3.0NaCl-1	2.0719	3	0.12	WIPP-Solubility-12 Pg. 63
PbO-4.0NaCl-1	2.2580	4.06	0.12	WIPP-Solubility-12 Pg. 63
PbO-5.0NaCl-1	2.5201	5.01	0.12	WIPP-Solubility-12 Pg. 63

Table 3-38 Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). pH data measured with pH electrode and meter.

	pH			
Set-up ID	**34 Days**	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	4.07	4.13	4.16	4.09
PbO-0.1NaCl-1	4.05	4.10	4.12	4.13
PbO-1.0NaCl-1	4.62	6.80	7.29	7.43
PbO-2.0NaCl-1	4.07	6.69	7.48	7.56
PbO-3.0NaCl-1	3.81	4.10	4.18	4.18
PbO-4.0NaCl-1	3.93	4.69	5.12	5.39
PbO-5.0NaCl-1	4.12	5.14	5.51	5.92
Reference	WIPP-Solubility-12 pg. 79	WIPP-Solubility-21 pg. 12	WIPP-Solubility-21 pg. 42	WIPP-Solubility-21 pg. 71

Table 3-38(continued) Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). Na measured with ICP-AES.

	[Na(I)] (m)			
Set-up ID	**34 Days**	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	1.59E-02	1.54E-02	1.56E-02	1.55E-02
PbO-0.1NaCl-1	9.52E-02	9.55E-02	9.56E-02	9.65E-02
PbO-1.0NaCl-1	9.23E-01	9.52E-01	9.59E-01	9.52E-01
PbO-2.0NaCl-1	1.92E+00	1.88E+00	1.71E+00	1.94E+00
PbO-3.0NaCl-1	2.69E+00	2.61E+00	2.62E+00	2.77E+00
PbO-4.0NaCl-1	3.52E+00	3.38E+00	3.20E+00	3.49E+00
PbO-5.0NaCl-1	4.15E+00	4.14E+00	3.41E+00	3.58E+00
Reference	WIPP-Solubility-19 Pg. 21	WIPP-Solubility-22 pg. 90	WIPP-Solubility-22 pg. 90	WIPP-Solubility-24 Pg. 94-95

Table 3-38 (continued) Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)		
Set-up ID	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	1.10E-03	1.13E-03	1.12E-03
PbO-0.1NaCl-1	1.22E-03	1.23E-03	1.21E-03
PbO-1.0NaCl-1	1.16E-02	2.00E-02	2.07E-02
PbO-2.0NaCl-1	7.69E-03	1.66E-02	1.87E-02
PbO-3.0NaCl-1	4.52E-03	4.73E-03	4.49E-03
PbO-4.0NaCl-1	9.38E-03	8.38E-03	7.78E-03
PbO-5.0NaCl-1	1.43E-02	1.24E-02	1.28E-02
Reference	WIPP-Solubility-22 Pg. 70	WIPP-Solubility-22 Pg. 70	WIPP-Solubility-24 Pg. 75

Table 3-38 (continued) Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)			
Set-up ID	**34 Days**	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	1.49E-01	1.46E-01	1.58E-01	1.51E-01
PbO-0.1NaCl-1	1.51E-01	1.47E-01	1.43E-01	1.49E-01
PbO-1.0NaCl-1	1.70E-01	1.62E-01	1.66E-01	1.51E-01
PbO-2.0NaCl-1	1.76E-01	1.68E-01	1.52E-01	1.47E-01
PbO-3.0NaCl-1	1.77E-01	1.68E-01	1.62E-01	1.45E-01
PbO-4.0NaCl-1	1.77E-01	1.68E-01	1.45E-01	1.31E-01
PbO-5.0NaCl-1	1.76E-01	1.62E-01	1.07E-01	1.07E-01
Reference	WIPP-Solubility-13 Pg. 87	WIPP-Solubility-22 pg. 27	WIPP-Solubility-24 Pg. 7	WIPP-Solubility-24 Pg. 68-69

Table 3-38 (continued) Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). Cl^- measured with IC.

	[Cl(-I)] (m)			
Set-up ID	**34 Days**	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	1.16E-02	1.31E-02	1.30E-02	1.29E-02
PbO-0.1NaCl-1	9.60E-02	8.69E-02	9.40E-02	9.55E-02
PbO-1.0NaCl-1	9.50E-01	9.84E-01	9.86E-01	9.88E-01
PbO-2.0NaCl-1	1.91E+00	1.94E+00	1.96E+00	1.96E+00
PbO-3.0NaCl-1	2.81E+00	2.87E+00	2.89E+00	2.87E+00
PbO-4.0NaCl-1	3.69E+00	3.76E+00	3.80E+00	3.78E+00
PbO-5.0NaCl-1	4.43E+00	4.60E+00	4.62E+00	4.62E+00
Reference	WIPP-Solubility-16 Pg. 99 & WIPP-Solubility-19 Pgs. 6, 25	WIPP-Solubility-24 Pg. 60 & WIPP-Solubility-26 Pg. 40	WIPP-Solubility-24 Pg. 60 & WIPP-Solubility-26 Pg. 42	WIPP-Solubility-24 Pg. 60 & WIPP-Solubility-26 Pg. 42

Table 3-38 (continued) Measured data for the solubility of PbO(s) in mixed NaCl and MgHCitrate solutions (the "Na^+—$PbCit^-$" experiment). Citrate measured with IC.

	[Citrate3-] (m)			
Set-up ID	**34 Days**	**83 Days**	**132 Days**	**181 Days**
PbO-0.01NaCl-1	1.62E-01	1.58E-01	1.65E-01	1.64E-01
PbO-0.1NaCl-1	1.61E-01	1.58E-01	1.66E-01	1.63E-01
PbO-1.0NaCl-1	1.35E-01	1.18E-01	1.38E-01	1.42E-01
PbO-2.0NaCl-1	1.47E-01	1.17E-01	1.40E-01	1.44E-01
PbO-3.0NaCl-1	1.62E-01	1.37E-01	1.54E-01	1.57E-01
PbO-4.0NaCl-1	1.64E-01	1.31E-01	1.32E-01	1.33E-01
PbO-5.0NaCl-1	1.59E-01	1.14E-01	1.23E-01	1.17E-01
Reference	WIPP-Solubility-26 Pg. 40-41	WIPP-Solubility-26 Pg. 40-41	WIPP-Solubility-26 Pg. 42	WIPP-Solubility-26 Pg. 42

3.21 Solubility of PbO(s) in mixed $MgCl_2$ and $C_6H_6MgO_7 \cdot xH_2O$ ($MgHCitrate \cdot xH_2O$) solutions (the "Mg^{2+}—$PbCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbO(s) (lead oxide) in mixed $MgCl_2$ (magnesium chloride) and $MgHCitrate \cdot xH_2O$ (magnesium hydrogen citrate hydrate) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Mg^{2+}—$PbCit^-$" (Item 21, Table 1-1).

A known mass of PbO from MP Biomedicals was added to 100 mL of mixed $MgCl_2$ and MgHCit solutions as shown in

Table 3-39 below. The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (magnesium, chloride, and citrate) are also determined. Experimental results gathered to date are shown in Table 3-40.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 331 days. As an example, the pH readings for PbO-0.01Mg-1 are between 8.8 and 8.9. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-39 Preparation of experimental set-ups for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment).

Set-up ID	PbO(s) (g)	$MgCl_2$ (m)	MgHCit (m)	Reference
Pb-0.01Mg-1	2.0053	0.005	0.12	WIPP-Solubility-3, p. 26
Pb-0.1Mg-1	2.0051	0.05	0.12	WIPP-Solubility-3, p. 26
Pb-1.0Mg-1	2.0063	0.5	0.12	WIPP-Solubility-3, p. 26
Pb-1.5Mg-1	2.0082	0.75	0.12	WIPP-Solubility-3, p. 26
Pb-2.0Mg-1	2.0078	1	0.12	WIPP-Solubility-3, p. 26
Pb-2.5Mg-1	2.0001	1.25	0.12	WIPP-Solubility-3, p. 26

Table 3-40 Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**331 Days**	**785 Days**	**960 Days**	**1009 Days**	**1057 Days**	**1107 Days**
PbO-0.01 Mg-1	8.72	8.90	8.91	8.91	8.82	8.89
PbO-0.1 Mg-1	7.97	7.88	8.01	8.01	7.88	7.93
PbO-1.0 Mg-1	6.76	6.71	6.64	6.69	6.51	6.69
PbO-1.5 Mg-1	6.10	6.11	6.02	6.06	5.96	6.04
PbO-2.0 Mg-1	5.87	5.71	5.73	5.84	5.68	5.81
PbO-2.5 Mg-1	5.86	5.75	5.96	6.01	5.91	5.93
Reference	WIPP-Solubility-3 pg. 66	WIPP-Solubility-12 pg. 45-46	WIPP-Solubility-12 pg. 78	WIPP-Solubility-21 pg. 11	WIPP-Solubility-21 pg. 40	WIPP-Solubility-21 pg. 70

Table 3-40 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)					
Set-up ID	**331 Days**	**785 Days**	**960 Days**	**1009 Days**	**1057 Days**	**1107 Days**
PbO-0.01 Mg-1	8.91E-02	9.18E-02	8.92E-02	9.05E-02	8.83E-02	8.80E-02
PbO-0.1 Mg-1	1.12E-01	1.16E-01	1.19E-01	1.13E-01	1.16E-01	1.15E-01
PbO-1.0 Mg-1	5.32E-01	5.56E-01	5.31E-01	5.46E-01	5.11E-01	5.08E-01
PbO-1.5 Mg-1	7.58E-01	7.63E-01	7.48E-01	7.38E-01	7.36E-01	7.05E-01
PbO-2.0 Mg-1	9.76E-01	1.00E+00	9.60E-01	9.53E-01	9.65E-01	9.23E-01
PbO-2.5 Mg-1	1.21E+00	1.17E+00	1.14E+00	1.13E+00	1.18E+00	1.14E+00
Reference	WIPP-Solubility-24 Pg. 66	WIPP-Solubility-17 pg. 9-10	WIPP-Solubility-13 pg. 86	WIPP-Solubility-22 pg. 27	WIPP-Solubility-24 Pg. 7	WIPP-Solubility-24 Pg. 68-69

Table 3-40 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)					
Set-up ID	**331 Days**	**785 Days**	**960 Days**	**1009 Days**	**1057 Days**	**1107 Days**
PbO-0.01 Mg-1	1.27E-02	1.77E-02	1.77E-02	1.92E-02	1.77E-02	1.85E-02
PbO-0.1 Mg-1	7.16E-03	7.15E-03	6.98E-03	6.94E-03	6.97E-03	6.59E-03
PbO-1.0 Mg-1	1.04E-03	1.02E-03	1.01E-03	1.14E-03	1.18E-03	1.15E-03
PbO-1.5 Mg-1	1.04E-03	1.13E-03	1.27E-03	1.31E-03	1.42E-03	1.54E-03
PbO-2.0 Mg-1	2.08E-03	2.34E-03	2.59E-03	2.83E-03	2.90E-03	2.88E-03
PbO-2.5 Mg-1	9.97E-03	9.60E-03	9.22E-03	9.78E-03	1.03E-02	1.05E-02
Reference	WIPP-Solubility-3 pg. 72	WIPP-Solubility-17 pg. 5	WIPP-Solubility-13 pg. 64	WIPP-Solubility-22 Pg. 71	WIPP-Solubility-22 Pg. 71	WIPP-Solubility-24 Pg. 76

Table 3-40 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment). Cl^- measured with IC.

	[Cl(-I)] (m)
Set-up ID	**960 Days**
PbO-0.01 Mg-1	5.61E-02
PbO-0.1 Mg-1	1.20E-01
PbO-1.0 Mg-1	9.16E-01
PbO-1.5 Mg-1	1.35E+00
PbO-2.0 Mg-1	1.79E+00
PbO-2.5 Mg-1	2.16E+00
Reference	WIPP-Solubility-16 Pg. 98,99 & WIPP-Solubility-19 Pg. 6

Table 3-40 (continued) Measured data for the solubility of PbO(s) in mixed $MgCl_2$ and MgHCitrate solutions (the "Mg^{2+}—$PbCit^-$" experiment). Citrate measured with IC.

	[$Citrate^{3-}$] (m)					
Set-up ID	**331 Days**	**785 Days**	**960 Days**	**1009 Days**	**1057 Days**	**1107 Days**
PbO-0.01 Mg-1	6.38E-02	6.50E-02	6.51E-02	6.68E-02	6.65E-02	6.37E-02
PbO-0.1 Mg-1	5.07E-02	5.20E-02	5.33E-02	5.05E-02	4.93E-02	4.92E-02
PbO-1.0 Mg-1	2.75E-02	2.55E-02	3.05E-02	2.62E-02	2.62E-02	2.82E-02
PbO-1.5 Mg-1	3.04E-02	2.25E-02	2.80E-02	2.62E-02	2.69E-02	2.71E-02
PbO-2.0 Mg-1	3.18E-02	1.97E-02	2.68E-02	2.50E-02	2.44E-02	2.38E-02
PbO-2.5 Mg-1	3.60E-02	2.10E-02	2.34E-02	2.32E-02	2.17E-02	2.11E-02
Reference	WIPP-Solubility-26 Pg. 43	WIPP-Solubility-26 Pg. 43	WIPP-Solubility-26 Pg. 43	WIPP-Solubility-26 Pg. 43	WIPP-Solubility-26 Pg. 43	WIPP-Solubility-26 Pg. 43

3.22 Solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbC_2O_4(s)$ (lead oxalate) in NaCl (sodium chloride) solutions and (2) determine Pitzer ion-interaction parameters for the ion pair, "PbOx(aq)—Na^+" (Item 22, Table 1-1).

