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Third Milestone Report on Test Plan TP 12-02, "Experimental Investigation of Borate Interactions with Rare Earth Elements Under the WIPP Relevant Conditions at Sandia National Laboratories Carlsbad Facility"

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WIPP:4.4.2.2.2:TD:QA-L:RECERT:560221

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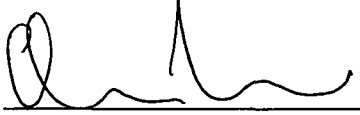
Management Reviewer:	 Antonio Triventi, 08882	*10/28/2020* Date

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DEFINITION OF ABBREVIATIONS, ACRONYMS AND INITIALISMS

Abbreviation or Acronym	Definition
(aq)	aqueous phase
$Am(OH)_3$	Americium Hydroxide
Am(III)	Trivalent Americium
$AmHB_4O_7^{2+}$	Americium Tetraborate
ASTM	American Society for Testing and Materials International
AVG	Average
BaCl	Barium Chloride
$Ba(OH)_2 \cdot 8H_2O$	Barium Hydroxide Octahydrate
CBFO	US DOE Carlsbad Field Office
CO_2	Carbon Dioxide
CV	Coefficient of Variation
DI	Deionized
DDI	De-aerated Deionized
EDS	Energy Dispersive Spectroscopy
ERDA-6	Energy Research and Development Administration well 6
ES&H	Environment, Safety and Health
g	gram
GWB	Generic Weep Brine (synthetic Salado Formation Brine)
$HB_4O_7^-$	Tetraborate
IC	Ion Chromatography
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectroscopy
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
m	Molality or Molal (mol/kg-H_2O)
M	Molarity or Molar (mol/L-solution)

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MAD	Median Absolute Deviation
$MgCl_2$	Magnesium Chloride
$MgCl_2 \cdot 6H_2O$	Magnesium Chloride Hexahydrate
$Mg(OH)_2$	Magnesium Hydroxide
mL	milliliter
mM	millimolar
n	number
N_2	Nitrogen gas
$Na_2B_4O_7 \cdot 10H_2O$	Sodium Tetraborate
NaCl	Sodium Chloride
Na_2SO_4	Sodium Sulfate
Nd_2O_3	Neodymium Oxide
$Nd(OH)_3$	Neodymium Hydroxide
Nd(III)	Trivalent Neodymium
$NdHB_4O_7^{2+}$	Neodymium Tetraborate
nm	nanometer
PDF	Powder Diffraction File
pH	Negative Logarithm of Hydrogen Ion Activity
pCH	Corrected pH Value
ppb	parts per billion
ppm	parts per million
$Pu(OH)_3$	Plutonium Hydroxide
Pu(III)	Trivalent Plutonium
QA	Quality Assurance
SEM	Scanning Electron Microscope
SNL	Sandia National Laboratories
SNL/CPG	Sandia National Laboratories Carlsbad Programs Group
(s)	solid phase or solid
TP	Test Plan
MΩ ·cm	Mega-ohm Per Centimeter

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WIPP	Waste Isolation Pilot Plant
XRD	X-Ray Diffractometer

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1.0 INTRODUCTION

The purpose of this milestone report is to summarize the progress completed to date for tasks related to Test Plan (TP) 12-02 Rev.2 (Xiong et al. 2015). The objectives of TP 12-02 are to establish the solubility of crystalline $Nd(OH)_3$ and determine a better understanding of the interactions between trivalent neodymium (Nd(III)) and tetraborate ($HB_4O_7^-$) in solutions containing the major components or ions of WIPP brine (Na^+, Mg^{2+}, Cl^- and SO_4^{2-}). Nd(III) has a molecule radius similar to that of Pu(III) and Am(III) and therefore can be used as an analog to model the equilibrium/solubility behavior of $Pu(OH)_3$ and $Am(OH)_3$. Although the concentration of the tetraborate ion ($HB_4O_7^-$) is relatively low [40 and 16 mM in GWB and ERDA-6 brines, respectively (Xiong, Y-L., 2008. SP 20-4)], it could form a relatively strong complex with trivalent neodymium (Nd(III)) (Borkowski et al., 2010) thus impacting the solubility of Nd(III). To accurately account for the contributions of $AmHB_4O_7^{2+}$ to the total solubility of Am(III) in the WIPP thermodynamic database, TP 12-02 was written to obtain the needed Pitzer parameters related to the neodymium borate analog system (Neodymium tetraborate complex,, $NdHB_4O_7^{2+}$). The following tasks have been identified for completion in this study as per TP 12-02 Rev.2:

- *Task 1: Experimental determination of binary interaction parameters (i.e. $\beta^{(0)},\beta^{(1)},C^{\phi}$) for $NdHB_4O_7^{2+}$—SO_4^{2-}*
- *Task 2: Experimental determination of theta parameters (θ) for $NdHB_4O_7^{2+}$—Na^+ and $NdHB_4O_7^{2+}$—Mg^{2+}*
- *Task 3: Experimental determination of psi parameters (Ψ) for $NdHB_4O_7^{2+}$—Na^+—Cl^- and $NdHB_4O_7^{2+}$—Mg^{2+}—Cl^-*
- *Task 4: Experimental validation of determined Pitzer parameters for $NdHB_4O_7^{2+}$ in GWB and ERDA-6 brine*
- *Task 5: Experimental determination of speciation of Nd(III) and solubility of $Nd(OH)_3$ in the alkaline region*

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2.0 MATERIALS AND METHODS

All solutions were prepared from reagent grade chemicals from Fisher Scientific or analogous vendors, and DI water. All DI water used for experimental set-up had a resistivity of ≥18 MΩ ·cm Type 1 water (ASTM D1193-99e1(2018)). The DI water for experiments was degassed inside a glove box, using pre-purified inert gas (e.g., N_2) to remove dissolved oxygen and any potentially dissolved CO_2, forming de-aerated water (DDI). All solutions and experimental set-ups were prepared inside a nitrogen atmosphere glovebox with <1 ppm oxygen, as verified by Pls and technologists at the time of sampling. Solids needed for the experiments were either purchased or synthesized. Chemicals used for synthesis and solution preparation were reagent grade commercial salts. For undersaturation solubility experiments, high purity crystalline $Nd(OH)_3$ was prepared. The $Nd(OH)_3$ starting material was synthesized in the lab per the procedure described by Wood et al. (2002). $Nd(OH)_3$ was synthesized by reacting high purity Nd_2O_3 with DDI water at 200 °C, as prescribed by the Wood et al. 2002 synthesis procedure, in a Paar® reaction vessel for a time period of approximately two weeks.

Densities in these experiments were measured by taring a Class A volumetric flask (ASTM E288-10(2017), ASTM E1272-02(2019)) on a calibrated balance and recording the weight. References for measured densities are listed next to the density in the subsequent tables. Volume measurements will be conducted by utilizing only Class A glassware for all solution preparation and calibrated pipettes if needed.

2.1 Solid Materials Characterization

Solid starting materials were analyzed using X-Ray Diffraction (XRD) as per SP 12-8 Rev. 3, "Use and Maintenance of Bruker Analytical X-Ray Systems D8 Advance X-Ray Diffractometer," (Xiong, Y.L., 2013) and by utilizing Scanning Electron Microscopy,(SEM) equipped with a Energy Dispersive X-Ray Spectrometer (EDS) as per SP 12-17 Rev. 3 "Scanning Electron Microscope Imaging and Energy Dispersive Spectroscopy" (Kirkes, 2016a). XRD patterns for the synthesized $Nd(OH)_3$ batch #14 are displayed in Figure 1 and

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show sharp narrow peaks consistent with a highly crystalline material. Numerous other batches were also verified using XRD with similar results, see WIPP-Nd-Borate scientific notebook series for additional data (see Reference section for WIPP-Nd-Borate-1 through 5). The peaks present in the XRD spectra in Figure 1 correspond to that of $Nd(OH)_3$ PDF pattern 01-070-0214. SEM image analysis of $Nd(OH)_3$ batch #1 can be seen in Figure 2. SEM imaging at higher resolution reveals microcrystalline material with maximum dimensions from 100 to 200 nm. High resolution SEM images from Texas Tech University show the crystals are manifested as well-defined hexagonal plates (Figure 3).

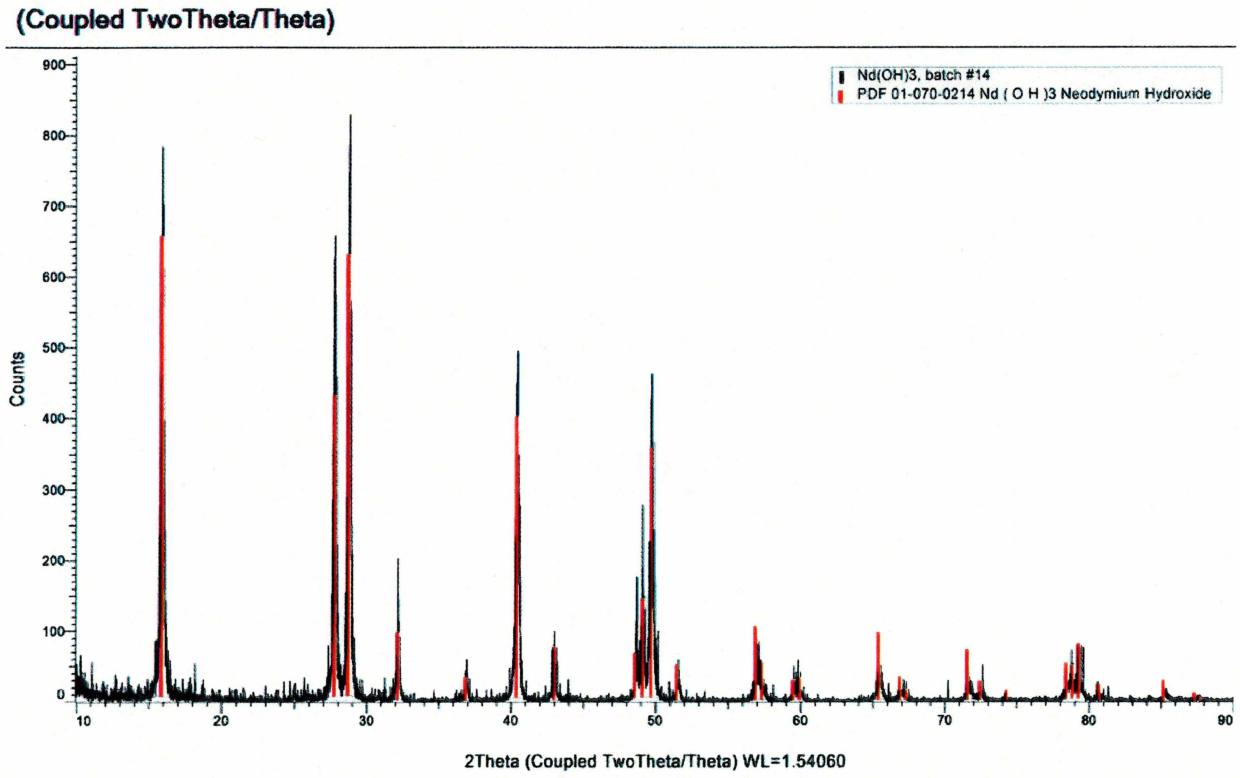

Figure 1 XRD Pattern for Synthetic $Nd(OH)_3$ batch #14 (WIPP-Nd-Borate-2 Pgs. 37 and 102)

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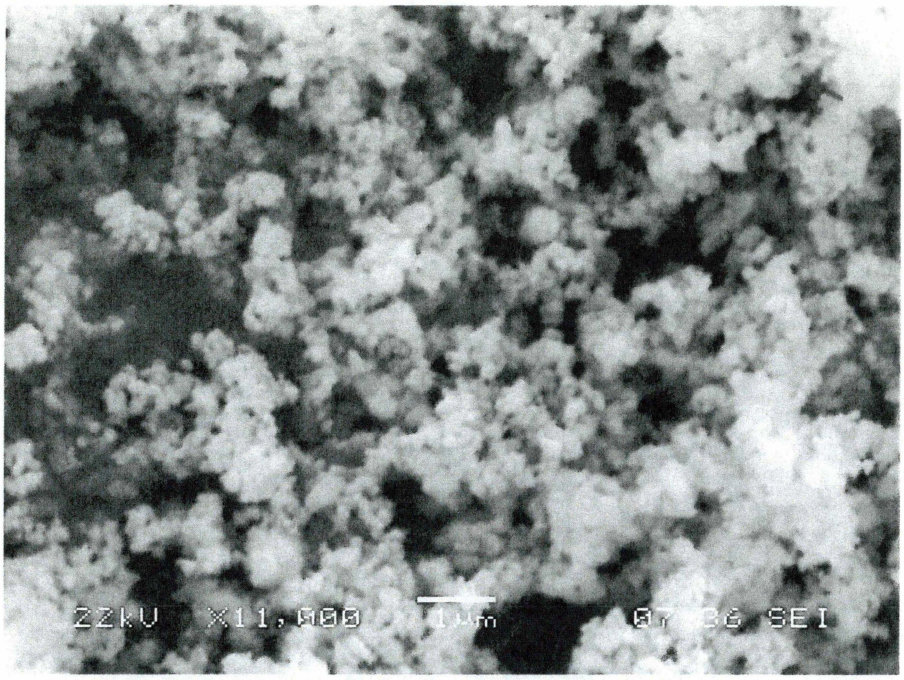

Figure 2 SEM image of $Nd(OH)_3$ batch #1 (WIPP-Nd-Borate-4 Pg. 98 (Image #4))

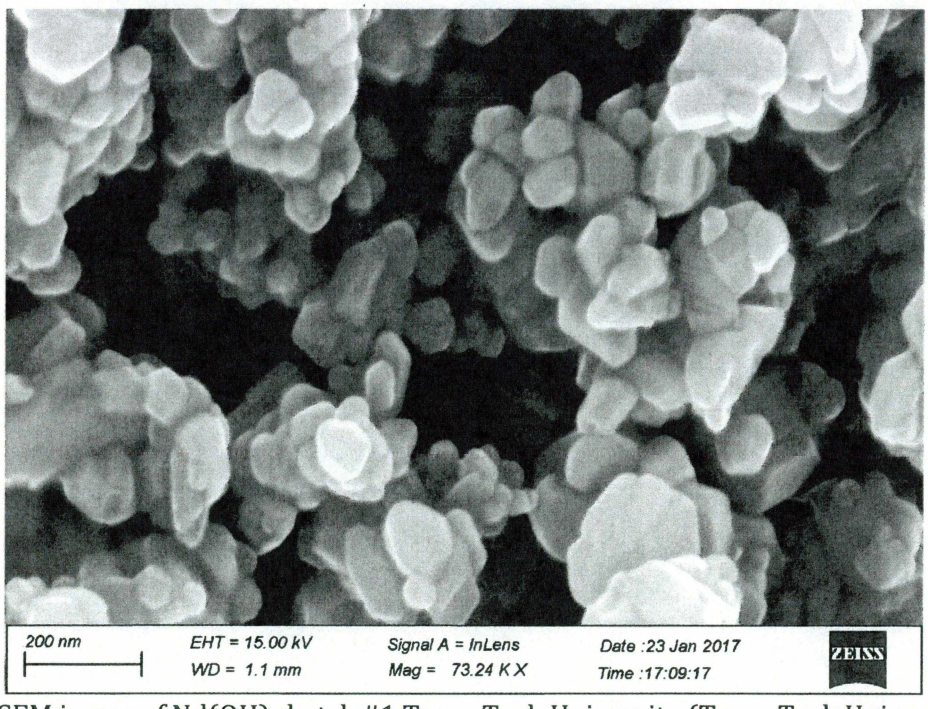

Figure 3 SEM image of $Nd(OH)_3$ batch #1 Texas Tech University (Texas Tech University, College of Arts & Sciences Microscopy. Do not Cite or Reproduce.)