In this set of experiments, a known mass of $PbC_2O_4(s)$ was added to NaCl solutions ranging from 0.010 m to 5.0 m (see Table 3-41). These solutions were prepared with ACS reagent grade NaCl and deionized water. The solubility-controlling phase is lead oxalate (PbC_2O_4) with a purity of 99.999%, which is from Alfa Aesar.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, chloride, and oxalate) are also determined. Experimental results gathered to date are shown in Table 3-42.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 831 days. As an example, the pH readings for PbOx-0.01-1 are between 6.4 and 6.5. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-41 Preparation of experimental set-ups for the solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment).

Set-up ID	$PbC_2O_4(s)$ (g)	NaCl (m)	Reference
PbOx-0.01-1	0.508	0.01	WIPP-Solubility-3, p. 8
PbOx-0.01-2	0.5028	0.01	WIPP-Solubility-3, p. 8
PbOx-0.1-1	0.5016	0.1	WIPP-Solubility-3, p. 8
PbOx-0.1-2	0.5114	0.1	WIPP-Solubility-3, p. 8
PbOx-1.0-1	0.5111	1.0	WIPP-Solubility-3, p. 8
PbOx-1.0-2	0.5078	1.0	WIPP-Solubility-3, p. 8
PbOx-2.0-1	0.5122	2.1	WIPP-Solubility-3, p. 8
PbOx-2.0-2	0.5079	2.1	WIPP-Solubility-3, p. 8
PbOx-3.0-1	0.5059	3.2	WIPP-Solubility-3, p. 8
PbOx-3.0-2	0.5055	3.2	WIPP-Solubility-3, p. 8
PbOx-4.0-1	0.4999	4.4	WIPP-Solubility-3, p. 8
PbOx-4.0-2	0.506	4.4	WIPP-Solubility-3, p. 8
PbOx-5.0-1	0.5091	5.0	WIPP-Solubility-3, p. 8
PbOx-5.0-2	0.5037	5.0	WIPP-Solubility-3, p. 8

Table 3-42 Measured data for the solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment). pH data measured with pH electrode and meter.

	pH							
Set-up ID	**110 Days**	**551 Days**	**780 Days**	**831 Days**	**1062 Days**	**1111 Days**	**1159 Days**	**1209 Days**
PbOx-0.01-1	6.40	6.30	6.01	6.30	6.46	6.53	6.45	6.41
PbOx-0.01-2	6.51	6.30	6.00	6.54	6.37	6.52	6.55	6.44
PbOx-0.1-1	6.03	6.06	5.77	6.22	6.24	6.34	6.35	6.29
PbOx-0.1-2	5.88	5.49	5.21	5.43	5.31	5.34	5.41	5.37
PbOx-1.0-1	6.55	6.80	6.88	6.88	6.77	7.00	7.02	6.94
PbOx-1.0-2	6.53	6.81	6.93	6.73	6.81	7.03	7.06	6.97
PbOx-2.0-1	6.11	5.86	5.70	5.66	5.63	5.68	5.72	5.58
PbOx-2.0-2	6.19	6.10	6.38	6.00	6.19	6.35	6.44	6.32
PbOx-3.0-1	6.14	5.85	5.98	5.63	5.71	5.74	5.82	5.71
PbOx-3.0-2	6.23	6.07	6.30	5.85	6.13	6.29	6.37	6.29
PbOx-4.0-1	6.56	6.38	6.58	6.12	6.37	6.61	6.70	6.60
PbOx-4.0-2	6.62	6.37	6.46	6.44	6.38	6.60	6.70	6.65
PbOx-5.0-1	7.12	6.88	7.05	6.72	6.87	7.01	7.11	7.00
PbOx-5.0-2	7.15	6.95	7.27	7.09	6.95	7.06	7.13	7.06
Reference	WIPP-Solubility -3 pg.28	WIPP Solubility -3 pg.76	WIPP-Solubility -12 pg. 18-20	WIPP-Solubility -12 pg. 38,40	WIPP-Solubility -12 pg. 80	WIPP-Solubility -21 pg. 13	WIPP-Solubility -21 pg. 43	WIPP-Solubility -21 pg. 73

Table 3-42 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment). Na measured with ICP-AES.

	[Na (I)] (m)							
Set-up ID	**110 Days**	**551 Days**	**780 Days**	**831 Days**	**1062 Days**	**1111 Days**	**1159 Days**	**1209 Days**
PbOx-0.01-1	3.48E-02	2.41E-02	1.04E-02	1.08E-02	1.18E-02	1.05E-02	1.04E-02	1.10E-02
PbOx-0.01-2	3.65E-02	2.15E-02	1.08E-02	1.06E-02	1.18E-02	1.06E-02	1.10E-02	1.15E-02
PbOx-0.1-1	1.31E-01	NA	1.06E-01	1.08E-01	1.14E-01	1.09E-01	1.04E-01	1.11E-01
PbOx-0.1-2	1.28E-01	NA	1.05E-01	1.04E-01	1.10E-01	1.08E-01	1.05E-01	1.09E-01
PbOx-1.0-1	9.87E-01	NA	9.41E-01	9.44E-01	9.23E-01	9.50E-01	9.12E-01	9.60E-01
PbOx-1.0-2	9.67E-01	NA	9.54E-01	9.37E-01	8.99E-01	9.51E-01	9.39E-01	9.63E-01
PbOx-2.0-1	2.07E+00	2.45E+00	1.87E+00	1.90E+00	1.90E+00	1.98E+00	1.98E+00	2.01E+00
PbOx-2.0-2	2.45E+00	2.02E+00	1.90E+00	2.10E+00	1.89E+00	1.96E+00	1.94E+00	2.05E+00
PbOx-3.0-1	2.80E+00	2.79E+00	2.82E+00	2.79E+00	2.72E+00	2.75E+00	2.54E+00	2.88E+00
PbOx-3.0-2	2.65E+00	2.70E+00	2.73E+00	2.87E+00	2.75E+00	2.83E+00	2.50E+00	2.79E+00
PbOx-4.0-1	3.61E+00	4.21E+00	3.65E+00	3.51E+00	3.40E+00	3.67E+00	3.35E+00	3.68E+00
PbOx-4.0-2	3.25E+00	3.11E+00	3.62E+00	3.61E+00	3.62E+00	3.39E+00	3.34E+00	3.75E+00
PbOx-5.0-1	3.81E+00	4.16E+00	4.18E+00	4.20E+00	4.06E+00	3.96E+00	3.92E+00	4.31E+00
PbOx-5.0-2	3.99E+00	4.22E+00	4.19E+00	3.79E+00	3.96E+00	4.12E+00	3.77E+00	4.24E+00
Reference	WIPP-Solubility -22 Pg. 82-83	WIPP-Solubility -22 Pg. 82-83	WIPP-Solubility -22 Pg. 82-83	WIPP-Solubility -22 Pg. 82-83	WIPP-Solubility -13 pg. 81	WIPP-Solubility -22 Pg. 84	WIPP-Solubility -22 Pg. 84	WIPP-Solubility -24 Pg. 93

Table 3-42 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)							
Set-up ID	**110 Days**	**551 Days**	**780 Days**	**831 Days**	**1062 Days**	**1111 Days**	**1159 Days**	**1209 Days**
PbOx-0.01-1	2.52E-05	2.93E-05	2.02E-05	2.23E-05	3.45E-05	2.14E-05	2.45E-05	2.43E-05
PbOx-0.01-2	2.38E-05	3.15E-05	2.14E-05	2.66E-05	2.81E-05	2.35E-05	2.42E-05	2.55E-05
PbOx-0.1-1	3.84E-05	2.67E-05	3.04E-05	3.19E-05	3.41E-05	3.65E-05	3.75E-05	4.42E-05
PbOx-0.1-2	3.84E-05	2.82E-05	3.17E-05	3.36E-05	3.53E-05	3.60E-05	3.74E-05	4.02E-05
PbOx-1.0-1	1.38E-04	1.20E-04	1.04E-04	1.08E-04	1.48E-04	1.29E-04	1.38E-04	1.34E-04
PbOx-1.0-2	1.40E-04	1.21E-04	1.05E-04	1.11E-04	1.39E-04	1.32E-04	1.46E-04	1.37E-04
PbOx-2.0-1	3.05E-04	1.99E-04	2.76E-04	2.71E-04	3.17E-04	3.28E-04	3.39E-04	3.37E-04
PbOx-2.0-2	3.73E-04	1.91E-04	2.73E-04	2.72E-04	3.19E-04	3.23E-04	3.37E-04	3.67E-04
PbOx-3.0-1	7.17E-04	6.30E-04	6.93E-04	6.73E-04	7.69E-04	8.01E-04	8.39E-04	8.23E-04
PbOx-3.0-2	7.30E-04	6.22E-04	6.90E-04	6.89E-04	7.76E-04	8.17E-04	8.67E-04	8.46E-04
PbOx-4.0-1	1.65E-03	1.61E-03	1.62E-03	1.62E-03	1.77E-03	1.93E-03	2.05E-03	1.92E-03
PbOx-4.0-2	1.67E-03	1.62E-03	1.68E-03	1.64E-03	1.84E-03	1.90E-03	1.97E-03	1.97E-03
PbOx-5.0-1	3.05E-03	3.13E-03	3.17E-03	3.05E-03	3.52E-03	3.81E-03	4.25E-03	3.84E-03
PbOx-5.0-2	3.04E-03	3.16E-03	3.17E-03	3.09E-03	3.29E-03	3.50E-03	4.50E-03	3.70E-03
Reference	WIPP-Solubility -3 pg. 30	WIPP-Solubility -3 pg. 79	WIPP-Solubility -10 pg. 94	WIPP-Solubility -14 pg. 19 & WIPP-Solubility -13 Pg. 62	WIPP-Solubility -13 pg. 65	WIPP-Solubility -22 Pg. 74-75	WIPP-Solubility -22 Pg. 74-75	WIPP-Solubility -24 Pg. 75

Table 3-42 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in NaCl solutions (the "PbOx(aq)—Na^+" experiment). Cl^- measured with ICP-AES.

	[Cl(-I)] (m)							
Set-up ID	**110 Days**	**551 Days**	**780 Days**	**831 Days**	**1062 Days**	**1111 Days**	**1159 Days**	**1209 Days**
PbOx-0.01-1	NA	NA	1.06E-02	1.07E-02	1.10E-02	1.07E-02	1.03E-02	1.04E-02
PbOx-0.01-2	NA	NA	1.10E-02	1.09E-02	1.10E-02	9.82E-03	1.04E-02	1.07E-02
PbOx-0.1-1	1.28E-01	NA	1.06E-01	1.05E-01	1.06E-01	1.05E-01	1.00E-01	1.02E-01
PbOx-0.1-2	1.31E-01	NA	1.06E-01	1.05E-01	1.05E-01	1.02E-01	9.94E-02	1.02E-01
PbOx-1.0-1	1.10E+00	NA	1.02E+00	9.93E-01	9.98E-01	1.04E+00	9.82E-01	1.00E+00
PbOx-1.0-2	1.08E+00	NA	1.03E+00	1.03E+00	1.05E+00	1.05E+00	1.03E+00	1.01E+00
PbOx-2.0-1	2.13E+00	1.81E+00	2.08E+00	2.05E+00	2.11E+00	2.08E+00	2.01E+00	2.02E+00
PbOx-2.0-2	2.39E+00	2.09E+00	2.07E+00	2.21E+00	2.11E+00	2.09E+00	2.00E+00	2.06E+00
PbOx-3.0-1	3.15E+00	3.05E+00	3.08E+00	3.11E+00	2.99E+00	3.06E+00	2.91E+00	2.87E+00
PbOx-3.0-2	3.18E+00	3.05E+00	3.02E+00	3.01E+00	2.37E+00	3.08E+00	3.13E+00	2.88E+00
PbOx-4.0-1	4.06E+00	4.00E+00	4.05E+00	4.09E+00	4.05E+00	4.07E+00	3.89E+00	3.76E+00
PbOx-4.0-2	4.16E+00	4.05E+00	4.10E+00	4.07E+00	3.81E+00	3.94E+00	3.89E+00	3.77E+00
PbOx-5.0-1	4.56E+00	4.63E+00	4.64E+00	4.67E+00	4.62E+00	4.69E+00	4.54E+00	4.21E+00
PbOx-5.0-2	4.63E+00	4.67E+00	4.61E+00	4.72E+00	4.63E+00	4.56E+00	4.31E+00	4.19E+00
Reference	WIPP-Solubility -24 Pg. 54	WIPP-Solubility -24 Pg. 54	WIPP-Solubility -24 Pg. 54- 55	WIPP-Solubility -24 Pg. 55	WIPP-Solubility -24 Pg. 55 & WIPP-Solubility -24 Pg. 63-64	WIPP-Solubility -24 Pg. 63-64	WIPP-Solubility -24 Pg. 32	WIPP-Solubility -24 Pg. 98-99

3.23 Solubility of $PbC_2O_4(s)$ in $MgCl_2$ solutions (the "PbOx(aq)—Mg^{2+}" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbC_2O_4(s)$ (lead oxalate) in $MgCl_2$ (magnesium chloride) solutions and (2) determine Pitzer ion-interaction parameters for the ion pair, "PbOx(aq)—Mg^{2+}" (Item 23, Table 1-1).