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2.2 Ion and Anion Concentration Measurements

Hydrogen ion concentrations were determined using pH readings measured with a Ross pH electrode and meter as per SP 12-14 Rev.5 "Use of pH Meters and Electrodes" (Kirkes, 2018). Where relevant, concentrations of anions such as chloride and sulfate were determined using Ion Chromatography (IC) as per SP 12-22 Rev. 3 and 4 "Calibration, Use and Maintenance of the Dionex Ion Chromatograph (IC) 6000" (Marrs, 2019).

2.3 Total Cation Concentrations

Elemental concentrations of interest are determined using anInductively Coupled Plasma Atomic Emission Spectrometer (ICP-AES) as per SP 12-9 Rev. 5 "Calibration, Use and Maintenance of the Perkin Elmer Optima 8300 Dual View (DV) ICP-AES" (Kirkes, 2017) and Inductively Coupled Plasma Mass Spectrometer (ICP-MS) as per SP 12-31 Rev.1 "Calibration, Use and Maintenance of the Perkin Elmer NexIon 300D ICP-MS" (Kirkes, 2016b). Specifically, the ICP-AES is used to measure the total sodium (Na), magnesium (Mg) and boron (B) concentrations. The ICP-MS is utilized to measure total concentrations of neodymium (Nd).

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3.0 RESULTS

The following sections describe the preparation and aqueous chemistry results for the experiments to the cut-off date of 5/31/20. These experiments are on-going and additional data will be added in a follow-on report. The data charts identify parameters that have not yet been analyzed or need to be re-analyzed as "NA". In some cases, the samples being analyzed have been depleted and not all parameters could be obtained. In that case, the table will say "Depleted" instead of having data presented. All solid characterization data of the experiments will be presented in an alternate report.

Potentially large uncertainties can be present when analyzing components at low concentrations, especially when large dilutions are needed to reduce the matrix effects of the brine solution. This is the case for the neodymium analysis at low concentrations and therefore within this report a method for outlier determination for the neodymium results will be applied for data quality control in future reports. Outliers exist due to experimental errors that can be attributed to factors such as: dilution, human error, measured concentration being at or close to the limit of detection, instrumental error, matrix interference, colloidal presence etc. In scientific data analysis the Z-score method is often used for outlier determination in a defined dataset. Z-scores (z_i) are used to determine outliers in parametric data sets with a normal distribution. Z-scores are calculated using the equation seen in Equation 1:

Equation 1

$$z_i = \frac{(x_i - \mu)}{\sigma}$$

Where, x_i is the number being analyzed, μ is the mean and σ is the standard deviation. When this method is utilized to determine outliers, it is common for data to be labeled as an outlier if it falls outside the normal distribution curve, which means an absolute value of greater than 3 (Iglewicz and Hoaglin 1993). However, it has been questioned whether this method can be utilized for small sample sizes. In the table below, maximum Z-scores were

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calculated using the expression $(n-1)/\sqrt{n}$ for sample sizes n= 5 to 20 as follows (Iglewicz and Hoaglin 1993):

n	Z_{max}
5	1.79
10	2.85
11	3.02
15	3.61
20	4.25

As demonstrated in the chart, a criterion of labeling a number as an outlier if it has an absolute value of 3 or greater, is not appropriate for small sample sizes when using the traditional Z-score method. This is primarily because of the fact that the μ and σ are too greatly affected by the outlier itself. Therefore, the traditional Z-score method is not appropriate for outlier determination with small sample sizes. For this reason, Iglewicz and Hoaglin 1993 developed a new method for determination of outliers that is appropriate for small sample sizes. This new method is termed the Modified Z-score method. This method replaces the highly affected terms μ and σ with more robust terms $\tilde{x}$ (median) and MAD (Median Absolute Deviation) respectively. The research conducted by Iglewicz and Hoaglin 1993 showed that the median and MAD terms were more "resistant" to affects from the outlier itself in small sample sizes (<10). The equation for determination of the Modified Z-score (M_i) can be seen in Equation 2 (Iglewicz and Hoaglin 1993).

Equation 2

$$M_i = \frac{0.6745(x_i - \tilde{x})}{MAD}$$

Where x_i denotes the number being analyzed, $\tilde{x}$ denotes the median and 0.6745 is a constant that is determined by the expected value of MAD=0.6745 σ for a large sample size and is the 0.75th quartile of the standard normal distribution. In Equation 2, MAD stands for the Median Absolute Deviation and is represented by Equation 3.

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Equation 3

$$MAD = median_i(|x_i - \tilde{x}|)$$

Iglewicz and Hoaglin 1993, suggest flagging a number as an outlier if it has a Modified Z-Score of >3.5 based on a simulation study of 10,000 replications of *n* pseudo-normal observations for each sample size.

In this report the Modified Z-Score has been chosen as the method for outlier determination, however it is important to note that there are a variety of other statistical methods that can be used for this purpose. The Modified Z-Score is suitable for use with data sets that have a normal distribution and small sample size. In this report, outliers will be determined using Equation 2 and flagged as outliers if they have a Modified Z-Score of > the absolute value of 3.5. If outliers are found to exist within the data set, they will be denoted with a red highlight, and called out in the text of that section. If a number is denoted as an outlier, it will not be used to calculate the average in the respective chart. The Modified Z-Score is used as a tool to highlight outliers in order to guide future analyses in determining outliers, but this does not exclude data from being used in future reports or analyses, if deemed acceptable.

The general equation for conversion between molarity (M) and molality (m) of the starting solutions is (Xiong, Y-L et al. 2010):

Equation 4

$$m_i = \frac{1000M_i}{1000\rho - \sum_i^j M_i E_i} \qquad M_i = \frac{1000 m_i \rho}{1000 + \sum_i^j m_i E_i}$$

where M_i is concentration of i species on a molarity scale, ρ is density of solution in g/mL or kg/L, m_i is concentration of i species on a molality scale, and E_i the molecular weight of i species in g/mol. Starting solution concentrations will be presented in both molarity and molality for ease of comparison to the measured data.

Appendix A contains a description of the equations used in the data spreadsheet for this work. The data spreadsheet for this report can be found at the following file path:

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/cvs/CVSLIB/WIPP_EXTERNAL/Geochem2020/milestones. The data spreadsheet at this file path also contains calculations to correct the $MgCl_2$ starting solution concentrations. Initially, when these concentrations were reported, the waters of hydration were not considered in the calculation and were therefore reported erroneously high. In addition, this spreadsheet contains all the calculations to convert the initial starting solutions from molality to molarity, using Equation 4 above. The $Na_2B_4O_7 \cdot 10H_2O$ used in several of the experiments in this study, may have a similar "waters of hydration" issue to the $MgCl_2 \cdot 6H_2O$. This component was added as a solid and was allowed to dissolve at its solubility rate in the matrix. Therefore, we do not know yet the fate of these waters of hydration. XRD analysis may help determine this and will be reported in a follow-on report.

Calculated averages for the purpose of this report are for information only. Further analysis will be completed in future analysis reports and the data will be more thoroughly examined and filtered at that time.

3.1 Task 1: Experimental determination of binary interaction parameters (i.e. $\beta^{(0)},\beta^{(1)},C^{\phi}$) for $NdHB_4O_7^{2+}$—SO_4^{2-}.

Undersaturation experiments were set-up with $Nd(OH)_3$ as the solid phase and Na_2SO_4 as the aqueous phase ranging from 0.01 m – 1.8 m. Table 3-1 shows the experimental set-up and Tables 3-2 to 3-5 show the collected data to date. Identified outliers for neodymium data:

Day 546: Nd(OH)3-0.01 SO4-1, Nd(OH)3-0.5 SO4-1, Nd(OH)3-0.5 SO4-2, Nd(OH)3-1.5 SO4-1, Nd(OH)3-1.8 SO4-2;

Day 1315: Nd(OH)3-0.01 SO4-2

Day 2289: Nd(OH)3-0.01 SO4-2

A second set of undersaturation experiments were set-up with the addition of $Nd(OH)_3$ and $Na_2B_4O_7 \cdot 10H_2O$ together as the solid phases, and Na_2SO_4 as the aqueous phase ranging in concentration from 0.01 m to 1.8 m. Table 3-6 shows the experimental set-up and Tables 3-7 to 3-11 show the collected data to date. Identified outliers for neodymium data:

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Day 454: Nd(OH)3-B- 0.1 SO4-1

Table 3-1 Experimental set-up for undersaturation experiments investigating $Nd(OH)_3$ and Na_2SO_4 interaction

Set-up ID	$Nd(OH)_3(s)$ (g)	Na_2SO_4 (m)	Na_2SO_4 (M)	Reference	Density g/mL	Reference
Nd(OH)3-0.01 SO4-1	0.35	0.01	0.01	WIPP-Nd-Borate-1 Pg. 50	0.999	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.01 SO4-2	0.35	0.01	0.01	WIPP-Nd-Borate-1 Pg. 50	0.999	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.1 SO4-1	0.36	0.10	0.10	WIPP-Nd-Borate-1 Pg. 50	1.009	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.1 SO4-2	0.37	0.10	0.10	WIPP-Nd-Borate-1 Pg. 50	1.009	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.5 SO4-1	0.36	0.50	0.49	WIPP-Nd-Borate-1 Pg. 50	1.057	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.5 SO4-2	0.36	0.50	0.49	WIPP-Nd-Borate-1 Pg. 50	1.057	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.0 SO4-1	0.35	1.00	0.98	WIPP-Nd-Borate-1 Pg. 50	1.115	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.0 SO4-2	0.35	1.00	0.98	WIPP-Nd-Borate-1 Pg. 50	1.115	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.5 SO4-1	0.35	1.50	1.44	WIPP-Nd-Borate-1 Pg. 50	1.165	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.5 SO4-2	0.35	1.50	1.44	WIPP-Nd-Borate-1 Pg. 50	1.165	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.8 SO4-1	0.38	1.80	1.71	WIPP-Nd-Borate-1 Pg. 50	1.191	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.8 SO4-2	0.44	1.80	1.71	WIPP-Nd-Borate-1 Pg. 50	1.191	WIPP-Nd-Borate-7 Pg. 75

Note: Densities used to convert starting solutions from Molality to Molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-2 Measured pH data for undersaturation experiments investigating $Nd(OH)_3$ and Na_2SO_4 interaction

	pH								
Set-up ID	103 Days	133 Days	278 Days	*546 Days	909 Days	1315 Days	2289 Days	2371 Days	AVG
Nd(OH)3-0.01 SO4-1	9.93	9.86	9.78	10.06	9.82	9.64	9.71	9.75	9.82
Nd(OH)3-0.01 SO4-2	9.94	9.90	9.81	10.10	9.86	9.68	9.74	9.80	9.85
Nd(OH)3-0.1 SO4-1	9.91	9.88	9.77	10.06	9.86	9.69	9.79	9.81	9.85
Nd(OH)3-0.1 SO4-2	9.95	9.91	9.77	10.09	9.91	9.69	9.61	9.61	9.82
Nd(OH)3-0.5 SO4-1	9.84	9.83	9.68	9.97	9.74	9.58	9.68	9.73	9.76
Nd(OH)3-0.5 SO4-2	9.80	9.79	9.67	9.94	9.78	9.56	9.66	9.64	9.73

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Nd(OH)3-1.0 SO4-1	9.79	9.75	9.63	9.89	9.69	9.49	9.55	9.56	9.67
Nd(OH)3-1.0 SO4-2	9.67	9.70	9.56	9.82	9.62	9.38	9.37	9.40	9.57
Nd(OH)3-1.5 SO4-1	9.67	9.73	9.60	9.88	9.67	9.46	9.48	9.52	9.63
Nd(OH)3-1.5 SO4-2	9.76	9.75	9.61	9.89	9.73	9.43	9.40	9.52	9.64
Nd(OH)3-1.8 SO4-1	9.74	9.76	9.58	9.82	9.68	9.46	9.47	9.56	9.63
Nd(OH)3-1.8 SO4-2	9.57	9.65	9.54	9.93	9.62	9.33	9.25	9.35	9.53
Reference	WIPP-Nd-Borate-1 Pg. 59-60	WIPP-Nd-Borate-1 Pg. 72-73	WIPP-Nd-Borate-1 Pg. 96-97	WIPP-Nd-Borate-2 Pg. 42-44	WIPP-Nd-Borate-4 Pg. 27-29	WIPP-Nd-Borate-4 Pg. 69-70	WIPP-Nd-Borate-6 Pg. 87	WIPP-Nd-Borate-7 Pg. 54	

*NOTE: pH data for 546 Days does not look consistent with other samplings. In the analysis of this data (in future reports i.e. analysis report) it should be considered whether this data should be used.

Table 3-3 Measured neodymium molar concentration data for undersaturation experiments investigating $Nd(OH)_3$ and Na_2SO_4 interaction

	[Nd(III)] (M)										
Set-up ID	**103 Days**	**133 Days**	**278 Days**	**546 Days**	**909 Days**	**1315 Days**	**2289 Days**	**2371 Days**	$\tilde{x}$	**MAD**	**AVG**
Nd(OH) 3-0.01 SO4-1	1.36E-07	2.83E-08	5.29E-08	3.52E-07	4.33E-08	1.01E-07	9.64E-08	1.21E-07	9.87E-08	4.16E-08	8.28E-08
Nd(OH) 3-0.01 SO4-2	5.28E-08	3.69E-08	3.91E-08	8.20E-08	4.53E-08	2.52E-07	3.24E-07	8.05E-08	6.66E-08	2.44E-08	5.61E-08
Nd(OH) 3-0.1 SO4-1	3.58E-08	4.59E-08	6.42E-08	2.27E-07	7.03E-08	2.20E-07	1.17E-07	1.08E-07	8.92E-08	3.56E-08	1.11E-07
Nd(OH) 3-0.1 SO4-2	1.58E-07	5.03E-08	3.22E-08	1.73E-07	5.96E-08	7.44E-08	2.71E-07	8.43E-08	7.94E-08	3.81E-08	1.13E-07
Nd(OH) 3-0.5 SO4-1	6.90E-08	1.33E-07	6.96E-08	3.88E-07	5.33E-08	1.35E-07	1.70E-07	9.67E-08	1.15E-07	4.54E-08	1.04E-07
Nd(OH) 3-0.5 SO4-2	6.52E-08	5.83E-08	5.79E-08	2.89E-07	1.08E-07	1.16E-07	1.29E-07	7.02E-08	8.89E-08	2.90E-08	8.64E-08
Nd(OH) 3-1.0 SO4-1	3.56E-07	5.27E-08	7.03E-08	3.27E-07	1.27E-07	6.71E-07	2.16E-07	1.27E-07	1.71E-07	1.10E-07	2.43E-07
Nd(OH) 3-1.0 SO4-2	8.93E-08	5.87E-07	7.81E-08	2.40E-07	1.11E-07	1.70E-07	2.64E-07	2.19E-07	1.94E-07	7.63E-08	2.20E-07
Nd(OH) 3-1.5	1.35E-07	9.84E-08	1.18E-07	5.91E-07	2.08E-07	1.63E-07	2.46E-07	1.51E-07	1.57E-07	4.50E-08	1.60E-07

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SO4-1											
Nd(OH)3-1.5 SO4-2	8.50E-08	2.40E-07	9.91E-08	2.30E-07	8.81E-08	1.88E-07	2.94E-07	2.95E-07	2.09E-07	8.52E-08	1.90E-07
Nd(OH)3-1.8 SO4-1	1.59E-07	7.77E-08	9.44E-08	2.77E-07	1.11E-07	2.85E-07	2.58E-07	2.73E-07	2.09E-07	7.28E-08	1.92E-07
Nd(OH)3-1.8 SO4-2	1.86E-07	1.07E-07	1.38E-07	1.80E-06	1.81E-07	3.21E-07	5.21E-07	3.69E-07	2.53E-07	1.15E-07	2.60E-07
Reference	WIPP-Nd-Borate-6 Pg. 21-23	WIPP-Nd-Borate-6 Pg. 21-23	WIPP-Nd-Borate-6 Pg. 21-23	WIPP-Nd-Borate-2 Pg. 46, 48 and WIPP-Nd-Borate-6 Pg. 21-23	WIPP-Nd-Borate-6 Pg. 26	WIPP-Nd-Borate-6 Pg. 26	WIPP-Nd-Borate-6 Pg. 92	WIPP-Nd-Borate-7 Pg. 56	Note: Average does not contain outliers		

Modified Z-Score for the Nd(III) concentrations shown in Table 3-3

Set-up ID	103 Days	133 Days	278 Days	546 Days	909 Days	1315 Days	2289 Days	2371 Days
Nd(OH)3-0.01 SO4-1	0.61	1.14	0.74	4.11	0.90	0.04	0.04	0.37
Nd(OH)3-0.01 SO4-2	0.38	0.82	0.76	0.42	0.59	5.12	7.11	0.38
Nd(OH)3-0.1 SO4-1	1.01	0.82	0.47	2.62	0.36	2.49	0.53	0.36
Nd(OH)3-0.1 SO4-2	1.40	0.51	0.83	1.66	0.35	0.09	3.38	0.09
Nd(OH)3-0.5 SO4-1	0.68	0.27	0.67	4.06	0.91	0.30	0.82	0.27
Nd(OH)3-0.5 SO4-2	0.55	0.71	0.72	4.65	0.43	0.64	0.94	0.43
Nd(OH)3-1.0 SO4-1	1.13	0.73	0.62	0.96	0.27	3.06	0.27	0.28
Nd(OH)3-1.0 SO4-2	0.93	3.47	1.03	0.41	0.74	0.22	0.61	0.22
Nd(OH)3-1.5 SO4-1	0.33	0.88	0.59	6.52	0.76	0.08	1.33	0.08
Nd(OH)3-1.5 SO4-2	0.98	0.25	0.87	0.17	0.96	0.17	0.67	0.68
Nd(OH)3-1.8 SO4-1	0.46	1.21	1.06	0.64	0.91	0.71	0.46	0.59
Nd(OH)3-1.8 SO4-2	0.40	0.85	0.67	9.02	0.43	0.40	1.56	0.68

Table 3-4 Measured sodium molar concentration data for the undersaturation experiments investigating $Nd(OH)_3$ and Na_2SO_4 interaction

Information Only

	[Na(I)] (M)								
Set-up ID	**103 Days**	**133 Days**	**278 Days**	**546 Days**	**909 Days**	**1315 Days**	**2289 Days**	**2371 Days**	**AVG**
Nd(OH)3-0.01 SO4-1	2.03E-02	1.85E-02	2.10E-02	2.08E-02	2.09E-02	2.04E-02	2.15E-02	2.28E-02	2.08E-02
Nd(OH)3-0.01 SO4-2	1.92E-02	1.96E-02	2.06E-02	2.02E-02	2.14E-02	2.07E-02	2.20E-02	2.37E-02	2.09E-02
Nd(OH)3-0.1 SO4-1	1.97E-01	1.86E-01	2.10E-01	2.09E-01	2.02E-01	1.76E-01	2.18E-01	2.06E-01	2.00E-01
Nd(OH)3-0.1 SO4-2	1.93E-01	1.94E-01	2.03E-01	2.13E-01	2.06E-01	1.77E-01	2.17E-01	2.16E-01	2.02E-01
Nd(OH)3-0.5 SO4-1	9.29E-01	9.45E-01	9.86E-01	1.06E+00	1.04E+00	1.05E+00	9.50E-01	9.77E-01	9.92E-01
Nd(OH)3-0.5 SO4-2	9.62E-01	9.65E-01	9.35E-01	1.05E+00	1.07E+00	1.05E+00	9.40E-01	9.96E-01	9.95E-01
Nd(OH)3-1.0 SO4-1	1.95E+00	1.92E+00	1.87E+00	2.07E+00	2.14E+00	2.21E+00	1.94E+00	2.01E+00	2.01E+00
Nd(OH)3-1.0 SO4-2	1.97E+00	1.90E+00	1.92E+00	2.06E+00	2.05E+00	2.20E+00	1.93E+00	2.18E+00	2.03E+00
Nd(OH)3-1.5 SO4-1	2.73E+00	2.80E+00	2.88E+00	2.99E+00	3.37E+00	3.14E+00	3.04E+00	3.45E+00	3.05E+00
Nd(OH)3-1.5 SO4-2	2.72E+00	3.15E+00	2.94E+00	3.00E+00	3.07E+00	2.97E+00	3.03E+00	3.65E+00	3.07E+00
Nd(OH)3-1.8 SO4-1	3.23E+00	3.21E+00	3.13E+00	3.55E+00	3.68E+00	3.70E+00	3.55E+00	3.20E+00	3.41E+00
Nd(OH)3-1.8 SO4-2	3.16E+00	3.21E+00	3.40E+00	3.53E+00	3.62E+00	3.34E+00	3.47E+00	3.11E+00	3.36E+00
Reference	WIPP-Nd-Borate-1 Pg. 66	WIPP-Nd-Borate-1 Pg. 89-90	WIPP-Nd-Borate-2 Pg. 11 and WIPP-Nd-Borate-8 Pg. 9	WIPP-Nd-Borate-4 Pg. 38	WIPP-Nd-Borate-4 Pg. 38	WIPP-Nd-Borate-4 Pg. 85	WIPP-Nd-Borate-6 Pg. 90	WIPP-Nd-Borate-8 Pg. 24	

Table 3-5 Measured sulfate molar concentration data for the undersaturation experiments investigating $Nd(OH)_3$ and Na_2SO_4 interaction

	[SO4(II-)] (M)								
Set-up ID	**103 Days**	**133 Days**	**278 Days**	**546 Days**	**909 Days**	**1315 Days**	**2289 Days**	**2371 Days**	**AVG**
Nd(OH)3-0.01 SO4-1	1.04E-02	1.04E-02	1.05E-02	8.97E-03	9.27E-03	1.29E-02	1.12E-02	1.09E-02	1.06E-02
Nd(OH)3-0.01 SO4-2	1.04E-02	1.05E-02	1.01E-02	9.10E-03	9.19E-03	1.35E-02	1.14E-02	1.11E-02	1.07E-02
Nd(OH)3-0.1 SO4-1	1.05E-01	1.06E-01	1.02E-01	9.81E-02	9.83E-02	1.36E-01	9.78E-02	1.08E-01	1.06E-01
Nd(OH)3-0.1 SO4-2	1.07E-01	1.06E-01	1.01E-01	1.00E-01	9.85E-02	1.34E-01	1.13E-01	1.06E-01	1.08E-01
Nd(OH)3-0.5	5.23E-	5.34E-	5.19E-	5.07E-	4.93E-	5.39E-	5.31E-	4.95E-	5.18E-01

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SO4-1	01	01	01	01	01	01	01	01	
Nd(OH)3-0.5 SO4-2	5.19E-01	5.38E-01	4.97E-01	4.97E-01	5.02E-01	5.36E-01	5.40E-01	5.04E-01	5.17E-01
Nd(OH)3-1.0 SO4-1	1.02E+00	1.03E+00	9.62E-01	9.29E-01	9.78E-01	1.36E+00	1.11E+00	1.11E+00	1.06E+00
Nd(OH)3-1.0 SO4-2	1.03E+00	1.03E+00	9.75E-01	9.39E-01	9.36E-01	1.30E+00	1.10E+00	1.09E+00	1.05E+00
Nd(OH)3-1.5 SO4-1	1.52E+00	1.50E+00	1.50E+00	1.39E+00	1.56E+00	1.64E+00	1.69E+00	1.59E+00	1.55E+00
Nd(OH)3-1.5 SO4-2	1.50E+00	1.51E+00	1.49E+00	1.34E+00	1.44E+00	1.76E+00	1.70E+00	1.60E+00	1.54E+00
Nd(OH)3-1.8 SO4-1	1.77E+00	1.79E+00	1.58E+00	1.51E+00	1.72E+00	2.05E+00	1.99E+00	1.64E+00	1.76E+00
Nd(OH)3-1.8 SO4-2	1.77E+00	1.76E+00	1.78E+00	1.67E+00	1.71E+00	1.91E+00	2.01E+00	1.63E+00	1.78E+00
Reference	WIPP-Nd-Borate-2 Pg. 24-25	WIPP-Nd-Borate-2 Pg. 24-25	WIPP-Nd-Borate-2 Pg. 24-25	WIPP-Nd-Borate-5 Pg. 43-44	WIPP-Nd-Borate-5 Pg. 43-44	WIPP-Nd-Borate-5 Pg. 85	WIPP-Nd-Borate-6 Pg. 93	WIPP-Nd-Borate-7 Pg.58	

Table 3-6 Experimental set-up for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7{\cdot}10H_2O$ interaction.

Set-up ID	$Nd(OH)_3$(s) (g)	$Na_2B_4O_7$ (s) (g)	Na_2SO_4 (m)	Na_2SO_4 (M)	Reference	Density g/mL	Reference
Nd(OH)3-B-0.01-SO4-1	0.35	10.04	0.01	0.01	WIPP-Nd-Borate-2 Pg. 66	1.028	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-0.01-SO4-2	0.35	10.01	0.01	0.01	WIPP-Nd-Borate-2 Pg. 66	1.028	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-0.1-SO4-1	0.35	10.90	0.10	0.1	WIPP-Nd-Borate-2 Pg. 66	1.032	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-0.1-SO4-2	0.35	10.94	0.10	0.1	WIPP-Nd-Borate-2 Pg. 66	1.032	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-0.5-SO4-1	0.35	10.84	0.50	0.49	WIPP-Nd-Borate-2 Pg. 66	1.072	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-0.5-SO4-2	0.35	10.08	0.50	0.49	WIPP-Nd-Borate-2 Pg. 66	1.072	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-1.0-SO4-1	0.34	10.02	1.00	0.98	WIPP-Nd-Borate-2 Pg. 66	1.126	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-1.0-SO4-2	0.35	10.06	1.00	0.98	WIPP-Nd-Borate-2 Pg. 66	1.126	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-1.5-SO4-1	0.35	10.56	1.50	1.44	WIPP-Nd-Borate-2 Pg. 66	1.176	WIPP-Nd-Borate-7 Pg. 75

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Nd(OH)3-B-1.5-SO4-2	0.34	10.09	1.50	1.44	WIPP-Nd-Borate-2 Pg. 66	1.176	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-1.8-SO4-1	0.36	10.03	1.80	1.71	WIPP-Nd-Borate-2 Pg. 66	1.203	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-B-1.8-SO4-2	0.36	10.10	1.80	1.71	WIPP-Nd-Borate-2 Pg. 66	1.203	WIPP-Nd-Borate-7 Pg. 75

Note: Densities used to convert starting solutions from Molality to Molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-7 Measured pH data for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	pH						
Set-up ID	**454 Days**	**762 Days**	**791 Days**	**811 Days**	**1120 Days**	**1721 Days**	**AVG**
Nd(OH)3-B-0.01-SO4-1	9.23	9.24	9.25	9.35	9.03*	9.32	9.28
Nd(OH)3-B-0.01-SO4-2	9.24	9.21	9.25	9.25	9.30	9.30	9.26
Nd(OH)3-B-0.1-SO4-1	9.16	9.12	9.17	9.17	9.22	9.23	9.18
Nd(OH)3-B-0.1-SO4-2	9.15	9.12	9.16	9.17	9.19	9.21	9.17
Nd(OH)3-B-0.5-SO4-1	8.99	8.97	9.00	9.00	9.02	9.05	9.01
Nd(OH)3-B-0.5-SO4-2	8.99	8.97	8.99	9.01	9.02	9.04	9.00
Nd(OH)3-B-1.0-SO4-1	8.90	8.89	8.91	8.91	8.91	8.96	8.91
Nd(OH)3-B-1.0-SO4-2	8.90	8.88	8.91	8.92	8.92	8.97	8.92
Nd(OH)3-B-1.5-SO4-1	8.84	8.82	8.85	8.85	8.86	8.90	8.85
Nd(OH)3-B-1.5-SO4-2	8.84	8.83	8.85	8.85	8.85	8.88	8.85
Nd(OH)3-B-1.8-SO4-1	8.84	8.81	8.83	8.83	8.82	8.87	8.83
Nd(OH)3-B-1.8-SO4-2	8.84	8.81	8.83	8.83	8.83	8.90	8.84
Reference	WIPP-Nd-Borate-4 Pg. 34-35	WIPP-Nd-Borate-5 Pg. 56-57	WIPP-Nd-Borate-4 Pg. 82-83	WIPP-Nd-Borate-4 Pg. 95-97	WIPP-Nd-Borate-6 Pg. 49	WIPP-Nd-Borate-6 Pg. 96	

NOTE: *This pH value is different from all other values for this sample. It will not be used.