In this set of experiments, a known mass of $PbC_2O_4(s)$ was added to $MgCl_2$ solutions ranging from 0.01 m to 2.5 m (Table 3-43). These solutions were prepared by using ACS reagent grade $MgCl_2 \cdot 6H_2O$ and deionized water. The solubility-controlling phase is lead oxalate (PbC_2O_4) with a purity of 99.999%, which is from Alfa Aesar. The pmH's can be obtained based on pH readings by applying the correction factors for $MgCl_2$ solutions determined by Hansen (2001), and they will be reported elsewhere. The total dissolved lead concentrations were determined using the ICP-AES. The oxalate concentrations were determined using the IC.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (magnesium, chloride, and oxalate) are also determined. Experimental results gathered to date are shown in Table 3-44.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 553 days. As an example, the pH readings for PbOx-0.01Mg-1 are between 6.0 and 6.2. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-43 Preparation of experimental set-ups for the solubility $PbC_2O_4(s)$ in $MgCl_2$ solutions (the "PbOx(aq)—Mg^{2+}" experiment).

Set-up ID	$PbC_2O_4(s)$ (g)	$MgCl_2$, m	Reference
PbOx-0.01Mg-1	0.5129	0.01	WIPP-Solubility-3, p. 9
PbOx-0.01Mg-2	0.5111	0.01	WIPP-Solubility-3, p. 9
PbOx-0.1Mg-1	0.4945	0.1	WIPP-Solubility-3, p. 9
PbOx-0.1Mg-2	0.4988	0.1	WIPP-Solubility-3, p. 9
PbOx-1.0Mg-1	0.5128	1.0	WIPP-Solubility-3, p. 9
PbOx-1.0Mg-2	0.5082	1.0	WIPP-Solubility-3, p. 9
PbOx-1.5Mg-1	0.4999	1.5	WIPP-Solubility-3, p. 9
PbOx-1.5Mg-2	0.5042	1.5	WIPP-Solubility-3, p. 9
PbOx-2.0Mg-1	0.5002	2.0	WIPP-Solubility-3, p. 9
PbOx-2.0Mg-2	0.5193	2.0	WIPP-Solubility-3, p. 9
PbOx-2.5Mg-1	0.5095	2.5	WIPP-Solubility-3, p. 9
PbOx-2.5Mg-2	0.5093	2.5	WIPP-Solubility-3, p. 9

Table 3-44 Measured data for solubility of $PbC_2O_4(s)$ in $MgCl_2$ solutions (the "PbOx(aq)—Mg^{2+}" experiment). pH data measured with pH electrode and meter.

	pH						
Set-up ID	**113 Days**	**254 Days**	**553 Days**	**1059 Days**	**1107 Days**	**1155 Days**	**1211 Days**
PbOx-0.01 Mg-1	6.57	6.38	6.01	6.06	6.16	6.11	5.98
PbOx-0.01 Mg-2	6.08	6.19	6.22	6.20	6.35	6.37	6.24
PbOx-0.1 Mg-1	5.86	5.86	5.88	5.95	6.10	5.98	6.07
PbOx-0.1 Mg-2	5.86	5.87	5.87	5.94	6.06	6.01	6.06
PbOx-1.0 Mg-1	5.36	5.22	5.04	5.23	5.23	5.30	5.31
PbOx-1.0 Mg-2	5.37	5.30	5.13	5.26	5.29	5.37	5.34
PbOx-1.5 Mg-1	5.01	4.92	4.82	4.94	4.96	5.06	5.02
PbOx-1.5 Mg-2	5.00	4.93	4.80	4.85	4.87	4.91	4.90
PbOx-2.0 Mg-1	4.64	4.68	4.65	4.73	4.76	4.87	4.80
PbOx-2.0 Mg-2	4.62	4.67	4.65	4.71	4.75	4.85	4.81
PbOx-2.5 Mg-1	4.35	4.44	4.39	4.46	4.53	4.62	4.58
PbOx-2.5 Mg-2	4.33	4.35	4.32	4.39	4.46	4.51	4.52
Reference	WIPP-Solubility-3 pg .31-32	WIPP-Solubility-3 pg. 41	WIPP-Solubility-3 pg . 81-82	WIPP-Solubility-12 pg.84	WIPP-Solubility-21 pg. 15	WIPP-Solubility -21 pg. 46	WIPP-Solubility-21 pg. 76

Table 3-44 (continued) Measured data for solubility of $PbC_2O_4(s)$ in $MgCl_2$ solutions (the "PbOx(aq)—Mg^{2+}" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)						
Set-up ID	**113 Days**	**254 Days**	**553 Days**	**1059 Days**	**1107 Days**	**1155 Days**	**1211 Days**
PbOx-0.01 Mg-1	NA	1.23E-02	1.03E-02	9.82E-03	9.91E-03	9.78E-03	9.95E-03
PbOx-0.01 Mg-2	NA	1.07E-02	1.01E-02	9.80E-03	9.80E-03	9.75E-03	9.93E-03
PbOx-0.1 Mg-1	NA	1.17E-01	9.82E-02	9.37E-02	9.59E-02	9.50E-02	9.61E-02
PbOx-0.1 Mg-2	NA	1.06E-01	9.82E-02	9.29E-02	9.61E-02	9.04E-02	9.62E-02
PbOx-1.0 Mg-1	9.68E-01	9.57E-01	9.31E-01	9.11E-01	9.16E-01	8.10E-01	9.16E-01
PbOx-1.0 Mg-2	9.66E-01	9.47E-01	9.27E-01	9.19E-01	9.30E-01	9.38E-01	9.43E-01
PbOx-1.5 Mg-1	1.43E+00	1.43E+00	1.40E+00	1.33E+00	1.36E+00	1.30E+00	1.30E+00
PbOx-1.5 Mg-2	1.41E+00	1.43E+00	1.39E+00	1.34E+00	1.35E+00	1.26E+00	1.40E+00
PbOx-2.0 Mg-1	1.88E+00	1.87E+00	1.84E+00	1.72E+00	1.81E+00	1.61E+00	1.85E+00
PbOx-2.0 Mg-2	1.95E+00	1.82E+00	1.85E+00	1.74E+00	1.82E+00	1.75E+00	1.83E+00
PbOx-2.5 Mg-1	2.28E+00	2.31E+00	2.29E+00	2.07E+00	2.26E+00	2.19E+00	2.20E+00
PbOx-2.5 Mg-2	2.41E+00	2.29E+00	2.27E+00	2.08E+00	2.26E+00	2.11E+00	2.08E+00
Reference	WIPP-Solubility-24 Pg. 8	WIPP-Solubility-24 Pg. 8	WIPP-Solubility-24 Pg. 8	WIPP-Solubility-13 Pg. 75	WIPP-Solubility-24 Pg. 9	WIPP-Solubility -24 Pg. 9	WIPP-Solubility-24 pg. 81

Table 3-44 (continued) Measured data for solubility of $PbC_2O_4(s)$ in $MgCl_2$ solutions (the "PbOx(aq)—Mg^{2+}" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)						
Set-up ID	**113 Days**	**254 Days**	**553 Days**	**1059 Days**	**1107 Days**	**1155 Days**	**1211 Days**
PbOx-0.01 Mg-1	4.96E-05	3.28E-05	4.06E-05	4.69E-05	4.69E-05	4.73E-05	4.57E-05
PbOx-0.01 Mg-2	4.06E-05	2.86E-05	4.16E-05	4.65E-05	4.67E-05	4.71E-05	4.60E-05
PbOx-0.1 Mg-1	2.09E-04	1.59E-04	1.66E-04	1.74E-04	1.81E-04	1.97E-04	1.85E-04
PbOx-0.1 Mg-2	2.07E-04	1.25E-04	1.67E-04	1.77E-04	1.81E-04	1.95E-04	1.84E-04
PbOx-1.0 Mg-1	8.57E-04	8.21E-04	8.15E-04	1.03E-03	1.08E-03	1.02E-03	9.93E-04
PbOx-1.0 Mg-2	9.18E-04	8.22E-04	8.21E-04	1.02E-03	1.06E-03	1.09E-03	1.02E-03
PbOx-1.5 Mg-1	3.34E-03	2.94E-03	3.04E-03	3.25E-03	3.64E-03	3.71E-03	3.50E-03
PbOx-1.5 Mg-2	3.35E-03	2.84E-03	2.83E-03	3.32E-03	3.44E-03	3.55E-03	3.54E-03
PbOx-2.0 Mg-1	1.19E-02	9.79E-03	9.62E-03	1.07E-02	1.19E-02	1.13E-02	1.21E-02
PbOx-2.0 Mg-2	1.16E-02	9.91E-03	9.58E-03	1.11E-02	1.19E-02	1.27E-02	1.36E-02
PbOx-2.5 Mg-1	1.52E-02	1.55E-02	1.49E-02	1.63E-02	1.82E-02	1.99E-02	1.65E-02
PbOx-2.5 Mg-2	1.70E-02	1.48E-02	1.45E-02	1.62E-02	1.79E-02	2.00E-02	1.58E-02
Reference	WIPP-Solubility-3 pg. 36	WIPP-Solubility-3 pg. 44	WIPP-Solubility-3 pg. 82	WIPP-Solubility-13 Pg. 67	WIPP-Solubility-22 Pg. 75	WIPP-Solubility -24 Pg. 21	WIPP-Solubility -24 Pg. 77

3.24 Solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $PbC_2O_4(s)$ (lead oxalate, Alfa Aesar, puratronic, 99.999%) in mixed NaCl (sodium chloride) and $MgCl_2$ (magnesium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "PbOx(aq)—Cl^-" (Item 24, Table 1-1).

A known mass of $PbC_2O_4(s)$ was added to 100 mL of mixed NaCl and $MgCl_2$ solutions ranging from as shown in Table 3-45 below.

The experimental set-ups are periodically monitored for pH and dissolved lead. Concentrations of other dissolved components (sodium, magnesium, chloride, and oxalate) are also determined. Experimental results gathered to date are shown in Table 3-46.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 755 days. As an example, the pH readings for PbOx-$MgCl_2$-A-1 are between 5.7 and 5.9. The corresponding lead concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-45 Preparation of experimental set-ups for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment).

Set-up ID	$PbC_2O_4(s)$ (g)	NaCl (m)	$MgCl_2$ (m)	Reference
PbOx-$MgCl_2$-A-1	0.9331	5	0.5	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-A-2	1.369	5	0.5	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-B-1	1.146	3.5	0.8	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-B-2	1.2838	3.5	0.8	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-C-1	1.1885	3	1.25	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-C-2	1.22	3	1.25	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-D-1	1.2549	2	1.5	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-D-2	1.4222	2	1.5	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-E-1	0.7271	1.5	1.75	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-E-2	0.5815	1.5	1.75	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-F-1	0.642	0.5	2	WIPP-Solubility-3, p. 40
PbOx-$MgCl_2$-F-2	0.6298	0.5	2	WIPP-Solubility-3, p. 40

Table 3-46 Measured data for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**75 Days**	**269 Days**	**755 Days**	**822 Days**	**852 Days**	**907 Days**
PbOx-$MgCl_2$-A-1	5.50	5.44	5.71	5.84	5.94	5.85
PbOx-$MgCl_2$-A-2	5.40	5.30	5.57	5.69	5.79	5.64
PbOx-$MgCl_2$-B-1	5.45	5.42	5.59	5.74	5.75	5.66
PbOx-$MgCl_2$-B-2	5.46	5.39	5.61	5.73	5.81	5.69
PbOx-$MgCl_2$-C-1	4.93	4.93	5.19	5.39	5.46	5.34
PbOx-$MgCl_2$-C-2	5.12	5.03	5.33	5.49	5.54	5.43
PbOx-$MgCl_2$-D-1	4.91	4.96	5.05	5.22	5.33	5.18
PbOx-$MgCl_2$-D-2	4.84	4.67	4.61	4.71	4.76	4.66
PbOx-$MgCl_2$-E-1	4.83	4.57	4.55	4.64	4.65	4.56
PbOx-$MgCl_2$-E-2	4.62	4.54	4.84	5.00	5.10	4.99
PbOx-$MgCl_2$-F-1	4.53	4.40	4.56	4.67	4.79	4.67
PbOx-$MgCl_2$-F-2	4.47	4.42	4.57	4.65	4.77	4.67
Reference	WIPP-Solubility-3 pg . 47	WIPP-Solubility-3 pg. 84-86	WIPP-Solubility-12 pg. 83	WIPP-Solubility-21 pg. 24	WIPP-Solubility-21 pg. 44	WIPP-Solubility-21 pg. 74

Table 3-46 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment). Na measured with ICP-AES.