Table 3-8 Measured neodymium molar concentration data for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	[Nd(III)] (M)						
Set-up ID	**454 Days**	**762 Days**	**791 Days**	**1721 Days**	$\tilde{x}$	**MAD**	**AVG**
Nd(OH)3-B-0.01-SO4-1	1.26E-07	7.10E-08	4.10E-08	1.77E-07	9.85E-08	4.24E-08	1.04E-07
Nd(OH)3-B-0.01-SO4-2	1.36E-07	6.70E-08	7.62E-09	1.16E-07	9.15E-08	3.47E-08	8.17E-08
Nd(OH)3-B-0.1-SO4-1	5.19E-07	6.65E-08	1.87E-08	1.28E-07	9.72E-08	5.46E-08	7.11E-08
Nd(OH)3-B-0.1-SO4-2	2.08E-07	7.77E-08	1.56E-08	1.79E-07	1.28E-07	6.50E-08	1.20E-07
Nd(OH)3-B-0.5-	1.66E-07	5.69E-08	3.46E-08	1.92E-07	1.11E-07	6.56E-08	1.12E-07

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SO4-1							
Nd(OH)3-B-0.5-SO4-2	1.23E-06	5.71E-08	6.21E-08	1.87E-06	6.45E-07	5.85E-07	8.04E-07
Nd(OH)3-B-1.0-SO4-1	2.89E-07	8.45E-08	1.89E-08	5.54E-07	1.87E-07	1.35E-07	2.36E-07
Nd(OH)3-B-1.0-SO4-2	3.61E-07	7.23E-08	3.69E-08	2.23E-07	1.48E-07	9.33E-08	1.73E-07
Nd(OH)3-B-1.5-SO4-1	2.06E-07	9.80E-08	6.83E-08	2.72E-07	1.52E-07	6.91E-08	1.61E-07
Nd(OH)3-B-1.5-SO4-2	1.33E-06	8.64E-08	4.47E-08	2.13E-06	7.06E-07	6.41E-07	8.97E-07
Nd(OH)3-B-1.8-SO4-1	3.45E-07	1.53E-07	2.32E-08	3.05E-07	2.29E-07	9.63E-08	2.07E-07
Nd(OH)3-B-1.8-SO4-2	3.95E-07	1.33E-07	3.07E-08	2.16E-07	1.75E-07	9.29E-08	1.94E-07
Reference	WIPP-Nd-Borate-5 Pg. 25	WIPP-Nd-Borate-5 Pg. 58-59	WIPP-Nd-Borate-2 Pg. 54	WIPP-Nd-Borate-7 Pg.19,23	Note: Average does not contain outliers		

Note: Days 811 and 1120 have not been analyzed for Nd to date

Modified Z-Score for the Nd(III) concentrations shown in Table 3-8

Set-up ID	454 Days	762 Days	791 Days	1721 Days
Nd(OH)3-B-0.01-SO4-1	0.44	0.44	0.91	1.25
Nd(OH)3-B-0.01-SO4-2	0.87	0.48	1.63	0.48
Nd(OH)3-B-0.1-SO4-1	5.21	0.38	0.97	0.38
Nd(OH)3-B-0.1-SO4-2	0.82	0.52	1.17	0.52
Nd(OH)3-B-0.5-SO4-1	0.56	0.56	0.79	0.83
Nd(OH)3-B-0.5-SO4-2	0.67	0.68	0.67	1.41
Nd(OH)3-B-1.0-SO4-1	0.51	0.51	0.84	1.84
Nd(OH)3-B-1.0-SO4-2	1.54	0.55	0.80	0.55
Nd(OH)3-B-1.5-SO4-1	0.53	0.53	0.82	1.17
Nd(OH)3-B-1.5-SO4-2	0.65	0.65	0.70	1.50
Nd(OH)3-B-1.8-SO4-1	0.81	0.54	1.44	0.54
Nd(OH)3-B-1.8-SO4-2	1.60	0.30	1.05	0.30

Table 3-9 Measured sodium molar concentration data for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7{\cdot}10H_2O$ interaction.

	[Na(I)] (M)						
Set-up ID	**454 Days**	**762 Days**	**791 Days**	**811 Days**	**1120 Days**	**1721 Days**	**AVG**
Nd(OH)3-B-0.01-SO4-1	2.86E-01	5.41E-01	3.29E-01	2.82E-01	3.09E-01	2.60E-01	3.35E-01
Nd(OH)3-B-0.01-SO4-2	2.88E-01	Depleted	3.11E-01	2.99E-01	5.48E-01	2.59E-01	3.41E-01
Nd(OH)3-B-0.1-SO4-1	4.27E-01	3.95E-01	4.21E-01	3.85E-01	4.30E-01	3.59E-01	4.03E-01
Nd(OH)3-B-0.1-SO4-2	4.24E-01	6.60E-01	4.21E-01	3.83E-01	4.28E-01	3.57E-01	4.46E-01
Nd(OH)3-B-0.5-SO4-1	1.00E+00	Depleted	1.18E+00	1.08E+00	1.17E+00	9.55E-01	1.08E+00
Nd(OH)3-B-0.5-SO4-2	1.18E+00	Depleted	1.18E+00	1.09E+00	1.09E+00	9.77E-01	1.11E+00
Nd(OH)3-B-1.0-SO4-1	2.18E+00	Depleted	2.28E+00	1.89E+00	2.22E+00	1.85E+00	2.08E+00
Nd(OH)3-B-1.0-SO4-2	2.16E+00	Depleted	2.33E+00	1.71E+00	2.18E+00	1.87E+00	2.05E+00

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Nd(OH)3-B-1.5-SO4-1	3.22E+00	Depleted	3.34E+00	2.91E+00	3.18E+00	2.70E+00	3.07E+00
Nd(OH)3-B-1.5-SO4-2	3.27E+00	Depleted	3.26E+00	3.00E+00	3.28E+00	2.76E+00	3.11E+00
Nd(OH)3-B-1.8-SO4-1	3.30E+00	Depleted	3.96E+00	3.24E+00	3.67E+00	3.01E+00	3.44E+00
Nd(OH)3-B-1.8-SO4-2	3.28E+00	Depleted	Depleted	3.36E+00	4.00E+00	3.08E+00	3.43E+00
Reference	WIPP-Nd-Borate-4 Pg. 42-43	WIPP-Nd-Borate-7 Pg. 79	WIPP-Nd-Borate-7 Pg. 79	WIPP-Nd-Borate-6 Pg. 48	WIPP-Nd-Borate-7 Pg. 80	WIPP-Nd-Borate-6 Pg. 98	

Table 3-10 Measured sulfate molar concentration data for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7{\cdot}10H_2O$ interaction.

	[SO4(II-)] (M)						
Set-up ID	**454 Days**	**762 Days**	**791 Days**	**811 Days**	**1120 Days**	**1721 Days**	**AVG**
Nd(OH)3-B-0.01-SO4-1	1.18E-02	1.26E-02	1.35E-02	1.18E-02	1.10E-02	1.07E-02	1.19E-02
Nd(OH)3-B-0.01-SO4-2	1.24E-02	1.31E-02	1.33E-02	1.10E-02	1.09E-02	1.10E-02	1.20E-02
Nd(OH)3-B-0.1-SO4-1	1.25E-01	1.32E-01	1.33E-01	6.24E-02	1.03E-01	1.08E-01	1.11E-01
Nd(OH)3-B-0.1-SO4-2	1.24E-01	1.33E-01	1.33E-01	6.99E-02	1.05E-01	1.09E-01	1.12E-01
Nd(OH)3-B-0.5-SO4-1	5.21E-01	5.39E-01	5.28E-01	5.80E-01	5.20E-01	5.17E-01	5.34E-01
Nd(OH)3-B-0.5-SO4-2	5.33E-01	5.47E-01	5.41E-01	5.04E-01	5.26E-01	5.25E-01	5.29E-01
Nd(OH)3-B-1.0-SO4-1	1.30E+00	1.34E+00	1.14E+00	7.66E-01	1.08E+00	1.07E+00	1.12E+00
Nd(OH)3-B-1.0-SO4-2	1.24E+00	1.30E+00	1.21E+00	1.04E+00	1.09E+00	1.09E+00	1.16E+00
Nd(OH)3-B-1.5-SO4-1	1.79E+00	1.63E+00	1.69E+00	1.03E+00	1.50E+00	1.60E+00	1.54E+00
Nd(OH)3-B-1.5-SO4-2	1.79E+00	1.72E+00	1.75E+00	1.10E+00	1.48E+00	1.61E+00	1.57E+00
Nd(OH)3-B-1.8-SO4-1	1.68E+00	1.84E+00	2.03E+00	1.74E+00	1.57E+00	1.75E+00	1.77E+00
Nd(OH)3-B-1.8-SO4-2	1.73E+00	1.92E+00	2.05E+00	1.42E+00	1.90E+00	1.86E+00	1.81E+00
Reference	WIPP-Nd-Borate-5 Pg. 50	WIPP-Nd-Borate-5 Pg. 82-83	WIPP-Nd-Borate-5 Pg. 82-83	WIPP-Nd-Borate-7 Pg. 91 and WIPP-Nd-Borate-16	WIPP-Nd-Borate-7 Pg. 91	WIPP-Nd-Borate-6 Pg. 99	

Table 3-11 Measured boron molar concentration data for undersaturation experiments investigating $Nd(OH)_3$, Na_2SO_4 and $Na_2B_4O_7{\cdot}10H_2O$ interaction.

	[B] (M)						
Set-up ID	**454 Days**	**762 Days**	**791 Days**	**811 Days**	**1120 Days**	**1721 Days**	**AVG**
Nd(OH)3-B-0.01-SO4-1	5.44E-01	5.41E-01	6.67E-01	5.67E-01	6.58E-01	5.97E-01	5.96E-01
Nd(OH)3-B-0.01-SO4-2	5.32E-01	5.51E-01	6.30E-01	5.68E-01	6.57E-01	6.08E-01	5.91E-01
Nd(OH)3-B-0.1-SO4-1	4.33E-01	4.61E-01	5.23E-01	4.78E-01	5.44E-01	5.05E-01	4.91E-01
Nd(OH)3-B-0.1-SO4-2	4.20E-01	4.69E-01	5.16E-01	4.82E-01	5.33E-01	5.13E-01	4.89E-01
Nd(OH)3-B-0.5-SO4-1	2.43E-01	2.72E-01	2.80E-01	3.25E-01	3.68E-01	3.64E-01	3.09E-01
Nd(OH)3-B-0.5-SO4-2	2.93E-01	2.77E-01	2.86E-01	3.18E-01	3.64E-01	3.51E-01	3.15E-01
Nd(OH)3-B-1.0-SO4-1	2.61E-01	2.61E-01	2.52E-01	2.85E-01	3.31E-01	3.23E-01	2.86E-01

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Nd(OH)3-B-1.0-SO4-2	2.59E-01	2.50E-01	2.62E-01	2.78E-01	3.29E-01	3.23E-01	2.84E-01
Nd(OH)3-B-1.5-SO4-1	2.98E-01	2.36E-01	2.43E-01	2.67E-01	3.08E-01	3.15E-01	2.78E-01
Nd(OH)3-B-1.5-SO4-2	2.61E-01	2.33E-01	2.44E-01	2.56E-01	3.12E-01	3.15E-01	2.70E-01
Nd(OH)3-B-1.8-SO4-1	2.77E-01	2.55E-01	2.46E-01	2.47E-01	2.98E-01	3.07E-01	2.72E-01
Nd(OH)3-B-1.8-SO4-2	2.78E-01	2.50E-01	2.45E-01	2.59E-01	2.98E-01	3.11E-01	2.73E-01
Reference	WIPP-Nd-Borate-4 Pg. 44	WIPP-Nd-Borate-5 Pg. 99 and WIPP-Nd-Borate-6 Pg. 17	WIPP-Nd-Borate-5 Pg. 99 and WIPP-Nd-Borate-6 Pg. 17-18	WIPP-Nd-Borate-6 Pg. 33	WIPP-Nd-Borate-7 Pg. 61	WIPP-Nd-Borate-6 Pg. 98	

3.2 Task 2: Experimental Determination of theta parameters (θ) for $NdHB_4O_7^{2+}$—Na^+ and $NdHB_4O_7^{2+}$—Mg^{2+}

Undersaturation experiments were set-up with $Nd(OH)_3$ as the solid phase and NaCl as the aqueous phase ranging from 0.01 m – 5.0 m. Table 3-12 shows the experimental set-up and Tables 3-13 to 3-16 show the collected data to date. Identified outliers for neodymium data:

Day 7: Nd(OH)3-0.01-1

Day 35: Nd(OH)3-2.0-2

Day 270: Nd(OH)3-1.0-1, Nd(OH)3-1.0-2

Day 445: Nd(OH)3-0.1-1, Nd(OH)3-1.0-1

Day 712: Nd(OH)3-0.01-1, Nd(OH)3-0.01-2, Nd(OH)3-0.1-2, Nd(OH)3-1.0-1, Nd(OH)3-3.0-1,Nd(OH)3-4.0-1, Nd(OH)3-4.0-2, Nd(OH)3-5.0-1

A second set of undersaturation experiments were set-up with the addition of $Nd(OH)_3$ and $Na_2B_4O_7{\cdot}10H_2O$ together as the solid phases, and NaCl as the aqueous phase ranging in concentration from 0.01 m to 5.0 m. Table 3-17 shows the experimental set-up and Tables 3-18 to 3-22 show the collected data to date. Identified outliers for neodymium data:

Day 412: All samples on this day are different than samples Day 1100+

A third set of undersaturation experiments were set-up with the addition of $Nd(OH)_3$ as the solid phase, and $MgCl_2$ as the aqueous phase ranging in concentration from 0.01 m

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to 2.0 m. Table 3-23 shows the experimental set-up and Tables 3-24 to 3-27 show the collected data to date. Identified outliers for neodymium data:

Day 986: Nd(OH)3-2.0 Mg-2

Day 1874: Nd(OH)3-0.1 Mg-2

Day 1972: Nd(OH)3-0.01 Mg-2

A fourth set of undersaturation experiments were set-up with the addition of $Nd(OH)_3$ and $Na_2B_4O_7{\cdot}10H_2O$ together as the solid phases, and $MgCl_2$ as the aqueous phase ranging in concentration from 0.01 m to 2.0 m. Table 3-28 shows the experimental set-up and Tables 3-29 to 3-33 show the collected data to date. Identified outliers for neodymium data:

Day 704: Nd(OH)3-B-0.01 Mg-1, Nd(OH)3-B-0.1 Mg-1, Nd(OH)3-B-2.0 Mg-1

Day 1015: Nd(OH)3-B-1.0 Mg-1, Nd(OH)3-B-1.0 Mg-2

Table 3-12 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$ and NaCl interaction

Set-up ID	$Nd(OH)_3$(s) (g)	NaCl (m)	NaCl (M)	Reference	Density g/mL	Reference
Nd(OH)3-0.01-1	0.35	0.01	0.01	WIPP-Nd-Borate-1 Pg. 10	1.000	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.01-2	0.35	0.01	0.01	WIPP-Nd-Borate-1 Pg. 10	1.000	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.1-1	0.35	0.10	0.10	WIPP-Nd-Borate-1 Pg. 10	1.005	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-0.1-2	0.35	0.10	0.10	WIPP-Nd-Borate-1 Pg. 10	1.005	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.0-1	0.37	1.00	0.99	WIPP-Nd-Borate-1 Pg. 10	1.044	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-1.0-2	0.36	1.00	0.99	WIPP-Nd-Borate-1 Pg. 10	1.044	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-2.0-1	0.36	2.00	1.92	WIPP-Nd-Borate-1 Pg. 10	1.074	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-2.0-2	0.36	2.00	1.92	WIPP-Nd-Borate-1 Pg. 10	1.074	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-3.0-1	0.35	3.00	2.82	WIPP-Nd-Borate-1 Pg. 10	1.106	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-3.0-2	0.35	3.00	2.82	WIPP-Nd-Borate-1 Pg. 10	1.106	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-4.0-1	0.35	4.00	3.69	WIPP-Nd-Borate-1 Pg. 10	1.138	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-4.0-2	0.35	4.00	3.69	WIPP-Nd-Borate-1 Pg. 10	1.138	WIPP-Nd-Borate-7 Pg. 75
Nd(OH)3-5.0-1	0.35	5.00	4.52	WIPP-Nd-Borate-1	1.168	WIPP-Nd-Borate-7

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Nd(OH)3-5.0-2	0.35	5.00	4.52	Pg. 10 WIPP-Nd-Borate-1 Pg. 10	1.168	Pg. 75 WIPP-Nd-Borate-7 Pg. 75

Note: Densities used to convert starting solutions from molality to molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-13 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$ and NaCl interaction

	pH										
Set-up ID	**7 Days**	**35 Days**	**167 Days**	**270 Days**	**298 Days**	**445 Days**	**712 Days**	**741 Days**	**1146 Days**	**2609 Days**	**AVG**
Nd(OH)3-0.01-1	9.09	9.07	9.01	9.08	9.11	8.83	8.87	9.08	8.87	8.94	9.00
Nd(OH)3-0.01-2	9.45	9.54	9.54	9.56	9.64	9.47	9.47	9.58	9.22	9.22	9.50
Nd(OH)3-0.1-1	9.42	9.52	9.50	9.52	9.58	9.41	9.41	9.51	9.07	9.03	9.44
Nd(OH)3-0.1-2	9.52	9.62	9.62	9.61	9.72	9.65	9.59	9.66	9.18	9.17	9.57
Nd(OH)3-1.0-1	9.43	9.41	9.40	9.32	9.47	9.28	9.33	9.45	9.12	9.02	9.36
Nd(OH)3-1.0-2	9.44	9.44	9.48	9.26	9.50	9.33	9.35	9.45	9.12	9.12	9.37
Nd(OH)3-2.0-1	9.30	9.24	9.28	8.99	9.29	9.14	9.07	9.26	8.98	8.97	9.17
Nd(OH)3-2.0-2	9.26	9.24	9.28	9.16	9.28	9.13	9.08	9.25	8.91	8.94	9.18
Nd(OH)3-3.0-1	9.24	9.23	9.26	9.15	9.28	9.13	9.09	9.20	8.90	8.94	9.16
Nd(OH)3-3.0-2	9.23	9.21	9.27	9.18	9.27	9.15	9.13	9.23	8.95	8.96	9.18
Nd(OH)3-4.0-1	8.93	8.99	9.07	8.95	9.07	8.41	8.93	9.12	8.81	8.90	8.92
Nd(OH)3-4.0-2	8.92	8.98	9.10	8.86	9.10	8.97	8.90	9.13	8.89	8.97	8.98
Nd(OH)3-5.0-1	8.99	9.00	9.08	8.76	9.11	8.99	8.99	9.15	8.86	8.94	8.99
Nd(OH)3-5.0-2	8.95	8.86	9.04	8.75	9.09	8.98	8.92	9.13	8.84	9.04	8.95
Reference	WIPP-Nd-Borate -1 Pg. 13-15	WIPP-Nd-Borate -1 Pg. 28-29	WIPP-Nd-Borate -1 Pg. 46-48	WIPP-Nd-Borate -1 Pg. 56-58	WIPP-Nd-Borate -1 Pg. 69-71	WIPP-Nd-Borate -1 Pg. 95-97	WIPP-Nd-Borate -2 Pg. 41,43-44	WIPP-Nd-Borate -2 Pg. 67,74	WIPP-Nd-Borate -4 Pg. 32-33	WIPP-Nd-Borate -7 Pg. 82-83	

Table 3-14 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and NaCl interaction

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[Nd(III)] (M)												
Set-up ID	7 Days	35 Days	167 Days	270 Days	298 Days	445 Days	712 Days	741 Days	1146 Days	$\tilde{x}$	MAD	AVG
Nd(OH) 3-0.01-1	5.21E -07	3.09E -08	5.01E -08	1.26E -07	1.89E -08	9.86E -08	7.84E -07	1.91E -08	6.02E -08	6.02E -08	4.11E -08	5.77E -08
Nd(OH) 3-0.01-2	1.72E -08	5.22E -08	3.78E -08	9.56E -08	3.09E -08	7.99E -08	3.23E -07	2.18E -08	7.47E -08	5.22E -08	2.77E -08	5.13E -08
Nd(OH) 3-0.1-1	1.95E -07	6.46E -08	1.16E -07	1.05E -07	2.13E -08	1.64E -06	5.06E -07	3.50E -08	1.51E -07	1.16E -07	7.89E -08	1.49E -07
Nd(OH) 3-0.1-2	4.24E -08	3.40E -07	3.47E -08	2.22E -07	2.14E -08	6.95E -08	1.01E -06	5.93E -09	1.77E -07	6.95E -08	6.35E -08	1.14E -07
Nd(OH) 3-1.0-1	2.58E -08	3.76E -08	2.77E -08	6.51E -07	2.07E -08	3.65E -07	3.65E -07	2.09E -08	9.22E -08	3.76E -08	1.69E -08	3.75E -08
Nd(OH) 3-1.0-2	4.62E -08	1.69E -07	5.53E -08	1.34E -06	7.33E -08	6.42E -08	3.82E -07	8.00E -09	2.31E -07	7.33E -08	6.53E -08	1.29E -07
Nd(OH) 3-2.0-1	4.08E -08	1.65E -07	7.53E -08	4.33E -07	5.00E -08	2.11E -07	2.61E -07	3.44E -08	1.08E -07	1.08E -07	6.69E -08	1.53E -07
Nd(OH) 3-2.0-2	1.08E -07	2.19E -06	7.54E -08	9.46E -08	2.55E -08	3.23E -07	5.05E -07	1.45E -08	1.21E -07	1.08E -07	8.24E -08	1.58E -07
Nd(OH) 3-3.0-1	1.27E -07	8.67E -08	1.37E -07	2.18E -07	2.81E -08	4.22E -07	3.45E -07	2.06E -08	9.86E -08	1.27E -07	9.10E -08	1.65E -07
Nd(OH) 3-3.0-2	1.71E -07	6.43E -08	5.44E -08	1.82E -07	6.54E -08	1.88E -07	1.06E -06	1.78E -08	1.45E -07	1.45E -07	7.96E -08	1.11E -07
Nd(OH) 3-4.0-1	3.10E -08	1.20E -07	6.86E -08	1.75E -07	4.56E -08	2.03E -07	1.04E -06	2.88E -08	2.29E -07	1.20E -07	8.26E -08	1.13E -07
Nd(OH) 3-4.0-2	1.13E -07	1.59E -08	1.03E -07	1.84E -07	7.98E -08	1.81E -07	1.11E -06	2.07E -08	1.45E -07	1.13E -07	6.84E -08	1.05E -07
Nd(OH) 3-5.0-1	1.48E -07	7.71E -08	1.12E -07	3.25E -07	4.33E -08	1.55E -06	4.78E -07	6.50E -08	9.45E -08	1.12E -07	4.71E -08	1.24E -07
Nd(OH) 3-5.0-2	1.57E -07	9.71E -08	2.29E -08	5.71E -07	5.33E -07	7.01E -07	7.78E -07	1.00E -07	1.16E -07	1.57E -07	1.34E -07	3.42E -07
Reference	WIPP-Nd-Borate-1 Pg. 40-42, 43-45	WIPP-Nd-Borate-1 Pg. 40-42, 43-45	WIPP-Nd-Borate-1 Pg. 52	WIPP-Nd-Borate-1 Pg. 67-68	WIPP-Nd-Borate-1 Pg. 78	WIPP-Nd-Borate-2 Pg. 53,55	WIPP-Nd-Borate-2 Pg. 45,47	WIPP-Nd-Borate-2 Pg. 75	WIPP-Nd-Borate-5 Pg. 23	Note: Average does not contain outliers		

Note: Day 2609 has not been analyzed for Nd to date.

Modified Z-Score for the Nd(III) concentrations shown in Table 3-14

Set-up ID	7 Days	35 Days	167 Days	270 Days	298 Days	445 Days	712 Days	741 Days	1146 Days
Nd(OH) 3-0.01-1	7.57	0.48	0.17	1.08	0.68	0.63	11.88	0.67	0.00
Nd(OH) 3-0.01-2	0.85	0.00	0.35	1.06	0.52	0.67	6.58	0.74	0.55
Nd(OH) 3-0.1-1	0.67	0.44	0.00	0.10	0.81	13.01	3.34	0.69	0.30
Nd(OH) 3-0.1-2	0.29	2.87	0.37	1.62	0.51	0.00	9.95	0.67	1.14
Nd(OH) 3-1.0-1	0.47	0.00	0.39	24.43	0.67	13.02	13.05	0.67	2.18
Nd(OH)	0.28	0.99	0.19	13.03	0.00	0.09	3.19	0.67	1.63

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3-1.0-2									
Nd(OH) 3-2.0-1	0.67	0.57	0.33	3.28	0.58	1.04	1.54	0.74	0.00
Nd(OH) 3-2.0-2	0.00	17.02	0.27	0.11	0.67	1.76	3.25	0.76	0.10
Nd(OH) 3-3.0-1	0.00	0.30	0.07	0.67	0.74	2.18	1.61	0.79	0.21
Nd(OH) 3-3.0-2	0.22	0.68	0.77	0.31	0.67	0.37	7.75	1.08	0.00
Nd(OH) 3-4.0-1	0.73	0.00	0.42	0.45	0.61	0.67	7.53	0.74	0.89
Nd(OH) 3-4.0-2	0.00	0.96	0.10	0.70	0.33	0.67	9.86	0.91	0.31
Nd(OH) 3-5.0-1	0.52	0.50	0.00	3.05	0.99	20.58	5.24	0.67	0.25
Nd(OH) 3-5.0-2	0.00	0.30	0.67	2.08	1.89	2.74	3.12	0.28	0.21

Table 3-15 Measured sodium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and NaCl interaction

	[Na(I)] (M)										
Set-up ID	**7 Days**	**35 Days**	**167 Days**	**270 Days**	**298 Days**	**445 Days**	**712 Days**	**741 Days**	**1146 Days**	**2609 Days**	**AVG**
Nd(OH)3-0.01-1	1.06E-02	1.12E-02	1.10E-02	1.17E-02	1.02E-02	1.30E-02	7.40E-03	9.07E-03	1.05E-02	1.15E-02	1.05E-02
Nd(OH)3-0.01-2	1.04E-02	1.10E-02	1.12E-02	1.08E-02	1.07E-02	1.19E-02	9.91E-03	9.24E-03	9.79E-03	1.14E-02	1.05E-02
Nd(OH)3-0.1-1	9.16E-02	9.38E-02	9.53E-02	9.28E-02	9.55E-02	9.20E-02	9.23E-02	9.47E-02	9.95E-02	8.53E-02	9.42E-02
Nd(OH)3-0.1-2	9.36E-02	9.25E-02	9.45E-02	9.41E-02	9.28E-02	9.02E-02	9.96E-02	8.05E-02	1.01E-01	8.64E-02	9.33E-02
Nd(OH)3-1.0-1	9.35E-01	9.24E-01	9.02E-01	9.23E-01	6.51E-01	9.11E-01	9.78E-01	1.43E+00	1.02E+00	8.54E-01	9.64E-01
Nd(OH)3-1.0-2	9.15E-01	9.31E-01	9.14E-01	9.23E-01	9.20E-01	9.24E-01	9.88E-01	9.27E-01	9.68E-01	8.69E-01	9.34E-01
Nd(OH)3-2.0-1	1.93E+00	1.82E+00	2.04E+00	1.88E+00	2.06E+00	2.03E+00	1.98E+00	1.79E+00	2.06E+00	1.87E+00	1.95E+00
Nd(OH)3-2.0-2	1.81E+00	1.86E+00	1.87E+00	1.89E+00	2.02E+00	1.97E+00	2.03E+00	1.70E+00	2.01E+00	1.91E+00	1.91E+00
Nd(OH)3-3.0-1	2.74E+00	2.75E+00	2.77E+00	2.59E+00	2.44E+00	2.84E+00	2.77E+00	1.48E+00	2.97E+00	2.71E+00	2.60E+00
Nd(OH)3-3.0-2	2.65E+00	2.59E+00	2.58E+00	2.67E+00	2.49E+00	2.81E+00	2.94E+00	2.45E+00	2.93E+00	2.65E+00	2.68E+00
Nd(OH)3-4.0-1	3.44E+00	3.41E+00	3.40E+00	3.29E+00	3.37E+00	3.06E+00	3.54E+00	3.13E+00	3.79E+00	3.48E+00	3.38E+00
Nd(OH)3-4.0-2	3.32E+00	3.39E+00	3.33E+00	3.43E+00	3.28E+00	3.55E+00	3.44E+00	2.99E+00	3.77E+00	3.37E+00	3.39E+00
Nd(OH)3-5.0-1	4.16E+00	4.33E+00	4.13E+00	4.01E+00	4.10E+00	4.21E+00	4.33E+00	3.92E+00	4.46E+00	4.11E+00	4.18E+00
Nd(OH)3-5.0-2	4.36E+00	4.04E+00	4.06E+00	4.16E+00	3.97E+00	4.17E+00	4.34E+00	3.84E+00	4.53E+00	4.16E+00	4.16E+00