	[Na (I)] (m)					
Set-up ID	**75 Days**	**269 Days**	**755 Days**	**822 Days**	**852 Days**	**907 Days**
PbOx-$MgCl_2$-A-1	3.23E+00	4.15E+00	4.10E+00	4.18E+00	3.94E+00	3.87E+00
PbOx-$MgCl_2$-A-2	3.35E+00	4.16E+00	4.14E+00	3.63E+00	3.70E+00	4.16E+00
PbOx-$MgCl_2$-B-1	2.45E+00	2.96E+00	2.93E+00	2.75E+00	2.60E+00	2.90E+00
PbOx-$MgCl_2$-B-2	2.38E+00	2.93E+00	3.01E+00	2.88E+00	2.82E+00	2.93E+00
PbOx-$MgCl_2$-C-1	2.09E+00	2.60E+00	2.68E+00	2.60E+00	2.45E+00	2.54E+00
PbOx-$MgCl_2$-C-2	2.11E+00	2.64E+00	2.60E+00	2.60E+00	2.40E+00	2.44E+00
PbOx-$MgCl_2$-D-1	1.52E+00	1.64E+00	1.78E+00	1.86E+00	1.67E+00	1.85E+00
PbOx-$MgCl_2$-D-2	1.46E+00	1.87E+00	1.83E+00	1.88E+00	1.67E+00	1.91E+00
PbOx-$MgCl_2$-E-1	1.47E+00	1.39E+00	1.33E+00	1.37E+00	1.24E+00	1.37E+00
PbOx-$MgCl_2$-E-2	1.46E+00	1.34E+00	1.34E+00	1.40E+00	1.26E+00	1.42E+00
PbOx-$MgCl_2$-F-1	5.11E-01	4.72E-01	4.65E-01	4.76E-01	4.27E-01	4.43E-01
PbOx-$MgCl_2$-F-2	5.11E-01	4.72E-01	4.30E-01	4.69E-01	4.52E-01	4.50E-01
Reference	WIPP-Solubility-22 Pg. 58	WIPP-Solubility-22 Pg. 56	WIPP-Solubility-13 Pg. 84	WIPP-Solubility-22 Pg. 57	WIPP-Solubility-24 Pg. 51	WIPP-Solubility-24 Pg. 93

Table 3-46 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment). Mg measured with ICP-AES.

	[Mg (II)] (m)					
Set-up ID	**75 Days**	**269 Days**	**755 Days**	**822 Days**	**852 Days**	**907 Days**
PbOx-$MgCl_2$-A-1	3.07E-01	4.70E-01	4.34E-01	3.75E-01	3.96E-01	3.39E-01
PbOx-$MgCl_2$-A-2	3.13E-01	4.63E-01	4.30E-01	3.57E-01	3.75E-01	3.48E-01
PbOx-$MgCl_2$-B-1	6.04E-01	8.11E-01	7.77E-01	6.79E-01	6.54E-01	6.82E-01
PbOx-$MgCl_2$-B-2	6.00E-01	8.15E-01	7.83E-01	6.94E-01	7.00E-01	6.72E-01
PbOx-$MgCl_2$-C-1	8.71E-01	1.17E+00	1.14E+00	1.05E+00	1.07E+00	1.03E+00
PbOx-$MgCl_2$-C-2	9.00E-01	1.17E+00	1.15E+00	1.04E+00	1.04E+00	1.04E+00
PbOx-$MgCl_2$-D-1	1.10E+00	1.39E+00	1.31E+00	1.31E+00	1.27E+00	1.28E+00
PbOx-$MgCl_2$-D-2	1.05E+00	1.38E+00	1.35E+00	1.29E+00	1.25E+00	1.29E+00
PbOx-$MgCl_2$-E-1	1.69E+00	1.60E+00	1.53E+00	1.54E+00	1.46E+00	1.51E+00
PbOx-$MgCl_2$-E-2	1.62E+00	1.56E+00	1.53E+00	1.54E+00	1.50E+00	1.52E+00
PbOx-$MgCl_2$-F-1	1.95E+00	1.82E+00	1.74E+00	1.84E+00	1.67E+00	1.65E+00
PbOx-$MgCl_2$-F-2	1.94E+00	1.84E+00	1.60E+00	1.77E+00	1.77E+00	1.68E+00
Reference	WIPP-Solubility-22 Pg. 61	WIPP-Solubility-10 Pg. 97 & WIPP-Solubility-22 Pg. 61	WIPP-Solubility-13 Pg. 74	WIPP-Solubility-22 Pg. 68	WIPP-solubility-24 Pg. 11	WIPP-Solubility-24 pg. 81

Table 3-46 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment). Pb measured with ICP-AES.

	[Pb(II)] (m)					
Set-up ID	**75 Days**	**269 Days**	**755 Days**	**822 Days**	**852 Days**	**907 Days**
PbOx-$MgCl_2$-A-1	5.56E-02	5.73E-02	6.23E-02	7.01E-02	6.85E-02	6.29E-02
PbOx-$MgCl_2$-A-2	5.97E-02	6.33E-02	7.09E-02	7.71E-02	7.80E-02	7.78E-02
PbOx-$MgCl_2$-B-1	2.86E-02	3.02E-02	3.45E-02	3.95E-02	3.65E-02	3.96E-02
PbOx-$MgCl_2$-B-2	2.97E-02	3.03E-02	3.37E-02	3.86E-02	3.94E-02	3.91E-02
PbOx-$MgCl_2$-C-1	3.22E-02	3.34E-02	3.97E-02	4.89E-02	4.34E-02	4.28E-02
PbOx-$MgCl_2$-C-2	3.37E-02	3.39E-02	3.92E-02	4.23E-02	4.19E-02	4.43E-02
PbOx-$MgCl_2$-D-1	2.18E-02	2.22E-02	2.36E-02	2.86E-02	2.71E-02	2.85E-02
PbOx-$MgCl_2$-D-2	2.24E-02	2.18E-02	2.52E-02	2.70E-02	2.65E-02	2.87E-02
PbOx-$MgCl_2$-E-1	1.66E-02	2.09E-02	2.26E-02	2.56E-02	2.44E-02	2.64E-02
PbOx-$MgCl_2$-E-2	1.72E-02	2.05E-02	2.20E-02	2.55E-02	2.49E-02	2.63E-02
PbOx-$MgCl_2$-F-1	1.32E-02	1.30E-02	1.44E-02	1.56E-02	1.52E-02	1.64E-02
PbOx-$MgCl_2$-F-2	1.35E-02	1.29E-02	1.30E-02	1.54E-02	1.62E-02	1.54E-02
Reference	WIPP-Solubility-3 pg. 53 & 58	WIPP-Solubility-10 pg. 25	WIPP-Solubility-13 pg. 68	WIPP-Solubility-22 Pg. 69	WIPP-Solubility-24 Pg. 61	WIPP-Solubility-24 Pg. 76

Table 3-46 (continued) Measured data for the solubility of $PbC_2O_4(s)$ in mixed NaCl and $MgCl_2$ solutions (the "PbOx(aq)—Cl^-" experiment). Cl^- measured with ICP-AES.

	[Cl(-I)] (m)					
Set-up ID	**75 Days**	**269 Days**	**755 Days**	**822 Days**	**852 Days**	**907 Days**
PbOx-$MgCl_2$-A-1	4.05E+00	5.67E+00	6.16E+00	5.97E+00	5.47E+00	5.30E+00
PbOx-$MgCl_2$-A-2	3.75E+00	5.92E+00	6.00E+00	5.94E+00	5.32E+00	5.34E+00
PbOx-$MgCl_2$-B-1	3.44E+00	5.39E+00	5.40E+00	5.13E+00	4.63E+00	4.55E+00
PbOx-$MgCl_2$-B-2	3.73E+00	5.44E+00	5.08E+00	5.15E+00	4.60E+00	4.47E+00
PbOx-$MgCl_2$-C-1	3.94E+00	5.75E+00	5.50E+00	5.83E+00	5.00E+00	4.92E+00
PbOx-$MgCl_2$-C-2	4.03E+00	5.98E+00	5.76E+00	5.91E+00	4.88E+00	4.82E+00
PbOx-$MgCl_2$-D-1	3.91E+00	5.97E+00	5.21E+00	5.39E+00	4.43E+00	4.52E+00
PbOx-$MgCl_2$-D-2	3.78E+00	5.37E+00	5.21E+00	5.50E+00	4.38E+00	4.50E+00
PbOx-$MgCl_2$-E-1	NA	5.94E+00	5.35E+00	5.36E+00	4.41E+00	4.57E+00
PbOx-$MgCl_2$-E-2	NA	5.83E+00	5.22E+00	5.44E+00	4.41E+00	4.56E+00
PbOx-$MgCl_2$-F-1	NA	4.92E+00	5.08E+00	4.95E+00	3.81E+00	4.09E+00
PbOx-$MgCl_2$-F-2	NA	5.38E+00	4.68E+00	4.91E+00	4.14E+00	4.05E+00
Reference	WIPP-Solubility-22 Pg. 66	WIPP-Solubility-22 Pg. 66	WIPP-Solubility-22 Pg. 66	WIPP-Solubility-22 pg. 66	WIPP-Solubility-24 Pg. 32	WIPP-Solubility-24 Pg. 98-99

3.25 Solubility of $Na_2(B_4O_7)•10H_2O(s)$ in NaHS solutions (the "Na^+—HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Na_2(B_4O_7)\cdot 10H_2O(s)$ (sodium tetraborate decahydrate) in NaHS (sodium bisulfide) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Na^+—HS^-" (Item 25, Table 1-1).

This set of experiments has not been started yet. It is planned to use $Na_2B_4O_7•10H_2O(s)$ as a starting material. The supporting solutions will be NaHS solution. A known mass of $Na_2B_4O_7•10H_2O(s)$ will be added to 100 mL of NaHS solutions as to be shown in Table 3-47 below.

The experimental set-ups will be periodically monitored for pH and dissolved sodium. Once stable pH readings are achieved, concentrations of other dissolved components (sodium, borate, and sulfide) are to be determined. Experimental results gathered to date will be shown in Table 3-48.

Table 3-47 Preparation of experimental set-ups for the solubility of $Na_2(B_4O_7)(s)$ in NaHS solutions (the "Na^+—HS^-" experiment).

Set-up ID	$Na_2(B_4O_7)(s)$ (g)	NaHS(m)	Reference
No Data to Date			

Table 3-48 Measured data for the solubility of $Na_2(B_4O_7)(s)$ in NaHS solutions (the "Na^+—HS^-" experiment).

Set-up ID	pH	[Na(I)]	[B(IV)]	[S(-II)]
Reference	No Data to Date			

3.26 Solubility of $Mg(OH)_2(s)$ in mixed NaHS and Na_2S solutions (the "Mg^{2+}–HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of $Mg(OH)_2$ (magnesium hydroxide) in NaHS/Na_2S solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Mg^{2+}–HS^-" (Item 26, Table 1-1). This investigation is under preparation. Experimental set-ups will be listed in Table 3-49, and they will be periodically monitored for one or more component(s) among those listed in Table 3-50. Once stable readings are achieved for the selected component(s), concentrations of other components are to be determined.

Table 3-49 Preparation of experimental set-ups for the solubility of $Mg(OH)_2(s)$ in NaHS/Na_2S solutions (the "Mg^{2+}–HS^-" experiment).

Set-up ID	$Mg(OH)_2(s)$ (g)	NaHS/Na_2S (m)	Reference
No Data to Date			

Table 3-50 Measured data for the solubility of $Mg(OH)_2(s)$ in NaHS/Na_2S solutions (the "Mg^{2+}–HS^-" experiment).

Set-up ID	pH	[Mg(II)]	[S(-II)]	[Na(I)]
Reference	No Data to Date			

3.27 Solubility of PbS(s) in NaCl solutions (the "Cl^-—HS^-" experiment)

The objectives of this set of experiments are to (1) determine the solubility of PbS(s) (lead sulfide) in NaCl (sodium chloride) solutions, and (2) determine the Pitzer ion-interaction parameters for the ion pair, "Cl^-—HS^-" (Item 27, Table 1-1). This investigation is under preparation. The preparation of experimental set-ups will be shown in Table 3-51, and measured data will be listed in Table 3-52.

Table 3-51 Preparation of experimental set-ups for the solubility of PbS(s) in NaCl solutions (the "Cl^-—HS^-" experiment).

Set-up ID	PbS(s) (g)	HCl (m)	Reference
No Data to Date			

Table 3-52 Measured data for the solubility of PbS(s) in NaCl solutions (the "Cl^-—HS^-" experiment).

Set-up ID	pH	[Pb(II)]	[S(-II)]	[Cl(-I)]
Reference	No Data to Date			

3.28 Solubility of $FeC_2O_4 \cdot 2H_2O$(s) in mixed $MgCl_2$ and NaCl solutions (the "FeOx(aq)—Mg^{2+}—Na^+" experiment).

The objectives of this set of experiments are to (1) measure solubility of $FeC_2O_4 \cdot 2H_2O$(s) (ferrous iron oxalate) in mixed $MgCl_2$ (magnesium chloride) and NaCl (sodium chloride) solutions, and (2) to determine the Pitzer ion-interaction parameters for the ion triplet "FeOx(aq)–Mg^{+2}–Na^+". This experiment is an addition to TP-08-02 and this triplet is not listed in Table 1-1. This triplet is listed in Table 1-2 (Item 28, Table 1-2).