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Reference	WIPP -Nd- Borate -1 Pg. 64-65	WIPP -Nd- Borate -1 Pg. 64-65	WIPP -Nd- Borate -1 Pg. 64-66	WIPP -Nd- Borate -1 Pg. 64-65	WIPP -Nd- Borate -1 Pg. 89 and WIPP -Nd- Borate -8 Pg. 9	WIPP -Nd- Borate -2 Pg. 10	WIPP -Nd- Borate -4 Pg. 39,47 and WIPP -Nd- Borate -8 Pg. 9	WIPP -Nd- Borate -4 Pg. 39	WIPP- Nd- Borate -4 Pg. 40 and WIPP- Nd- Borate -7 Pg. 96	WIPP- Nd- Borate -8 Pg. 12

Table 3-16 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and NaCl interaction

	[Cl-] (M)										
Set-up ID	**7 Days**	**35 Days**	**167 Days**	**270 Days**	**298 Days**	**445 Days**	**712 Days**	**741 Days**	**1146 Days**	**2609 Days**	**AVG**
Nd(OH)3-0.01-1	9.96E-03	9.90E-03	1.01E-02	1.04E-02	1.06E-02	1.07E-02	9.87E-03	1.01E-02	1.01E-02	1.12E-02	1.02E-02
Nd(OH)3-0.01-2	1.01E-02	9.97E-03	1.02E-02	1.04E-02	1.09E-02	1.05E-02	9.57E-03	9.82E-03	1.00E-02	1.13E-02	1.02E-02
Nd(OH)3-0.1-1	1.01E-01	9.86E-02	1.01E-01	1.00E-01	1.00E-01	1.01E-01	9.78E-02	8.63E-02	9.37E-02	1.08E-01	9.77E-02
Nd(OH)3-0.1-2	9.98E-02	9.98E-02	9.95E-02	1.02E-01	1.02E-01	9.90E-02	9.62E-02	8.72E-02	9.17E-02	1.09E-01	9.75E-02
Nd(OH)3-1.0-1	1.00E+00	9.65E-01	1.00E+00	1.00E+00	7.67E-01	1.00E+00	9.70E-01	8.70E-01	9.29E-01	1.08E+00	9.45E-01
Nd(OH)3-1.0-2	1.01E+00	9.93E-01	1.01E+00	9.96E-01	1.05E+00	1.00E+00	9.92E-01	8.84E-01	1.01E+00	1.10E+00	9.94E-01
Nd(OH)3-2.0-1	1.96E+00	1.94E+00	1.94E+00	1.87E+00	2.06E+00	1.86E+00	1.70E+00	1.82E+00	1.79E+00	2.12E+00	1.88E+00
Nd(OH)3-2.0-2	1.93E+00	1.89E+00	1.94E+00	1.92E+00	2.18E+00	1.86E+00	1.63E+00	1.84E+00	1.83E+00	2.12E+00	1.89E+00
Nd(OH)3-3.0-1	2.84E+00	2.83E+00	2.88E+00	2.81E+00	3.17E+00	2.80E+00	2.50E+00	2.75E+00	2.69E+00	3.06E+00	2.81E+00
Nd(OH)3-3.0-2	2.85E+00	2.87E+00	2.87E+00	2.81E+00	2.80E+00	2.77E+00	2.48E+00	2.81E+00	2.74E+00	3.18E+00	2.78E+00
Nd(OH)3-4.0-1	3.71E+00	3.79E+00	3.83E+00	3.65E+00	3.74E+00	3.08E+00	3.19E+00	3.75E+00	3.55E+00	4.07E+00	3.59E+00
Nd(OH)3-4.0-2	3.68E+00	3.74E+00	3.76E+00	3.63E+00	3.65E+00	3.67E+00	3.20E+00	3.72E+00	3.62E+00	3.98E+00	3.63E+00
Nd(OH)3-5.0-1	4.64E+00	4.55E+00	4.60E+00	4.49E+00	4.65E+00	4.53E+00	4.48E+00	4.69E+00	4.41E+00	5.08E+00	4.56E+00
Nd(OH)3-5.0-2	4.63E+00	4.52E+00	4.65E+00	4.51E+00	4.58E+00	4.43E+00	4.50E+00	4.71E+00	4.47E+00	4.98E+00	4.55E+00
Reference	WIPP -Nd- Borate -2 Pg. 4-5, 23	WIPP -Nd- Borate -2 Pg. 4-5, 23	WIPP -Nd- Borate -2 Pg. 4-5	WIPP -Nd- Borate -2 Pg. 21-22	WIPP -Nd- Borate -2 Pg. 21-23, 48	WIPP -Nd- Borate -2 Pg. 21-22	WIPP -Nd- Borate -5 Pg. 42,48	WIPP -Nd- Borate -5 Pg. 45	WIPP- Nd- Borate -5 Pg. 42,48	WIPP- Nd- Borate -8 Pg. 19	

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Table 3-17 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

Set-up ID	$Nd(OH)_3$ (s) (g)	$Na_2B_4O_7$ (s) (g)	NaCl (m)	NaCl (M)	Reference	Density g/mL	Reference
Nd(OH)3-0.01B-1	0.36	10.22	0.01	0.01	WIPP-Nd-Borate-2 Pg. 30	1.027	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-0.01B-2	0.35	10.07	0.01	0.01	WIPP-Nd-Borate-2 Pg. 30	1.027	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-0.1B-1	0.35	10.03	0.10	0.10	WIPP-Nd-Borate-2 Pg. 30	1.028	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-0.1B-2	0.35	10.07	0.10	0.10	WIPP-Nd-Borate-2 Pg. 30	1.028	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-1.0B-1	0.35	10.55	1.00	0.99	WIPP-Nd-Borate-2 Pg. 30	1.049	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-1.0B-2	0.35	10.30	1.00	0.99	WIPP-Nd-Borate-2 Pg. 30	1.049	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-2.0B-1	0.35	10.20	2.00	1.92	WIPP-Nd-Borate-2 Pg. 30	1.083	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-2.0B-2	0.35	10.17	2.00	1.92	WIPP-Nd-Borate-2 Pg. 30	1.083	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-3.0B-1	0.35	10.05	3.00	2.82	WIPP-Nd-Borate-2 Pg. 30	1.115	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-3.0B-2	0.35	10.29	3.00	2.82	WIPP-Nd-Borate-2 Pg. 30	1.115	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-4.0B-1	0.35	10.15	4.00	3.69	WIPP-Nd-Borate-2 Pg. 30	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-4.0B-2	0.35	10.22	4.00	3.69	WIPP-Nd-Borate-2 Pg. 30	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-5.0B-1	0.35	10.31	5.00	4.52	WIPP-Nd-Borate-2 Pg. 30	1.178	WIPP-Nd-Borate-8 Pg. 14
Nd(OH)3-5.0B-2	0.34	10.52	5.00	4.52	WIPP-Nd-Borate-2 Pg. 30	1.178	WIPP-Nd-Borate-8 Pg. 14

Note: Densities used to convert starting solutions from molality to molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-18 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	pH				
Set-up ID	412 Days	1176 Days	1218 Days	1972 Days	AVG
Nd(OH)3-0.01B-1	9.30	9.25	9.33	9.35	9.31
Nd(OH)3-0.01B-2	9.28	9.25	9.32	9.34	9.30
Nd(OH)3-0.1B-1	9.21	9.18	9.24	9.27	9.23
Nd(OH)3-0.1B-2	9.19	9.18	9.21	9.28	9.22
Nd(OH)3-1.0B-1	8.85	8.82	8.86	8.96	8.87
Nd(OH)3-1.0B-2	8.85	8.82	8.87	8.95	8.87
Nd(OH)3-2.0B-1	8.65	8.62	8.67	8.76	8.68
Nd(OH)3-2.0B-2	8.64	8.61	8.63	8.75	8.66
Nd(OH)3-3.0B-1	8.49	8.46	8.48	8.62	8.51

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Nd(OH)3-3.0B-2	8.50	8.46	8.49	8.62	8.52
Nd(OH)3-4.0B-1	8.34	8.34	8.39	8.50	8.39
Nd(OH)3-4.0B-2	8.37	8.33	8.36	8.50	8.39
Nd(OH)3-5.0B-1	8.24	8.23	8.25	8.40	8.28
Nd(OH)3-5.0B-2	8.23	8.23	8.25	8.38	8.27
Reference	WIPP-Nd-Borate-4 Pg. 21-23	WIPP-Nd-Borate-6 Pg. 19	WIPP-Nd-Borate-6 Pg.39	WIPP-Nd-Borate-7 Pg. 77	

Table 3-19 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	[Nd(III)] (M)	
Set-up ID	**412 Days**	**1176 Days**
Nd(OH)3-0.01B-1	3.64E-07	9.52E-08
Nd(OH)3-0.01B-2	3.08E-07	1.14E-07
Nd(OH)3-0.1B-1	4.48E-07	7.35E-08
Nd(OH)3-0.1B-2	1.85E-07	1.15E-07
Nd(OH)3-1.0B-1	4.87E-07	1.22E-07
Nd(OH)3-1.0B-2	4.36E-07	8.49E-08
Nd(OH)3-2.0B-1	7.47E-07	5.73E-08
Nd(OH)3-2.0B-2	4.01E-07	2.40E-07
Nd(OH)3-3.0B-1	9.80E-07	1.73E-08
Nd(OH)3-3.0B-2	3.79E-07	2.50E-08
Nd(OH)3-4.0B-1	3.48E-07	4.28E-08
Nd(OH)3-4.0B-2	4.83E-07	4.79E-08
Nd(OH)3-5.0B-1	3.17E-07	8.31E-08
Nd(OH)3-5.0B-2	2.67E-07	7.74E-08
Reference	WIPP-Nd-Borate-5 Pg. 15 and WIPP-Nd-Borate-7 Pg. 12-13	WIPP-Nd-Borate-7 Pg. 12-13

Note: Days 1218 and 1972 have not been analyzed for Nd to date. In addition, the 412 Day data is significantly different from the 1100+ Day data. Modified Z-Scores will not be calculated for this set of data until more data can be collected.

Table 3-20 Measured sodium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	[Na(I)] (M)				
Set-up ID	**412 Days**	**1176 Days**	**1218 Days**	**1972 Days**	**AVG**
Nd(OH)3-0.01B-1	2.94E-01	2.95E-01	2.99E-01	2.91E-01	2.95E-01
Nd(OH)3-0.01B-2	2.88E-01	2.91E-01	2.97E-01	2.94E-01	2.92E-01
Nd(OH)3-0.1B-1	2.89E-01	3.23E-01	3.41E-01	3.31E-01	3.21E-01
Nd(OH)3-0.1B-2	3.39E-01	3.19E-01	3.31E-01	3.29E-01	3.30E-01
Nd(OH)3-1.0B-1	1.04E+00	1.03E+00	1.01E+00	1.08E+00	1.04E+00
Nd(OH)3-1.0B-2	1.09E+00	1.00E+00	1.03E+00	1.08E+00	1.05E+00

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Nd(OH)3-2.0B-1	1.82E+00	2.09E+00	2.14E+00	1.95E+00	2.00E+00
Nd(OH)3-2.0B-2	1.96E+00	2.12E+00	2.12E+00	1.87E+00	2.02E+00
Nd(OH)3-3.0B-1	3.19E+00	2.94E+00	2.92E+00	2.81E+00	2.97E+00
Nd(OH)3-3.0B-2	3.17E+00	2.93E+00	2.93E+00	2.85E+00	2.97E+00
Nd(OH)3-4.0B-1	3.79E+00	3.79E+00	3.85E+00	3.76E+00	3.80E+00
Nd(OH)3-4.0B-2	3.86E+00	3.72E+00	3.76E+00	3.70E+00	3.76E+00
Nd(OH)3-5.0B-1	4.22E+00	4.39E+00	4.35E+00	4.46E+00	4.35E+00
Nd(OH)3-5.0B-2	4.61E+00	4.64E+00	4.65E+00	4.65E+00	4.64E+00
Reference	WIPP-Nd-Borate-4 Pg. 41, 43	WIPP-Nd-Borate-7 Pg. 99-100	WIPP-Nd-Borate-7 Pg. 99-100 and WIPP-Nd-Borate-8 Pg. 4	WIPP-Nd-Borate-8 Pg. 11	

Table 3-21 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	[Cl-] (M)				
Set-up ID	**412 Days**	**1176 Days**	**1218 Days**	**1972 Days**	**AVG**
Nd(OH)3-0.01B-1	1.02E-02	9.71E-03	9.98E-03	NA	9.95E-03
Nd(OH)3-0.01B-2	9.75E-03	9.61E-03	9.94E-03	NA	9.77E-03
Nd(OH)3-0.1B-1	9.88E-02	1.03E-01	1.05E-01	NA	1.02E-01
Nd(OH)3-0.1B-2	1.00E-01	1.00E-01	1.03E-01	NA	1.01E-01
Nd(OH)3-1.0B-1	9.89E+00	1.02E+00	1.07E+00	NA	3.99E+00
Nd(OH)3-1.0B-2	9.98E+00	1.06E+00	1.07E+00	NA	4.04E+00
Nd(OH)3-2.0B-1	2.02E+00	1.92E+00	2.08E+00	NA	2.01E+00
Nd(OH)3-2.0B-2	2.01E+00	2.05E+00	2.07E+00	NA	2.04E+00
Nd(OH)3-3.0B-1	3.69E+00	2.90E+00	2.97E+00	NA	3.19E+00
Nd(OH)3-3.0B-2	2.99E+00	2.95E+00	3.02E+00	NA	2.99E+00
Nd(OH)3-4.0B-1	3.88E+00	3.62E+00	3.75E+00	NA	3.75E+00
Nd(OH)3-4.0B-2	3.94E+00	3.80E+00	4.01E+00	NA	3.92E+00
Nd(OH)3-5.0B-1	4.71E+00	4.76E+00	4.85E+00	NA	4.78E+00
Nd(OH)3-5.0B-2	4.79E+00	4.91E+00	4.91E+00	NA	4.87E+00
Reference	WIPP-Nd-Borate-5 Pg. 48	WIPP-Nd-Borate-7 84, 92	WIPP-Nd-Borate-7 84, 92		

Table 3-22 Measured boron molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ NaCl and $Na_2B_4O_7 \cdot 10H_2O$ interaction.