Ferrous oxalate dihydrate ($FeC_2O_4 \cdot 2H_2O$) was purchased from Alfa Aesar (puratronic, 99.999 % metal basis), and magnesium chloride hexahydrate ($MgCl_2 \cdot 6H_2O$) and sodium chloride (NaCl) were purchased from Fisher. A known mass of $FeC_2O_4 \cdot 2H_2O$ was added to 50 mL of mixed $MgCl_2$ and NaCl solutions as shown in Table 3-53 below.

The experimental set-ups were periodically monitored for pH. Once stable pH readings were achieved, the concentrations of other dissolved components (ferrous iron, magnesium, sodium, and chloride) were or are measured. Experimental results gathered to date are shown in Table 3-54.

Table 3-53 Preparation of experimental set-ups for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in mixed $MgCl_2$ and NaCl solutions (the "FeOx(aq)—Mg^{2+}—Na^+" experiment).

Set-up ID	$FeC_2O_4 \cdot 2H_2O(s)$ (g)	$MgCl_2$ (m)	NaCl (m)	Reference
FeOxMgNa-1-1	0.1495	0.479	4.83	WIPP-Solubility-7, p.47
FeOxMgNa-1-2	0.1056	0.479	4.83	
FeOxMgNa-1-3	0.1167	0.479	4.83	
FeOxMgNa-2-1	0.1599	0.752	3.24	
FeOxMgNa-2-2	0.1447	0.752	3.24	
FeOxMgNa-2-3	0.1197	0.752	3.24	
FeOxMgNa-3-1	0.144	1.11	2.64	
FeOxMgNa-3-2	0.1276	1.11	2.64	
FeOxMgNa-3-3	0.1177	1.11	2.64	
FeOxMgNa-4-1	0.1377	1.3	1.76	
FeOxMgNa-4-2	0.1511	1.3	1.76	
FeOxMgNa-4-3	0.1112	1.3	1.76	
FeOxMgNa-5-1	0.1876	1.47	1.28	
FeOxMgNa-5-2	0.1323	1.47	1.28	
FeOxMgNa-5-3	0.105	1.47	1.28	
FeOxMgNa-6-1	0.1269	1.65	0.545	
FeOxMgNa-6-2	0.139	1.65	0.545	
FeOxMgNa-6-3	0.1283	1.65	0.545	

Table 3-54 Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in mixed $MgCl_2$ and NaCl solutions (the "FeOx(aq)—Mg^{2+}—Na^{+}" experiment).

	pH*							
Set-up ID	**(9 day)**	**(28 days)**	**(29 days)**	**(80 days)**	**(83 days)**	**(84 days)**	**(390 days)**	**(394 days)**
FeOxMgNa-1-1	6.391	6.272	-	5.529	-	-	5.325	-
FeOxMgNa-1-2	6.473	6.202	-	5.755	-	-	5.629	-
FeOxMgNa-1-3	6.325	6.289	-	5.729	-	-	5.924	-
FeOxMgNa-2-1	6.438	6.324	-	-	5.61	-	5.911	-
FeOxMgNa-2-2	6.637	6.417	-	-	5.914	-	5.878	-
FeOxMgNa-2-3	6.665	6.514	-	-	6.001	-	6.017	-
FeOxMgNa-3-1	5.925	-	5.694	-	5.347	-	-	5.682
FeOxMgNa-3-2	6.076	-	5.823	-	5.704	-	-	5.836
FeOxMgNa-3-3	6.149	-	5.916	-	5.743	-	-	5.574
FeOxMgNa-4-1	6.347	-	6.05	-	-	5.648	-	5.864
FeOxMgNa-4-2	6.376	-	6.084	-	-	5.824	-	5.970
FeOxMgNa-4-3	6.463	-	6.111	-	-	5.933	-	6.062
FeOxMgNa-5-1	5.734	-	5.458	-	5.554	-	-	5.162
FeOxMgNa-5-2	6.021	-	5.703	-	5.687	-	-	5.624
FeOxMgNa-5-3	6.07	-	5.784	-	5.755	-	-	5.715
FeOxMgNa-6-1	5.795	-	5.472	-	5.216	-	-	5.187
FeOxMgNa-6-2	5.783	-	5.426	-	5.342	-	-	5.366
FeOxMgNa-6-3	5.817	-	5.463	-	5.415	-	-	5.424
Reference	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48	WIPP-Solubility-7, p.48

* Measured with pH electrode and meter.

Table 3-54 (continued) Measured data for the solubility of $FeC_2O_4 \cdot 2H_2O(s)$ in mixed $MgCl_2$ and NaCl solutions (the "FeOx(aq)—Mg^{2+}—Na^{+}" experiment).

Set-up ID	$([Fe(II)]_{diss}$, (mol/L)[a] (520 days)	$[Na(I)]_{diss}$, (mol/L)[b] (520 days)	$[Mg(II)]_{diss}$, (mol/L)[b] (520 days)
FeOxMgNa-1-1	8.79E-03	4.12E+00	4.85E-01
FeOxMgNa-1-2	8.15E-03	4.26E+00	5.30E-01
FeOxMgNa-1-3	8.30E-03	4.34E+00	5.03E-01
FeOxMgNa-2-1	1.08E-02	2.87E+00	7.81E-01
FeOxMgNa-2-2	1.08E-02	3.02E+00	8.22E-01
FeOxMgNa-2-3	9.20E-03	2.91E+00	7.84E-01
FeOxMgNa-3-1	1.19E-02	2.32E+00	1.13E+00
FeOxMgNa-3-2	1.08E-02	2.45E+00	1.18E+00
FeOxMgNa-3-3	9.91E-03	2.31E+00	1.13E+00
FeOxMgNa-4-1	1.14E-02	1.56E+00	1.29E+00
FeOxMgNa-4-2	1.21E-02	1.55E+00	1.26E+00
FeOxMgNa-4-3	9.55E-03	1.60E+00	1.31E+00
FeOxMgNa-5-1	1.44E-02	1.16E+00	1.40E+00
FeOxMgNa-5-2	1.07E-02	1.17E+00	1.45E+00
FeOxMgNa-5-3	9.54E-03	1.15E+00	1.43E+00
FeOxMgNa-6-1	1.07E-02	5.55E-01	1.63E+00
FeOxMgNa-6-2	1.17E-02	5.30E-01	1.59E+00
FeOxMgNa-6-3	1.09E-02	5.39E-01	1.56E+00
Reference	WIPP-Solubility-15, p.53, 54	WIPP-Solubility-15, p.65	WIPP-Solubility-15, p.65

[a] Measured using the Ferrozine method

[b] Measured using the ICP-AES.

3.29 Solubility of $Ca_3(C_6H_5O_7)_2 \cdot 4H_2O(s)$ ($Ca_3[Citrate]_2 \cdot 4H_2O(s)$) in NaCl solutions (the "Na^+—$CaCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of earlandite ($Ca_3[Citrate]_2 \cdot 4H_2O(s)$, calcium citrate tribasic tetrahydrate) in NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Na^+—$CaCit^-$" (Item 29, Table 1-2).

A known mass of earlandite (calcium citrate tribasic tetrahydrate) from ACROS Organics was added to 100 mL of NaCl solutions as shown in Table 3-55 below.

The experimental set-ups are periodically monitored for pH and dissolved calcium. Concentrations of other dissolved components (sodium, chloride, and citrate) are also determined. Experimental results gathered to date are shown in Table 3-56.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 662 days. As an example, the pH readings for ACROS-ELDT-0.01-1 are between 7.6 and 7.7. The corresponding calcium concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-55 Preparation of experimental set-ups for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment).

Set-up ID	Earlandite (g)	NaCl (m)	Reference
ACROS-ELDT-0.01-1	2.0197	0.01	WIPP-Solubility-3, p. 62
ACROS-ELDT-0.01-2	2.01	0.01	WIPP-Solubility-3, p. 62
ACROS-ELDT-0.1-1	2.0176	0.1	WIPP-Solubility-3, p. 62
ACROS-ELDT-0.1-2	2.0199	0.1	WIPP-Solubility-3, p. 62
ACROS-ELDT-1.0-1	2.0128	1	WIPP-Solubility-3, p. 62
ACROS-ELDT-1.0-2	2.0254	1	WIPP-Solubility-3, p. 62
ACROS-ELDT-2.0-1	2.0162	2.1	WIPP-Solubility-3, p. 62
ACROS-ELDT-2.0-2	2.0198	2.1	WIPP-Solubility-3, p. 62
ACROS-ELDT-3.0-1	2.0146	3.2	WIPP-Solubility-3, p. 62
ACROS-ELDT-3.0-2	2.0057	3.2	WIPP-Solubility-3, p. 62
ACROS-ELDT-5.0-1	2.0108	5	WIPP-Solubility-3, p. 62
ACROS-ELDT-5.0-2	2.0009	5	WIPP-Solubility-3, p. 62

Table 3-56 Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**182 Days**	**375 Days**	**662 Days**	**712 Days**	**760 Days**	**815 Days**
ACROS-ELDT-0.01-1	6.98	7.15	7.55	7.69	7.68	7.72
ACROS-ELDT-0.01-2	6.96	7.27	7.54	7.70	7.65	7.71
ACROS-ELDT-0.1-1	6.46	6.84	7.36	7.52	7.65	7.62
ACROS-ELDT-0.1-2	6.52	6.97	7.44	7.59	7.62	7.62
ACROS-ELDT-1.0-1	6.27	6.62	7.01	7.14	7.13	7.21
ACROS-ELDT-1.0-2	6.36	6.24	6.44	6.47	6.42	6.48
ACROS-ELDT-2.0-1	5.77	5.51	5.67	5.73	5.78	5.89
ACROS-ELDT-2.0-2	5.80	5.48	5.74	5.81	5.85	5.98
ACROS-ELDT-3.0-1	5.03	5.13	5.51	5.60	5.72	5.94
ACROS-ELDT-3.0-2	4.81	4.91	5.11	5.14	5.65	5.27
ACROS-ELDT-5.0-1	4.17	3.94	4.06	3.94	3.93	3.92
ACROS-ELDT-5.0-2	4.14	3.98	4.06	3.92	3.94	3.93
Reference	WIPP-Solubililty-3 Pg. 87-89, WIPP-Solubility-12 pg. 8-9	WIPP-Solubility-12 pg. 21,23	WIPP-Solubility-12 pg. 87	WIPP-Solubility-21 pg. 18	WIPP-Solubility-21 pg. 52	WIPP-Solubility-21 pg. 79

Table 3-56 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment). Na measured with ICP-AES.

	[Na(I)] (m)					
Set-up ID	**182 Days**	**375 Days**	**662 Days**	**712 Days**	**760 Days**	**815 Days**
ACROS-ELDT-0.01-1	1.07E-02	1.09E-02	1.07E-02	1.18E-02	9.19E-03	9.76E-03
ACROS-ELDT-0.01-2	1.12E-02	1.12E-02	1.13E-02	9.81E-03	9.05E-03	9.70E-03
ACROS-ELDT-0.1-1	9.73E-02	1.05E-02	1.20E-01	1.01E-01	9.05E-02	9.91E-02
ACROS-ELDT-0.1-2	9.56E-02	1.14E-02	1.12E-01	9.56E-02	8.78E-02	9.06E-02
ACROS-ELDT-1.0-1	9.64E-01	8.80E-01	9.43E-01	1.00E+00	8.81E-01	8.75E-01
ACROS-ELDT-1.0-2	9.57E-01	9.76E-01	9.20E-01	9.98E-01	8.90E-01	9.52E-01
ACROS-ELDT-2.0-1	1.98E+00	1.82E+00	2.00E+00	1.94E+00	1.92E+00	1.93E+00
ACROS-ELDT-2.0-2	2.04E+00	1.75E+00	1.91E+00	1.92E+00	1.83E+00	1.84E+00
ACROS-ELDT-3.0-1	2.86E+00	2.77E+00	2.75E+00	3.09E+00	2.32E+00	2.78E+00
ACROS-ELDT-3.0-2	2.86E+00	2.76E+00	2.79E+00	2.97E+00	2.46E+00	2.72E+00
ACROS-ELDT-5.0-1	5.03E+00	4.40E+00	4.55E+00	4.84E+00	4.09E+00	4.50E+00
ACROS-ELDT-5.0-2	4.82E+00	4.82E+00	4.48E+00	4.53E+00	4.17E+00	4.20E+00
Reference	WIPP-Solubility-14 pg. 80 & WIPP-Solubility-13 Pg. 13	WIPP-Solubility-13 pg. 79 &WIPP-Solubility-10 Pg. 96	WIPP-Solubility-13 pg. 79	WIPP-Solubility-22 Pg. 50	WIPP-Solubility-24 Pg. 18-19	WIPP-Solubility-24 Pg. 94-95

Table 3-56 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment). Ca measured with ICP-AES.