	[B] (M)				
Set-up ID	**412 Days**	**1176 Days**	**1218 Days**	**1972 Days**	**AVG**
Nd(OH)3-0.01B-1	5.62E-01	6.05E-01	6.66E-01	6.28E-01	6.15E-01
Nd(OH)3-0.01B-2	5.40E-01	5.96E-01	6.51E-01	6.34E-01	6.05E-01
Nd(OH)3-0.1B-1	4.07E-01	5.15E-01	5.77E-01	5.54E-01	5.13E-01
Nd(OH)3-0.1B-2	4.63E-01	5.08E-01	5.63E-01	5.65E-01	5.25E-01

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Nd(OH)3-1.0B-1	2.27E-01	2.52E-01	2.75E-01	2.66E-01	2.55E-01
Nd(OH)3-1.0B-2	2.29E-01	2.57E-01	2.77E-01	2.70E-01	2.58E-01
Nd(OH)3-2.0B-1	1.85E-01	2.12E-01	2.32E-01	2.11E-01	2.10E-01
Nd(OH)3-2.0B-2	1.82E-01	2.10E-01	2.28E-01	2.09E-01	2.07E-01
Nd(OH)3-3.0B-1	2.09E-01	1.90E-01	2.03E-01	1.98E-01	2.00E-01
Nd(OH)3-3.0B-2	1.82E-01	2.07E-01	2.09E-01	1.98E-01	1.99E-01
Nd(OH)3-4.0B-1	1.63E-01	1.97E-01	1.79E-01	1.91E-01	1.83E-01
Nd(OH)3-4.0B-2	1.68E-01	1.91E-01	1.77E-01	1.89E-01	1.81E-01
Nd(OH)3-5.0B-1	1.65E-01	1.98E-01	2.09E-01	1.83E-01	1.89E-01
Nd(OH)3-5.0B-2	1.69E-01	2.00E-01	2.09E-01	1.80E-01	1.89E-01
Reference	WIPP-Nd-Borate-4 pg. 44	WIPP-Nd-Borate-7 Pg. 59	WIPP-Nd-Borate-7 Pg. 61	WIPP-Nd-Borate-8 Pg. 21	

Table 3-23 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$ and $MgCl_2$ interaction

Set-up ID	$Nd(OH)_3$ (s) (g)	$MgCl_2$ (m)	$MgCl_2$ (M)	Reference	Density g/mL	Reference
Nd(OH)3-0.01 Mg-1	0.36	0.01	0.01	WIPP-Nd-Borate-2 Pg. 18	1.001	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-0.01 Mg-2	0.36	0.01	0.01	WIPP-Nd-Borate-2 Pg. 18	1.001	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-0.1 Mg-1	0.36	0.10	0.10	WIPP-Nd-Borate-2 Pg. 18	1.006	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-0.1 Mg-2	0.35	0.10	0.10	WIPP-Nd-Borate-2 Pg. 18	1.006	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-1.0 Mg-1	0.35	0.90	0.88	WIPP-Nd-Borate-2 Pg. 18	1.065	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-1.0 Mg-2	0.36	0.90	0.88	WIPP-Nd-Borate-2 Pg. 18	1.065	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-1.5 Mg-1	0.36	1.29	1.26	WIPP-Nd-Borate-2 Pg. 18	1.099	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-1.5 Mg-2	0.36	1.29	1.26	WIPP-Nd-Borate-2 Pg. 18	1.099	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-2.0 Mg-1	0.36	1.64	1.59	WIPP-Nd-Borate-2 Pg. 18	1.115	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-2.0 Mg-2	0.36	1.64	1.59	WIPP-Nd-Borate-2 Pg. 18	1.115	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-2.5 Mg-1	0.36	1.97	1.89	WIPP-Nd-Borate-2 Pg. 18	1.138	WIPP-Nd-Borate-8 Pg. 13
Nd(OH)3-2.5 Mg-2	0.37	1.97	1.89	WIPP-Nd-Borate-2 Pg. 18	1.138	WIPP-Nd-Borate-8 Pg. 13

Note: Densities used to convert starting solutions from Molality to Molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-24 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$ and $MgCl_2$ interaction

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	pH					
Set-up ID	**671 Days**	**986 Days**	**1874 Days**	**1972 Days**	**2082 Days**	**AVG**
Nd(OH)3-0.01 Mg-1	8.88	9.02	8.95	8.94	8.90	8.95
Nd(OH)3-0.01 Mg-2	8.84	8.99	8.99	9.03	8.80	8.96
Nd(OH)3-0.1 Mg-1	8.71	8.81	8.88	8.93	8.81	8.83
Nd(OH)3-0.1 Mg-2	8.74	8.87	8.90	8.95	8.72	8.87
Nd(OH)3-1.0 Mg-1	7.99	8.13	8.15	8.22	7.98	8.12
Nd(OH)3-1.0 Mg-2	8.06	8.18	8.22	8.29	8.08	8.19
Nd(OH)3-1.5 Mg-1	7.75	7.89	7.94	7.94	7.85	7.88
Nd(OH)3-1.5 Mg-2	7.77	7.89	7.95	7.99	7.76	7.90
Nd(OH)3-2.0 Mg-1	7.54	7.68	7.75	7.80	7.59	7.69
Nd(OH)3-2.0 Mg-2	7.52	7.65	7.70	7.74	7.53	7.65
Nd(OH)3-2.5 Mg-1	7.35	7.49	7.58	7.57	7.45	7.50
Nd(OH)3-2.5 Mg-2	7.32	7.47	7.55	7.57	7.40	7.48
Reference	WIPP-Nd-Borate-4 Pg. 36-37	WIPP-Nd-Borate-4 Pg. 72-74	WIPP-Nd-Borate-6 Pg. 55	WIPP-Nd-Borate-7 Pg. 16	WIPP-Nd-Borate-7 Pg. 97	

Table 3-25 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $MgCl_2$ interaction

	[Nd(III)] (M)						
Set-up ID	**671 Days**	**986 Days**	**1874 Days**	**1972 Days**		**MAD**	**AVG**
Nd(OH)3-0.01 Mg-1	1.92E-07	1.60E-08	2.87E-07	2.13E-07	2.03E-07	4.74E-08	1.77E-07
Nd(OH)3-0.01 Mg-2	3.10E-08	4.67E-08	2.52E-07	2.75E-06	1.49E-07	1.10E-07	1.10E-07
Nd(OH)3-0.1 Mg-1	2.82E-07	6.09E-08	3.78E-07	1.44E-07	2.13E-07	1.11E-07	2.16E-07
Nd(OH)3-0.1 Mg-2	1.06E-07	5.77E-08	3.25E-07	6.80E-08	8.69E-08	2.41E-08	7.72E-08
Nd(OH)3-1.0 Mg-1	3.79E-06	3.21E-06	4.05E-06	3.41E-06	3.60E-06	2.91E-07	3.61E-06
Nd(OH)3-1.0 Mg-2	2.92E-06	2.61E-06	2.87E-06	2.43E-06	2.74E-06	1.56E-07	2.71E-06
Nd(OH)3-1.5 Mg-1	8.98E-06	9.44E-06	8.84E-06	7.70E-06	8.91E-06	2.99E-07	8.74E-06
Nd(OH)3-1.5 Mg-2	8.40E-06	8.06E-06	8.55E-06	7.35E-06	8.23E-06	2.47E-07	8.09E-06
Nd(OH)3-2.0 Mg-1	1.71E-05	1.56E-05	1.81E-05	1.59E-05	1.65E-05	7.60E-07	1.67E-05
Nd(OH)3-2.0 Mg-2	2.03E-05	3.51E-05	2.31E-05	1.95E-05	2.17E-05	1.84E-06	2.45E-05
Nd(OH)3-2.5 Mg-1	2.89E-05	2.63E-05	2.81E-05	2.60E-05	2.72E-05	1.06E-06	2.73E-05
Nd(OH)3-2.5 Mg-2	2.66E-05	2.91E-05	3.02E-05	2.69E-05	2.80E-05	1.26E-06	2.82E-05

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Reference	WIPP-Nd-Borate-5 Pg. 27-28	WIPP-Nd-Borate-5 Pg. 61	WIPP-Nd-Borate-6 Pg. 57	WIPP-Nd-Borate-7 Pg. 23-24		Note:Average does not contain outliers

Note: Day 2082 has not been analyzed for Nd to date.

Modified Z-Score for the Nd(III) concentrations shown in Table 3-25

Set-up ID	671 Days	986 Days	1874 Days	1972 Days
Nd(OH)3-0.01 Mg-1	0.15	2.65	1.20	0.15
Nd(OH)3-0.01 Mg-2	0.72	0.63	0.63	15.92
Nd(OH)3-0.1 Mg-1	0.42	0.93	1.01	0.42
Nd(OH)3-0.1 Mg-2	0.53	0.82	6.65	0.53
Nd(OH)3-1.0 Mg-1	0.44	0.91	1.03	0.44
Nd(OH)3-1.0 Mg-2	0.80	0.55	0.55	1.34
Nd(OH)3-1.5 Mg-1	0.15	1.20	0.15	2.74
Nd(OH)3-1.5 Mg-2	0.47	0.47	0.88	2.41
Nd(OH)3-2.0 Mg-1	0.53	0.82	1.41	0.53
Nd(OH)3-2.0 Mg-2	0.52	4.93	0.52	0.82
Nd(OH)3-2.5 Mg-1	1.09	0.60	0.60	0.75
Nd(OH)3-2.5 Mg-2	0.76	0.59	1.16	0.59

Table 3-26 Measured magnesium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $MgCl_2$ interaction

	[Mg(II)] (M)					
Set-up ID	**671 Days**	**986 Days**	**1874 Days**	**1972 Days**	**2082 Days**	**AVG**
Nd(OH)3-0.01 Mg-1	1.02E-02	1.03E-02	1.03E-02	8.44E-03	8.91E-03	9.48E-03
Nd(OH)3-0.01 Mg-2	1.07E-02	1.04E-02	1.05E-02	8.46E-03	8.92E-03	9.55E-03
Nd(OH)3-0.1 Mg-1	9.61E-02	9.57E-02	9.72E-02	8.13E-02	8.55E-02	8.99E-02
Nd(OH)3-0.1 Mg-2	9.61E-02	9.37E-02	9.59E-02	8.00E-02	8.64E-02	8.90E-02
Nd(OH)3-1.0 Mg-1	8.82E-01	8.52E-01	9.03E-01	7.45E-01	7.83E-01	8.21E-01
Nd(OH)3-1.0 Mg-2	8.87E-01	8.48E-01	8.46E-01	7.46E-01	7.86E-01	8.06E-01
Nd(OH)3-1.5 Mg-1	1.28E+00	1.24E+00	1.28E+00	1.05E+00	1.12E+00	1.17E+00
Nd(OH)3-1.5 Mg-2	1.15E+00	1.25E+00	1.27E+00	1.03E+00	1.12E+00	1.17E+00
Nd(OH)3-2.0 Mg-1	1.59E+00	1.59E+00	1.64E+00	1.33E+00	1.39E+00	1.48E+00
Nd(OH)3-2.0 Mg-2	1.58E+00	1.56E+00	1.64E+00	1.35E+00	1.49E+00	1.51E+00
Nd(OH)3-2.5 Mg-1	1.95E+00	1.87E+00	1.98E+00	1.59E+00	1.75E+00	1.80E+00
Nd(OH)3-2.5 Mg-2	1.85E+00	1.83E+00	1.99E+00	1.58E+00	1.71E+00	1.78E+00

Reference	WIPP-Nd-Borate-4 Pg. 45	WIPP-Nd-Borate-4 Pg. 87	WIPP-Nd-Borate-6 Pg. 58	WIPP-Nd-Borate-7 Pg. 74	WIPP-Nd-Borate-8 Pg. 22

Table 3-27 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $MgCl_2$ interaction

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	[Cl-] (M)					
Set-up ID	**671 Days**	**986 Days**	**1874 Days**	**1972 Days**	**2082 Days**	**AVG**
Nd(OH)3-0.01 Mg-1	2.14E-02	2.20E-02	2.16E-02	2.25E-02	2.05E-02	2.16E-02
Nd(OH)3-0.01 Mg-2	2.11E-02	2.21E-02	2.04E-02	2.14E-02	2.01E-02	2.10E-02
Nd(OH)3-0.1 Mg-1	2.04E-01	2.12E-01	2.02E-01	2.06E-01	2.03E-01	2.06E-01
Nd(OH)3-0.1 Mg-2	2.03E-01	2.05E-01	1.94E-01	2.07E-01	2.04E-01	2.03E-01
Nd(OH)3-1.0 Mg-1	1.87E+00	1.96E+00	1.78E+00	1.87E+00	1.89E+00	1.88E+00
Nd(OH)3-1.0 Mg-2	1.88E+00	1.97E+00	1.69E+00	1.87E+00	1.88E+00	1.85E+00
Nd(OH)3-1.5 Mg-1	2.69E+00	2.78E+00	2.57E+00	2.66E+00	2.68E+00	2.67E+00
Nd(OH)3-1.5 Mg-2	2.69E+00	2.71E+00	2.47E+00	2.66E+00	2.68E+00	2.63E+00
Nd(OH)3-2.0 Mg-1	3.32E+00	3.45E+00	3.18E+00	3.33E+00	3.38E+00	3.33E+00
Nd(OH)3-2.0 Mg-2	3.32E+00	3.47E+00	3.18E+00	3.36E+00	3.33E+00	3.34E+00
Nd(OH)3-2.5 Mg-1	4.01E+00	4.10E+00	3.75E+00	4.06E+00	4.02E+00	3.99E+00
Nd(OH)3-2.5 Mg-2	3.98E+00	4.11E+00	3.78E+00	4.04E+00	4.03E+00	3.99E+00
Reference	WIPP-Nd-Borate-5 Pg. 48-49	WIPP-Nd-Borate-5 Pg. 85	WIPP-Nd-Borate-6 Pg. 61	WIPP-Nd-Borate-7 Pg. 20, 87	WIPP-Nd-Borate-8 Pg. 17	