	[Ca(II)] (m)					
Set-up ID	**182 Days**	**375 Days**	**662 Days**	**712 Days**	**760 Days**	**815 Days**
ACROS-ELDT-0.01-1	5.23E-03	4.65E-03	4.84E-03	5.07E-03	5.20E-03	5.05E-03
ACROS-ELDT-0.01-2	5.39E-03	5.02E-03	4.73E-03	4.97E-03	5.04E-03	4.87E-03
ACROS-ELDT-0.1-1	7.25E-03	6.93E-03	6.75E-03	6.80E-03	6.99E-03	6.77E-03
ACROS-ELDT-0.1-2	7.89E-03	6.67E-03	6.75E-03	6.90E-03	6.79E-03	6.39E-03
ACROS-ELDT-1.0-1	1.38E-02	1.20E-02	1.17E-02	1.16E-02	1.17E-02	1.11E-02
ACROS-ELDT-1.0-2	1.85E-02	1.24E-02	1.16E-02	1.18E-02	1.19E-02	1.17E-02
ACROS-ELDT-2.0-1	1.55E-02	1.43E-02	1.77E-02	1.75E-02	1.78E-02	1.76E-02
ACROS-ELDT-2.0-2	1.54E-02	1.38E-02	1.72E-02	1.73E-02	1.72E-02	1.74E-02
ACROS-ELDT-3.0-1	2.84E-02	2.33E-02	2.60E-02	2.61E-02	2.57E-02	2.59E-02
ACROS-ELDT-3.0-2	2.97E-02	2.55E-02	2.62E-02	2.65E-02	2.58E-02	2.57E-02
ACROS-ELDT-5.0-1	4.23E-04	3.13E-02	3.43E-02	3.40E-02	3.39E-02	3.42E-02
ACROS-ELDT-5.0-2	4.62E-04	3.33E-02	3.45E-02	3.39E-02	3.38E-02	3.23E-02
Reference	WIPP-Solubility-10 Pg. 18, 20	WIPP-Solubility-10 pg. 98	WIPP-Solubility-13 pg. 89	WIPP-Solubility-22 pg. 20	WIPP-Solubility-24 Pg. 16	WIPP-Solubility-24 Pg. 83-84

Table 3-56 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment). Cl^- measured with IC.

	[Cl(-I)] (m)				
Set-up ID	**182 Days**	**375 Days**	**662 Days**	**760 Days**	**815 Days**
ACROS-ELDT-0.01-1	4.31E-02	2.39E-02	9.51E-03	1.01E-02	9.91E-03
ACROS-ELDT-0.01-2	3.85E-02	2.36E-02	9.55E-03	1.01E-02	9.90E-03
ACROS-ELDT-0.1-1	9.96E-02	9.44E-02	9.59E-02	1.01E-01	9.76E-02
ACROS-ELDT-0.1-2	9.79E-02	9.86E-02	9.30E-02	1.01E-01	9.95E-02
ACROS-ELDT-1.0-1	1.02E+00	8.78E-01	8.88E-01	1.02E+00	9.81E-01
ACROS-ELDT-1.0-2	9.47E-01	9.63E-01	8.99E-01	1.01E+00	9.81E-01
ACROS-ELDT-2.0-1	2.19E+00	1.88E+00	1.80E+00	2.04E+00	1.97E+00
ACROS-ELDT-2.0-2	2.16E+00	1.92E+00	1.82E+00	2.02E+00	1.96E+00
ACROS-ELDT-3.0-1	3.08E+00	2.92E+00	2.64E+00	3.03E+00	2.92E+00
ACROS-ELDT-3.0-2	3.23E+00	2.99E+00	2.86E+00	3.01E+00	2.90E+00
ACROS-ELDT-5.0-1	5.47E+00	4.87E+00	4.38E+00	4.99E+00	4.82E+00
ACROS-ELDT-5.0-2	5.29E+00	6.08E+00	4.23E+00	5.02E+00	4.84E+00
Reference	WIPP-Solubility-16 pg. 13 & WIPP-Solubility-24 Pg. 33, 42	WIPP-Solubility-14 Pg. 24 & WIPP-Solubility-24 Pg. 33.42	WIPP-Solubility-19 Pgs. 8, 26-27 & 30	WIPP-Solubility-24 Pg. 63-64	WIPP-Solubility-24 Pg. 98-99

Table 3-56 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in NaCl solutions (the "Na^+—$CaCit^-$" experiment). Citrate measured with IC.

	[$Citrate^{3-}$] (m)					
Set-up ID	**182 Days**	**375 Days**	**662 Days**	**712 Days**	**760 Days**	**815 Days**
ACROS-ELDT-0.01-1	3.11E-03	2.88E-03	2.84E-03	2.67E-03	2.77E-03	2.90E-03
ACROS-ELDT-0.01-2	3.47E-03	2.84E-03	2.83E-03	2.85E-03	2.82E-03	2.87E-03
ACROS-ELDT-0.1-1	5.16E-03	4.13E-03	4.15E-03	3.99E-03	3.99E-03	4.00E-03
ACROS-ELDT-0.1-2	4.94E-03	4.23E-03	3.95E-03	3.95E-03	4.06E-03	3.98E-03
ACROS-ELDT-1.0-1	NA	7.41E-03	7.06E-03	6.82E-03	7.42E-03	7.34E-03
ACROS-ELDT-1.0-2	NA	7.78E-03	7.18E-03	7.13E-03	7.85E-03	7.68E-03
ACROS-ELDT-2.0-1	8.15E-03	5.49E-03	4.27E-03	4.02E-03	4.61E-03	4.68E-03
ACROS-ELDT-2.0-2	8.68E-03	5.66E-03	4.46E-03	4.20E-03	4.59E-03	4.45E-03
ACROS-ELDT-3.0-1	NA	2.34E-03	2.18E-03	2.17E-03	2.02E-03	2.01E-03
ACROS-ELDT-3.0-2	NA	2.67E-03	2.30E-03	2.37E-03	2.31E-03	2.39E-03
ACROS-ELDT-5.0-1	1.43E-03	1.03E-03	4.55E-04	6.61E-04	5.45E-04	5.88E-04
ACROS-ELDT-5.0-2	1.35E-03	1.02E-03	5.25E-04	6.92E-04	6.32E-04	NA
Reference	WIPP-Solubility-26 Pg. 26	WIPP-Solubility-26 Pg. 26	WIPP-Solubility-26 Pg. 26	WIPP-Solubility-26 Pg. 26	WIPP-Solubility-26 Pg. 29	WIPP-Solubility-26 Pg. 29

3.30 Solubility of $Ca_3(C_6H_5O_7)_2 \cdot 4H_2O(s)$ ($Ca_3[Citrate]_2 \cdot 4H_2O(s)$) in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment)

The objectives of this set of experiments are to (1) determine the solubility of earlandite ($Ca_3[Citrate]_2 \cdot 4H_2O(s)$) in $MgCl_2$ (magnesium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Mg^{2+}—$CaCit^-$" (Item 30, Table 1-2).

A known mass of earlandite (calcium citrate tribasic tetrahydrate) from ACROS Organics was added to 100 mL of $MgCl_2$ solutions as shown in Table 3-57 below.

The experimental set-ups are periodically monitored for pH and dissolved calcium. Concentrations of other dissolved components (magnesium, chloride, and citrate) are also determined. Experimental results gathered to date are shown in Table 3-58.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 709 days. As an example, the pH readings for ACROS-ELDT-0.01Mg-1 are between 7.8 and 8.0. The corresponding calcium concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-57 Preparation of experimental set-ups for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment).

Set-up ID	Erlandite (g)	$MgCl_2$ (m)	Reference
ACROS-ELDT-0.01 Mg-1	2.0117	0.01	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-0.01 Mg-2	2.0028	0.01	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-0.1 Mg-1	2.0075	0.1	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-0.1 Mg-2	2.0142	0.1	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-1.0 Mg-1	2.0195	1	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-1.0 Mg-2	2.0067	1	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-1.5 Mg-1	2.0126	1.5	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-1.5 Mg-2	2.0048	1.5	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-2.0 Mg-1	2.0129	2	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-2.0 Mg-2	2.0167	2	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-2.5 Mg-1	2.0088	2.5	WIPP-Solubility-3 Pg. 62
ACROS-ELDT-2.5 Mg-2	2.0063	2.5	WIPP-Solubility-3 Pg. 62

Table 3-58 Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment). pH data measured with pH electrode and meter.

	pH						
Set-up ID	**203 Days**	**385 Days**	**458 Days**	**660 Days**	**709 Days**	**758 Days**	**813 Days**
ACROS-ELDT-0.01 Mg-1	6.93	7.24	7.46	7.63	7.80	7.77	7.96
ACROS-ELDT-0.01 Mg-2	7.01	7.40	7.64	7.69	7.80	7.80	7.78
ACROS-ELDT-0.1 Mg-1	5.68	5.32	5.56	5.54	5.58	5.56	5.70
ACROS-ELDT-0.1 Mg-2	5.68	5.34	5.60	5.54	5.59	5.55	5.71
ACROS-ELDT-1.0 Mg-1	4.36	4.15	4.34	4.35	4.36	4.38	4.42
ACROS-ELDT-1.0 Mg-2	4.37	4.27	4.39	4.39	4.38	4.52	4.46
ACROS-ELDT-1.5 Mg-1	4.16	3.92	3.76	4.16	4.14	4.22	4.22
ACROS-ELDT-1.5 Mg-2	4.19	3.91	3.98	4.17	4.14	4.11	4.21
ACROS-ELDT-2.0 Mg-1	4.12	3.84	4.03	4.14	4.12	4.05	4.19
ACROS-ELDT-2.0 Mg-2	4.46	4.23	4.18	4.52	4.20	4.38	4.56
ACROS-ELDT-2.5 Mg-1	4.00	3.76	3.87	3.95	4.06	4.04	4.12
ACROS-ELDT-2.5 Mg-2	3.76	3.31	3.50	3.61	3.62	3.53	3.69
Reference	WIPP-Solubility -3 pg. 89-92	WIPP-Solubility -12 pg. 23-24	WIPP-Solubility -12 pg. 42-43	WIPP-Solubility -12 pg. 89	WIPP-Solubility -21 pg. 19-20	WIPP-Solubility-21 pg. 53	WIPP-Solubility -21 pg. 80

Table 3-58 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)						
Set-up ID	**203 Days**	**385 Days**	**458 Days**	**660 Days**	**709 Days**	**758 Days**	**813 Days**
ACROS-ELDT-0.01 Mg-1	1.75E-02	9.78E-03	9.63E-03	9.49E-03	9.64E-03	9.73E-03	9.38E-03
ACROS-ELDT-0.01 Mg-2	1.28E-02	9.88E-03	9.81E-03	9.30E-03	9.59E-03	9.85E-03	9.36E-03
ACROS-ELDT-0.1 Mg-1	1.25E-01	8.47E-02	8.46E-02	7.83E-02	8.08E-02	7.67E-02	7.16E-02
ACROS-ELDT-0.1 Mg-2	1.24E-01	8.44E-02	8.58E-02	8.08E-02	7.98E-02	7.81E-02	7.60E-02
ACROS-ELDT-1.0 Mg-1	1.04E+00	9.40E-01	9.56E-01	9.33E-01	9.19E-01	9.13E-01	9.36E-01
ACROS-ELDT-1.0 Mg-2	1.01E+00	9.55E-01	9.49E-01	9.52E-01	9.39E-01	8.82E-01	9.44E-01
ACROS-ELDT-1.5 Mg-1	1.10E+00	1.30E+00	1.39E+00	1.36E+00	1.32E+00	1.37E+00	1.40E+00
ACROS-ELDT-1.5 Mg-2	1.07E+00	1.38E+00	1.39E+00	1.37E+00	1.35E+00	1.39E+00	1.39E+00
ACROS-ELDT-2.0 Mg-1	1.47E+00	1.69E+00	1.77E+00	1.77E+00	1.62E+00	1.76E+00	1.79E+00
ACROS-ELDT-2.0 Mg-2	1.42E+00	1.71E+00	1.78E+00	1.73E+00	1.69E+00	1.75E+00	1.81E+00
ACROS-ELDT-2.5 Mg-1	1.73E+00	1.72E+00	2.15E+00	2.04E+00	2.23E+00	2.32E+00	2.25E+00
ACROS-ELDT-2.5 Mg-2	1.72E+00	1.75E+00	2.26E+00	2.26E+00	2.36E+00	2.28E+00	2.33E+00
Reference	WIPP-Solubility-10 pg. 28	WIPP-Solubility-14 pg. 27	WIPP-Solubility -22 Pg. 24	WIPP-Solubility -13 pg. 73	WIPP-Solubility -22 Pg. 25	WIPP-Solubility -24 Pg. 10	WIPP-Solubility -26 Pg. 7

Table 3-58 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment). Ca measured with ICP-AES.

	[Ca(II)] (m)						
Set-up ID	**203 Days**	**385 Days**	**458 Days**	**660 Days**	**709 Days**	**758 Days**	**813 Days**
ACROS-ELDT-0.01 Mg-1	7.85E-03	7.82E-03	7.89E-03	7.90E-03	8.15E-03	8.12E-03	8.07E-03
ACROS-ELDT-0.01 Mg-2	7.87E-03	7.69E-03	7.87E-03	7.58E-03	8.04E-03	7.78E-03	7.85E-03
ACROS-ELDT-0.1 Mg-1	2.53E-02	2.70E-02	2.78E-02	3.01E-02	3.19E-02	3.07E-02	3.03E-02
ACROS-ELDT-0.1 Mg-2	2.32E-02	2.66E-02	2.87E-02	3.07E-02	3.14E-02	3.16E-02	3.19E-02
ACROS-ELDT-1.0 Mg-1	5.30E-02	4.12E-02	4.59E-02	4.88E-02	4.96E-02	4.93E-02	4.94E-02
ACROS-ELDT-1.0 Mg-2	5.11E-02	4.11E-02	4.56E-02	4.87E-02	4.91E-02	4.75E-02	4.91E-02
ACROS-ELDT-1.5 Mg-1	5.36E-02	3.61E-02	4.56E-02	4.91E-02	4.94E-02	5.06E-02	4.99E-02
ACROS-ELDT-1.5 Mg-2	5.34E-02	3.79E-02	4.59E-02	4.89E-02	4.79E-02	4.99E-02	4.99E-02
ACROS-ELDT-2.0 Mg-1	5.13E-02	3.49E-02	4.55E-02	4.87E-02	4.82E-02	4.93E-02	4.96E-02
ACROS-ELDT-2.0 Mg-2	5.24E-02	3.60E-02	4.59E-02	4.87E-02	4.98E-02	5.06E-02	4.98E-02
ACROS-ELDT-2.5 Mg-1	4.98E-02	3.15E-02	4.28E-02	4.65E-02	4.79E-02	4.85E-02	4.77E-02
ACROS-ELDT-2.5 Mg-2	4.93E-02	3.18E-02	4.27E-02	4.62E-02	4.85E-02	4.75E-02	4.73E-02
Reference	WIPP-Solubility -10 pg. 18, 20	WIPP-Solubility -10 pg. 98 & WIPP-Solubility -14 Pg. 3	WIPP-Solubility -14 pg. 36-37	WIPP-Solubility -13 pg. 93	WIPP-Solubility -22 pg. 20	WIPP-Solubility-24 Pg. 16	WIPP-Solubility -24 Pg. 83-84

Table 3-58 (continued) Measured data for the solubility of $Ca_3[Citrate]_2 \cdot 4H_2O(s)$ in $MgCl_2$ solutions (the "Mg^{2+}—$CaCit^-$" experiment). Citrate measured with IC.

	[Citrate3-] (m)		
Set-up ID	**203 Days**	**385 Days**	**458 Days**
ACROS-ELDT-0.01 Mg-1	5.26E-03	4.93E-03	4.16E-03
ACROS-ELDT-0.01 Mg-2	5.33E-03	4.80E-03	4.25E-03
ACROS-ELDT-0.1 Mg-1	NA	7.61E-03	6.66E-03
ACROS-ELDT-0.1 Mg-2	NA	7.55E-03	6.86E-03
ACROS-ELDT-1.0 Mg-1	1.53E-02	1.11E-02	9.80E-03
ACROS-ELDT-1.0 Mg-2	1.54E-02	1.11E-02	1.02E-02
ACROS-ELDT-1.5 Mg-1	1.52E-02	1.09E-02	9.77E-03
ACROS-ELDT-1.5 Mg-2	1.47E-02	1.10E-02	9.75E-03
ACROS-ELDT-2.0 Mg-1	1.33E-02	9.52E-03	NA
ACROS-ELDT-2.0 Mg-2	1.29E-02	9.49E-03	NA
ACROS-ELDT-2.5 Mg-1	1.10E-02	6.54E-03	NA
ACROS-ELDT-2.5 Mg-2	1.01E-02	6.58E-03	NA
Reference	WIPP-Solubility-26 Pg. 44-45	WIPP-Solubility-26 Pg. 44-45	WIPP-Solubility-26 Pg. 44-45

3.31 Solubility of $Ca_2C_{10}H_{12}N_2O_8$(s) (Ca_2EDTA(s)) in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment).

The objectives of this set of experiments are to (1) determine the solubility of Ca_2EDTA (dicalcium EDTA) in NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Cl^-—$HEDTA^{3-}$" (Item 31, Table 1-2).

A known mass of Ca_2EDTA from ACROS Organics was added to 100 mL of NaCl solutions as shown in Table 3-59 below.

The experimental set-ups are periodically monitored for pH and dissolved calcium. Concentrations of other dissolved components (sodium, chloride, and EDTA) are also determined. Experimental results gathered to date are shown in Table 3-60.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 965 days. As an example, the pH readings for Ca_2EDTA-0.01-1 are between 7.8 and 7.9. The corresponding calcium concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-59 Preparation of experimental set-ups for the solubility of Ca_2EDTA(s) in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment).

Set-up ID	Ca_2EDTA(s) (g)	NaCl (m)	Reference
Ca_2EDTA-0.01-1	2.007	0.01	WIPP-Solubility-3, p. 9-10
Ca_2EDTA-0.01-2	2.0029	0.01	WIPP-Solubility-3, p. 9-10
Ca_2EDTA-0.1-1	2.0075	0.1	WIPP-Solubility-3, p. 9-10
Ca_2EDTA-0.1-2	2.0052	0.1	WIPP-Solubility-3, p. 9-10
Ca_2EDTA-1.0-1	4.0081	1	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-1.0-2	4.0084	1	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-2.0-1	4.0088	2.1	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-2.0-2	4.013	2.1	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-3.0-1	4.0094	3.2	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-3.0-2	4.0072	3.2	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-4.0-1	4.0093	4.4	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-4.0-2	4.0087	4.4	WIPP-Solubility-3, p. 9-10, and p. 19
Ca_2EDTA-5.0-1	2.0034	5	WIPP-Solubility-3, p. 9-10
Ca_2EDTA-5.0-2	2.0011	5	WIPP-Solubility-3, p. 9-10

Table 3-60 Measured data for the solubility of $Ca_2EDTA(s)$ in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**390 Days**	**965 Days**	**1050 Days**	**1099 Days**	**1149 Days**	**1150 Days**
Ca_2EDTA-0.01-1	8.23	7.79	7.84	7.88	7.94	7.86
Ca_2EDTA-0.01-2	8.20	7.85	7.83	7.86	7.92	7.87
Ca_2EDTA-0.1-1	8.36	7.87	7.80	7.89	7.95	7.89
Ca_2EDTA-0.1-2	7.89	7.80	7.80	7.84	7.89	7.90
Ca_2EDTA-1.0-1	8.24	7.94	7.85	7.88	7.87	7.85
Ca_2EDTA-1.0-2	7.77	7.62	7.53	7.57	7.58	7.57
Ca_2EDTA-2.0-1	8.22	7.86	7.81	7.81	7.77	7.78
Ca_2EDTA-2.0-2	8.17	7.88	7.79	7.79	7.82	7.75
Ca_2EDTA-3.0-1	8.23	7.95	7.75	7.77	7.87	7.75
Ca_2EDTA-3.0-2	7.99	7.82	7.72	7.71	7.74	7.71
Ca_2EDTA-4.0-1	8.03	7.75	7.71	7.67	7.68	7.65
Ca_2EDTA-4.0-2	7.97	7.74	7.67	7.65	7.69	7.64
Ca_2EDTA-5.0-1	7.44	7.36	7.39	7.39	7.48	7.44
Ca_2EDTA-5.0-2	7.44	7.35	7.35	7.39	7.43	7.40
Reference	WIPP-Solubility-3 pg. 56	WIPP-Solubility-12 pgs. 55-56	WIPP-Solubility-12 pg. 72	WIPP-Solubility-21 pg. 5	WIPP-Solubility-21 pg. 37	WIPP-Solubility-21 pg. 65

Table 3-60 (continued) Measured data for the solubility of $Ca_2EDTA(s)$ in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment). Na measured with ICP-AES.

	[Na(I)] (m)					
Set-up ID	**390 Days**	**965 Days**	**1050 Days**	**1099 Days**	**1149 Days**	**1150 Days**
Ca_2EDTA-0.01-1	1.16E-02	1.09E-02	1.16E-02	1.17E-02	1.16E-02	1.09E-02
Ca_2EDTA-0.01-2	1.15E-02	1.09E-02	1.13E-02	1.15E-02	1.16E-02	1.10E-02
Ca_2EDTA-0.1-1	9.20E-02	8.47E-02	9.24E-02	9.49E-02	9.32E-02	9.15E-02
Ca_2EDTA-0.1-2	9.18E-02	8.69E-02	9.77E-02	9.18E-02	9.24E-02	9.17E-02
Ca_2EDTA-1.0-1	8.52E-01	8.90E-01	8.94E-01	9.08E-01	8.73E-01	8.77E-01
Ca_2EDTA-1.0-2	8.51E-01	8.99E-01	8.95E-01	9.20E-01	8.44E-01	8.89E-01
Ca_2EDTA-2.0-1	1.90E+00	1.94E+00	1.93E+00	1.93E+00	1.90E+00	1.83E+00
Ca_2EDTA-2.0-2	1.83E+00	1.92E+00	1.96E+00	1.91E+00	1.92E+00	1.86E+00
Ca_2EDTA-3.0-1	2.52E+00	2.84E+00	2.66E+00	2.91E+00	2.52E+00	2.59E+00
Ca_2EDTA-3.0-2	2.53E+00	2.90E+00	2.70E+00	2.65E+00	2.59E+00	2.65E+00
Ca_2EDTA-4.0-1	3.37E+00	3.32E+00	3.51E+00	3.42E+00	3.42E+00	3.45E+00
Ca_2EDTA-4.0-2	3.36E+00	3.26E+00	3.42E+00	3.29E+00	3.35E+00	3.40E+00
Ca_2EDTA-5.0-1	3.76E+00	3.69E+00	4.14E+00	3.89E+00	3.02E+00	3.89E+00
Ca_2EDTA-5.0-2	3.85E+00	3.83E+00	4.09E+00	3.89E+00	3.41E+00	3.72E+00
Reference	WIPP-Solubility-24 Pg. 51	WIPP-Solubility-16 pgs. 36,38,39	WIPP-Solubility-13 pg. 61	WIPP-Solubility-22 Pg. 55	WIPP-Solubility-22 Pg.92	WIPP-Solubility-24 Pg. 52

Table 3-60 (continued) Measured data for the solubility of $Ca_2EDTA(s)$ in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment). Ca measured with ICP-AES.

	[Ca(II)] (m)					
Set-up ID	**390 Days**	**965 Days**	**1050 Days**	**1099 Days**	**1149 Days**	**1150 Days**
Ca_2EDTA-0.01-1	7.14E-02	7.27E-02	7.30E-02	7.33E-02	7.24E-02	7.10E-02
Ca_2EDTA-0.01-2	7.16E-02	7.28E-02	7.27E-02	7.26E-02	6.64E-02	7.13E-02
Ca_2EDTA-0.1-1	8.63E-02	8.36E-02	8.49E-02	8.42E-02	8.39E-02	8.46E-02
Ca_2EDTA-0.1-2	8.69E-02	7.99E-02	8.52E-02	8.17E-02	8.40E-02	8.49E-02
Ca_2EDTA-1.0-1	1.35E-01	1.21E-01	1.21E-01	1.22E-01	1.20E-01	1.21E-01
Ca_2EDTA-1.0-2	1.35E-01	1.22E-01	1.21E-01	1.24E-01	1.18E-01	1.21E-01
Ca_2EDTA-2.0-1	1.39E-01	1.20E-01	1.20E-01	1.21E-01	1.20E-01	1.18E-01
Ca_2EDTA-2.0-2	1.42E-01	1.19E-01	1.23E-01	1.20E-01	1.24E-01	1.20E-01
Ca_2EDTA-3.0-1	1.35E-01	1.08E-01	1.09E-01	1.07E-01	1.09E-01	1.05E-01
Ca_2EDTA-3.0-2	1.30E-01	1.09E-01	1.08E-01	1.05E-01	1.11E-01	1.07E-01
Ca_2EDTA-4.0-1	1.17E-01	9.31E-02	9.15E-02	9.11E-02	9.62E-02	9.25E-02
Ca_2EDTA-4.0-2	1.18E-01	9.16E-02	9.41E-02	9.35E-02	9.28E-02	9.12E-02
Ca_2EDTA-5.0-1	1.10E-01	8.55E-02	8.97E-02	8.38E-02	8.12E-02	8.49E-02
Ca_2EDTA-5.0-2	1.10E-01	8.49E-02	8.57E-02	8.23E-02	8.14E-02	8.13E-02
Reference	WIPP-Solubility-3 Pg. 72-74	WIPP-Solubility-16 Pg. 33	WIPP-Solubility-13 pg. 56	WIPP-Solubility-22 pg. 21	WIPP-Solubility-24 Pg. 14	WIPP-Solubility-24 Pg. 65

Table 3-60 (continued) Measured data for the solubility of $Ca_2EDTA(s)$ in NaCl solutions (the "Cl^-—$HEDTA^{3-}$" experiment). EDTA measured with IC.

	[EDTA4-] (m)					
Set-up ID	**390 Days**	**965 Days**	**1050 Days**	**1099 Days**	**1149 Days**	**1150 Days**
Ca_2EDTA-0.01-1	5.84E-02	5.64E-02	5.75E-02	5.25E-02	5.42E-02	5.42E-02
Ca_2EDTA-0.01-2	3.69E-02	5.62E-02	5.79E-02	5.30E-02	5.37E-02	5.47E-02
Ca_2EDTA-0.1-1	6.79E-02	6.68E-02	7.11E-02	6.27E-02	6.33E-02	6.39E-02
Ca_2EDTA-0.1-2	6.70E-02	6.68E-02	6.84E-02	6.28E-02	6.35E-02	6.42E-02
Ca_2EDTA-1.0-1	9.08E-02	8.97E-02	9.20E-02	8.74E-02	8.85E-02	8.95E-02
Ca_2EDTA-1.0-2	9.05E-02	9.17E-02	8.96E-02	8.75E-02	8.97E-02	8.88E-02
Ca_2EDTA-2.0-1	9.04E-02	9.07E-02	8.97E-02	8.71E-02	8.80E-02	8.93E-02
Ca_2EDTA-2.0-2	9.19E-02	9.32E-02	8.88E-02	8.72E-02	8.78E-02	8.85E-02
Ca_2EDTA-3.0-1	8.38E-02	8.43E-02	8.24E-02	7.98E-02	8.10E-02	7.93E-02
Ca_2EDTA-3.0-2	8.15E-02	8.40E-02	8.17E-02	8.02E-02	8.05E-02	8.03E-02
Ca_2EDTA-4.0-1	5.23E-02	7.43E-02	7.28E-02	6.85E-02	7.01E-02	7.05E-02
Ca_2EDTA-4.0-2	7.40E-02	7.57E-02	7.39E-02	6.84E-02	6.96E-02	7.02E-02
Ca_2EDTA-5.0-1	6.70E-02	6.99E-02	6.88E-02	6.34E-02	6.47E-02	6.53E-02
Ca_2EDTA-5.0-2	6.82E-02	6.94E-02	6.84E-02	6.35E-02	6.49E-02	6.51E-02
Reference	WIPP-Solubility-13 pg. 45	WIPP-Solubility-13 pg. 36	WIPP-Solubility-16 Pg. 93-94	WIPP-Solubility-26 Pg. 20	WIPP-Solubility-26 Pg. 20	WIPP-Solubility-26 Pg. 20

3.32 Solubility of $Ca_2C_{10}H_{12}N_2O_8$(s) (Ca_2EDTA(s)) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment).

The objectives of this set of experiments are to (1) determine the solubility of Ca_2EDTA (calcium EDTA) in NaCl (sodium chloride) solutions and (2) determine the Pitzer ion-interaction parameters for the ion pair "Mg^{2+}—$HEDTA^{3-}$" (Item 32, Table 1-2).

A known mass of Ca_2EDTA from ACROS Organics was added to 100 mL of $MgCl_2$ (Fisher) solutions as shown in Table 3-61 below.

The experimental set-ups are periodically monitored for pH and dissolved calcium. Concentrations of other dissolved components (magnesium, chloride, and EDTA) are also determined. Experimental results gathered to date are shown in Table 3-62.

The results obtained so far demonstrate that the steady state/equilibrium has been attained. For instance, pH readings for all experiments at the same ionic strength are nearly constant after 780 days. As an example, the pH readings for Ca_2EDTA-0.01$MgCl_2$-1 are between 7.7 and 7.9. The corresponding calcium concentrations for all experiments at the same ionic strength are also nearly constant.

Table 3-61 Preparation of experimental set-ups for the solubility of Ca_2EDTA (s) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment).

Set-up ID	Ca_2EDTA(s) (g)	$MgCl_2$ (m)	Reference
Ca_2EDTA-0.01$MgCl_2$-1	2.0044	0.01	WIPP-Solubility-3, p. 12
Ca_2EDTA-0.01$MgCl_2$-2	2.0044	0.01	WIPP-Solubility-3, p. 12
Ca_2EDTA-0.1$MgCl_2$-1	4.0031	0.1	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-0.1$MgCl_2$-2	4.0062	0.1	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-1.0$MgCl_2$-1	6.0084	1	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-1.0$MgCl_2$-2	6.0074	1	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-1.5$MgCl_2$-1	8.0128	1.5	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-1.5$MgCl_2$-2	8.0087	1.5	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-2.0$MgCl_2$-1	8.0131	2	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-2.0$MgCl_2$-2	8.0078	2	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-2.5$MgCl_2$-1	10.0131	2.5	WIPP-Solubility-3, p. 12-19
Ca_2EDTA-2.5$MgCl_2$-2	10.0159	2.5	WIPP-Solubility-3, p. 12-19

Table 3-62 Measured data for the solubility of Ca_2EDTA (s) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment). pH data measured with pH electrode and meter.

	pH					
Set-up ID	**780 Days**	**954 Days**	**1038 Days**	**1088 Days**	**1137 Days**	**1189 Days**
Ca_2EDTA-0.01$MgCl_2$-1	7.90	7.74	7.79	7.86	7.92	7.81
Ca_2EDTA-0.01$MgCl_2$-2	7.82	7.75	7.71	7.75	7.71	7.67
Ca_2EDTA-0.1$MgCl_2$-1	7.76	7.75	7.72	7.76	7.78	7.73
Ca_2EDTA-0.1$MgCl_2$-2	7.30	7.46	7.44	7.50	7.54	7.44
Ca_2EDTA-1.0$MgCl_2$-1	7.07	7.15	7.08	7.15	7.17	7.18
Ca_2EDTA-1.0$MgCl_2$-2	7.11	7.13	7.08	7.14	7.19	7.17
Ca_2EDTA-1.5$MgCl_2$-1	6.73	6.95	6.93	6.99	6.85	6.98
Ca_2EDTA-1.5$MgCl_2$-2	6.68	6.89	6.90	6.96	6.93	6.95
Ca_2EDTA-2.0$MgCl_2$-1	6.47	6.75	6.73	6.79	6.76	6.80
Ca_2EDTA-2.0$MgCl_2$-2	6.65	6.75	6.72	6.75	6.82	6.83
Ca_2EDTA-2.5$MgCl_2$-1	6.35	6.58	6.52	6.58	6.63	6.63
Ca_2EDTA-2.5$MgCl_2$-2	6.50	6.53	6.50	6.54	6.62	6.61
Reference	WIPP-Solubility-12 pg. 26-27	WIPP-Solubility-12 pgs. 56-59	WIPP-Solubility-12 pg. 74	WIPP-Solubility-21 pg. 7	WIPP-Solubility-21 pg. 37	WIPP-Solubility-21 pg. 66

Table 3-62 (continued) Measured data for the solubility of Ca_2EDTA (s) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment). Mg measured with ICP-AES.

	[Mg(II)] (m)					
Set-up ID	**780 Days**	**954 Days**	**1038 Days**	**1088 Days**	**1137 Days**	**1189 Days**
Ca_2EDTA-0.01$MgCl_2$-1	1.19E-02	1.24E-02	1.16E-02	1.13E-02	1.14E-02	1.04E-02
Ca_2EDTA-0.01$MgCl_2$-2	1.22E-02	1.24E-02	1.14E-02	1.12E-02	1.15E-02	1.05E-02
Ca_2EDTA-0.1$MgCl_2$-1	1.01E-01	1.09E-01	9.77E-02	9.93E-02	1.02E-01	9.48E-02
Ca_2EDTA-0.1$MgCl_2$-2	1.01E-01	1.05E-01	9.72E-02	9.81E-02	1.01E-01	9.46E-02
Ca_2EDTA-1.0$MgCl_2$-1	8.01E-01	9.12E-01	8.52E-01	8.50E-01	7.03E-01	8.39E-01
Ca_2EDTA-1.0$MgCl_2$-2	7.80E-01	8.74E-01	8.28E-01	8.41E-01	8.14E-01	8.14E-01
Ca_2EDTA-1.5$MgCl_2$-1	1.09E+00	1.39E+00	1.22E+00	1.23E+00	1.22E+00	1.24E+00
Ca_2EDTA-1.5$MgCl_2$-2	1.11E+00	1.36E+00	1.17E+00	1.21E+00	1.12E+00	1.18E+00
Ca_2EDTA-2.0$MgCl_2$-1	1.41E+00	1.86E+00	1.60E+00	1.63E+00	1.67E+00	1.72E+00
Ca_2EDTA-2.0$MgCl_2$-2	1.39E+00	1.92E+00	1.66E+00	1.64E+00	1.75E+00	1.70E+00
Ca_2EDTA-2.5$MgCl_2$-1	NA	2.35E+00	1.95E+00	1.97E+00	2.00E+00	2.11E+00
Ca_2EDTA-2.5$MgCl_2$-2	NA	2.32E+00	1.71E+00	2.00E+00	2.13E+00	2.08E+00
Reference	WIPP-Solubility-16 pg. 8	WIPP-Solubility-16 Pg. 35	WIPP-Solubility-13 Pg. 72	WIPP-Solubility-22 pg. 26	WIPP-Solubility-24 pg. 10	WIPP-Solubility-24 Pg. 66

Table 3-62 (continued) Measured data for the solubility of Ca_2EDTA (s) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment). Ca measured with ICP-AES.

	[Ca(II)] (m)					
Set-up ID	**780 Days**	**954 Days**	**1038 Days**	**1088 Days**	**1137 Days**	**1189 Days**
Ca_2EDTA-0.01$MgCl_2$-1	7.27E-02	8.06E-02	7.65E-02	7.78E-02	8.24E-02	7.63E-02
Ca_2EDTA-0.01$MgCl_2$-2	7.24E-02	7.72E-02	7.37E-02	7.66E-02	7.82E-02	7.53E-02
Ca_2EDTA-0.1$MgCl_2$-1	1.10E-01	1.18E-01	1.12E-01	1.14E-01	1.20E-01	1.14E-01
Ca_2EDTA-0.1$MgCl_2$-2	1.11E-01	1.16E-01	1.11E-01	1.13E-01	1.18E-01	1.10E-01
Ca_2EDTA-1.0$MgCl_2$-1	1.74E-01	1.84E-01	1.79E-01	1.83E-01	1.57E-01	1.78E-01
Ca_2EDTA-1.0$MgCl_2$-2	1.59E-01	1.71E-01	1.64E-01	1.75E-01	1.75E-01	1.71E-01
Ca_2EDTA-1.5$MgCl_2$-1	2.10E-01	2.28E-01	2.21E-01	2.26E-01	2.26E-01	2.22E-01
Ca_2EDTA-1.5$MgCl_2$-2	2.07E-01	2.19E-01	2.08E-01	2.23E-01	2.10E-01	2.11E-01
Ca_2EDTA-2.0$MgCl_2$-1	2.24E-01	2.29E-01	2.26E-01	2.38E-01	2.42E-01	2.36E-01
Ca_2EDTA-2.0$MgCl_2$-2	2.05E-01	2.20E-01	2.25E-01	2.29E-01	2.42E-01	2.25E-01
Ca_2EDTA-2.5$MgCl_2$-1	2.96E-01	3.04E-01	2.90E-01	3.07E-01	3.05E-01	2.98E-01
Ca_2EDTA-2.5$MgCl_2$-2	2.88E-01	2.93E-01	2.52E-01	3.04E-01	3.17E-01	2.97E-01
Reference	WIPP-Solubility-14 pg. 3	WIPP-Solubility-16 Pg. 33	WIPP-Solubility-13 pg. 56	WIPP-Solubility-22 pg. 21,23	WIPP-Solubility-24 Pg. 14	WIPP-Solubility-24 Pg. 65

Table 3-62 (continued) Measured data for the solubility of Ca_2EDTA (s) in $MgCl_2$ solutions (the "Mg^{2+}—$HEDTA^{3-}$" experiment). EDTA measured with IC.

	[EDTA4-] (m)					
Set-up ID	**780 Days**	**954 Days**	**1038 Days**	**1088 Days**	**1137 Days**	**1189 Days**
Ca_2EDTA-0.01$MgCl_2$-1	5.82E-02	6.22E-02	6.17E-02	5.60E-02	5.76E-02	5.74E-02
Ca_2EDTA-0.01$MgCl_2$-2	5.97E-02	6.18E-02	5.93E-02	5.79E-02	5.81E-02	5.81E-02
Ca_2EDTA-0.1$MgCl_2$-1	8.59E-02	8.82E-02	8.28E-02	8.44E-02	8.40E-02	8.43E-02
Ca_2EDTA-0.1$MgCl_2$-2	8.62E-02	8.95E-02	8.39E-02	8.45E-02	8.40E-02	8.46E-02
Ca_2EDTA-1.0$MgCl_2$-1	5.74E-02	5.39E-02	5.28E-02	4.69E-02	4.54E-02	4.46E-02
Ca_2EDTA-1.0$MgCl_2$-2	3.39E-02	3.57E-02	3.74E-02	3.48E-02	3.57E-02	3.51E-02
Ca_2EDTA-1.5$MgCl_2$-1	4.49E-02	4.06E-02	4.11E-02	3.68E-02	3.64E-02	3.64E-02
Ca_2EDTA-1.5$MgCl_2$-2	3.53E-02	3.53E-02	3.87E-02	3.49E-02	3.50E-02	3.56E-02
Ca_2EDTA-2.0$MgCl_2$-1	6.88E-02	6.18E-02	5.83E-02	5.34E-02	5.26E-02	5.11E-02
Ca_2EDTA-2.0$MgCl_2$-2	3.57E-02	3.63E-02	3.96E-02	3.63E-02	3.70E-02	3.76E-02
Ca_2EDTA-2.5$MgCl_2$-1	1.06E-01	9.46E-02	8.33E-02	8.07E-02	7.83E-02	7.35E-02
Ca_2EDTA-2.5$MgCl_2$-2	1.01E-01	8.93E-02	8.00E-02	7.69E-02	7.48E-02	7.18E-02
Reference	WIPP-Solubility-13 pg. 39	WIPP-Solubility-13 pg. 37	WIPP-Solubility-16 Pg. 91-92	WIPP-Solubility-26 Pg. 16	WIPP-Solubility-26 Pg. 16	WIPP-Solubility-26 Pg. 16

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