Table 3-28 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7 \cdot 10H_2O$ and $MgCl_2$ interaction

Set-up ID	**$Nd(OH)_3$ (s) (g)**	**$Na_2B_4O_7$ (s) (g)**	**$MgCl_2$ (m)**	**$MgCl_2$ (M)**	**Reference**	**Density g/mL**	**Reference**
Nd(OH)3-B-0.01 Mg-1	0.36	10.02	0.01	0.01	WIPP-Nd-Borate-2 Pg. 16-17	1.028	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-0.01 Mg-2	0.36	10.56	0.01	0.01	WIPP-Nd-Borate-2 Pg. 16-17	1.028	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-0.1 Mg-1	0.36	10.02	0.10	0.10	WIPP-Nd-Borate-2 Pg. 16-17	1.029	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-0.1 Mg-2	0.37	10.04	0.10	0.10	WIPP-Nd-Borate-2 Pg. 16-17	1.029	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-1.0 Mg-1	0.36	10.04	0.90	0.88	WIPP-Nd-Borate-2 Pg. 16-17	1.077	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-1.0 Mg-2	0.35	10.00	0.90	0.88	WIPP-Nd-Borate-2 Pg. 16-17	1.077	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-1.5 Mg-1	0.36	10.02	1.29	1.26	WIPP-Nd-Borate-2 Pg. 16-17	1.104	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-1.5 Mg-2	0.36	10.05	1.29	1.26	WIPP-Nd-Borate-2 Pg. 16-17	1.104	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-2.0 Mg-1	0.35	10.04	1.64	1.59	WIPP-Nd-Borate-2 Pg. 16-17	1.128	WIPP-Nd-Borate-7 Pg.

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Nd(OH)3-B-2.0 Mg-2	0.36	10.04	1.64	1.59	WIPP-Nd-Borate-2 Pg. 16-17	1.128	76 WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-2.5 Mg-1	0.37	10.05	1.97	1.89	WIPP-Nd-Borate-2 Pg. 16-17	1.146	WIPP-Nd-Borate-7 Pg. 76
Nd(OH)3-B-2.5 Mg-2	0.37	10.80	1.97	1.89	WIPP-Nd-Borate-2 Pg. 16-17	1.146	WIPP-Nd-Borate-7 Pg. 76

Note: Densities used to convert starting solutions from molality to molarity can be found in Appendix B. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-29 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $MgCl_2$ interaction

	pH						
Set-up ID	**704 Days**	**994 Days**	**1015 Days**	**1307 Days**	**1883 Days**	**1986 Days**	**AVG**
Nd(OH)3-B-0.01 Mg-1	9.21	9.25	9.23	9.26	9.28	9.26	9.25
Nd(OH)3-B-0.01 Mg-2	9.18	9.25	9.23	9.28	9.27	9.26	9.24
Nd(OH)3-B-0.1 Mg-1	8.79	8.82	8.83	8.90	8.85	8.84	8.84
Nd(OH)3-B-0.1 Mg-2	9.04	9.08	9.09	8.88	8.82	8.79	8.98
Nd(OH)3-B-1.0 Mg-1	6.89	6.91	6.91	6.96	6.94	6.90	6.92
Nd(OH)3-B-1.0 Mg-2	6.92	6.80	6.80	6.75	6.73	6.68	6.80
Nd(OH)3-B-1.5 Mg-1	7.54	7.60	7.62	6.56	6.44	6.42	7.15
Nd(OH)3-B-1.5 Mg-2	7.53	7.60	7.62	6.69	6.45	6.36	7.18
Nd(OH)3-B-2.0 Mg-1	7.18	7.25	7.28	7.05	6.62	6.56	7.08
Nd(OH)3-B-2.0 Mg-2	7.19	7.25	7.28	7.21	6.58	6.54	7.10
Nd(OH)3-B-2.5 Mg-1	6.37	6.35	6.38	6.31	6.30	6.23	6.34
Nd(OH)3-B-2.5 Mg-2	6.42	6.39	6.42	6.36	6.24	6.29	6.37
Reference	WIPP-Nd-Borate-4 Pg. 48-49	WIPP-Nd-Borate-5 Pg. 62	WIPP-Nd-Borate-4 Pg. 90-91	WIPP-Nd-Borate-6 Pg. 37	WIPP-Nd-Borate-6 Pg. 59	WIPP-Nd-Borate-7 Pg. 25	

Table 3-30 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $MgCl_2$ interaction

	[Nd(III)] (M)						
Set-up ID	**704 Days**	**994 Days**	**1015 Days**	**1307 Days**	$\tilde{x}$	**MAD**	**AVG**
Nd(OH)3-B-0.01 Mg-1	8.50E-07	1.48E-07	1.45E-07	2.35E-07	1.92E-07	4.50E-08	1.76E-07
Nd(OH)3-B-0.01 Mg-2	3.94E-07	2.61E-07	1.43E-07	1.86E-07	2.23E-07	5.93E-08	2.46E-07
Nd(OH)3-B-0.1	7.24E-	1.60E-07	1.53E-07	1.60E-07	1.60E-07	3.71E-	1.58E-07

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Mg-1	07					09	
Nd(OH)3-B-0.1 Mg-2	4.69E-07	2.02E-07	1.37E-07	3.14E-07	2.58E-07	8.86E-08	2.80E-07
Nd(OH)3-B-1.0 Mg-1	4.86E-07	2.73E-07	1.08E-06	4.93E-07	4.90E-07	1.10E-07	4.17E-07
Nd(OH)3-B-1.0 Mg-2	4.32E-07	3.47E-07	1.70E-06	2.74E-07	3.90E-07	7.91E-08	3.51E-07
Nd(OH)3-B-1.5 Mg-1	4.88E-06	5.34E-06	8.11E-07	1.88E-06	3.38E-06	1.73E-06	3.23E-06
Nd(OH)3-B-1.5 Mg-2	4.82E-06	5.11E-06	7.07E-07	1.38E-06	3.10E-06	1.86E-06	3.00E-06
Nd(OH)3-B-2.0 Mg-1	1.55E-06	6.57E-07	2.58E-07	6.32E-07	6.44E-07	1.99E-07	7.75E-07
Nd(OH)3-B-2.0 Mg-2	1.60E-06	6.75E-07	8.37E-07	5.54E-07	7.56E-07	1.42E-07	6.89E-07
Nd(OH)3-B-2.5 Mg-1	2.51E-06	1.10E-06	2.94E-07	6.32E-07	8.66E-07	4.03E-07	1.13E-06
Nd(OH)3-B-2.5 Mg-2	1.42E-06	9.64E-07	2.91E-07	7.94E-07	8.79E-07	3.11E-07	8.66E-07
Reference	WIPP-Nd-Borate-6 Pg. 31-32 and WIPP-Nd-Borate-7 Pg. 10	WIPP-Nd-Borate-6 Pg. 31-32	WIPP-Nd-Borate-6 Pg. 51	WIPP-Nd-Borate-6 Pg. 31-32	Note: Average does not contain outliers		

Note: Days 1883 and 1986 have not been analyzed for Nd to date.

Modified Z-Score for the Nd(III) concentrations shown in Table 3-30

Set-up ID	704 Days	994 Days	1015 Days	1307 Days
Nd(OH)3-B-0.01 Mg-1	9.86	0.65	0.70	0.65
Nd(OH)3-B-0.01 Mg-2	1.94	0.43	0.92	0.43
Nd(OH)3-B-0.1 Mg-1	102.50	0.08	1.27	0.08
Nd(OH)3-B-0.1 Mg-2	1.60	0.43	0.92	0.43
Nd(OH)3-B-1.0 Mg-1	0.02	1.33	3.63	0.02
Nd(OH)3-B-1.0 Mg-2	0.37	0.37	11.18	0.98
Nd(OH)3-B-1.5 Mg-1	0.59	0.76	1.00	0.59
Nd(OH)3-B-1.5 Mg-2	0.62	0.73	0.87	0.62
Nd(OH)3-B-2.0 Mg-1	3.08	0.04	1.31	0.04
Nd(OH)3-B-2.0 Mg-2	4.00	0.39	0.39	0.96
Nd(OH)3-B-2.5 Mg-1	2.75	0.39	0.96	0.39
Nd(OH)3-B-2.5 Mg-2	1.16	0.18	1.28	0.18

Table 3-31 Measured magnesium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $MgCl_2$ interaction

[Mg(II)] (M)

Information Only

Set-up ID	704 Days	994 Days	1015 Days	1307 Days	1883 Days	1986 Days	AVG
Nd(OH)3-B-0.01 Mg-1	9.76E-03	9.31E-03	1.01E-02	6.46E-03	3.17E-03	1.88E-03	6.77E-03
Nd(OH)3-B-0.01 Mg-2	9.29E-03	9.83E-03	9.86E-03	9.81E-03	2.97E-03	1.71E-03	7.24E-03
Nd(OH)3-B-0.1 Mg-1	2.77E-03	2.82E-03	2.83E-03	3.03E-03	2.86E-03	1.80E-03	2.68E-03
Nd(OH)3-B-0.1 Mg-2	2.39E-02	2.51E-02	2.49E-02	1.21E-02	3.13E-03	2.13E-03	1.52E-02
Nd(OH)3-B-1.0 Mg-1	5.71E-01	5.98E-01	5.91E-01	6.13E-01	6.35E-01	6.32E-01	6.07E-01
Nd(OH)3-B-1.0 Mg-2	5.61E-01	5.72E-01	5.91E-01	5.82E-01	6.17E-01	6.45E-01	5.95E-01
Nd(OH)3-B-1.5 Mg-1	9.67E-01	1.01E+00	1.00E+00	9.82E-01	9.98E-01	9.95E-01	9.93E-01
Nd(OH)3-B-1.5 Mg-2	9.33E-01	1.03E+00	1.01E+00	9.82E-01	9.97E-01	9.78E-01	9.88E-01
Nd(OH)3-B-2.0 Mg-1	1.16E+00	1.37E+00	1.23E+00	1.31E+00	1.34E+00	1.29E+00	1.28E+00
Nd(OH)3-B-2.0 Mg-2	1.13E+00	1.11E+00	1.19E+00	1.34E+00	1.33E+00	1.28E+00	1.23E+00
Nd(OH)3-B-2.5 Mg-1	1.42E+00	1.21E+00	1.54E+00	1.58E+00	1.45E+00	1.55E+00	1.46E+00
Nd(OH)3-B-2.5 Mg-2	1.41E+00	1.45E+00	1.50E+00	1.59E+00	1.46E+00	1.55E+00	1.49E+00
Reference	WIPP-Nd-Borate-4 Pg. 46 and WIPP-Nd-Borate-5 Pg. 100	WIPP-Nd-Borate-5 Pg. 95, 100	WIPP-Nd-Borate-5 Pg. 95, 100	WIPP-Nd-Borate-6 Pg. 43-45	WIPP-Nd-Borate-6 Pg. 63	WIPP-Nd-Borate-7 Pg. 28	

Table 3-32 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $MgCl_2$ interaction

	[Cl-] (M)						
Set-up ID	704 Days	994 Days	1015 Days	1307 Days	1883 Days	1986 Days	Average
Nd(OH)3-B-0.01 Mg-1	2.08E-02	2.19E-02	2.11E-02	2.07E-02	2.02E-02	2.14E-02	2.10E-02
Nd(OH)3-B-0.01 Mg-2	2.05E-02	2.19E-02	2.12E-02	2.09E-02	2.00E-02	2.13E-02	2.10E-02
Nd(OH)3-B-0.1 Mg-1	1.92E-01	2.18E-01	2.04E-01	1.99E-01	1.89E-01	2.02E-01	2.01E-01
Nd(OH)3-B-0.1 Mg-2	1.99E-01	2.25E-01	2.04E-01	1.99E-01	1.89E-01	2.05E-01	2.04E-01
Nd(OH)3-B-1.0 Mg-1	1.84E+00	2.00E+00	1.89E+00	1.59E+00	1.71E+00	1.83E+00	1.81E+00
Nd(OH)3-B-1.0 Mg-2	1.83E+00	2.02E+00	1.86E+00	1.71E+00	1.68E+00	1.85E+00	1.82E+00
Nd(OH)3-B-1.5 Mg-1	2.57E+00	2.68E+00	2.56E+00	2.59E+00	2.41E+00	2.63E+00	2.57E+00
Nd(OH)3-B-1.5 Mg-2	2.56E+00	2.37E+00	2.60E+00	2.59E+00	2.41E+00	2.65E+00	2.53E+00
Nd(OH)3-B-2.0 Mg-1	3.33E+00	3.49E+00	3.37E+00	3.34E+00	3.22E+00	3.29E+00	3.34E+00
Nd(OH)3-B-2.0 Mg-2	3.32E+00	3.41E+00	3.33E+00	3.37E+00	3.28E+00	3.30E+00	3.33E+00
Nd(OH)3-B-2.5 Mg-1	3.86E+00	4.45E+00	3.97E+00	3.63E+00	3.85E+00	3.86E+00	3.94E+00
Nd(OH)3-B-2.5 Mg-2	3.90E+00	4.48E+00	4.03E+00	4.25E+00	3.86E+00	3.96E+00	4.08E+00
Reference	WIPP-Nd-Borate-5 Pg. 48-49	WIPP-Nd-Borate-5 Pg. 82-83, 98	WIPP-Nd-Borate-5 Pg. 86	WIPP-Nd-Borate-7 Pg. 87	WIPP-Nd-Borate-6 Pg. 61, 74	WIPP-Nd-Borate-7 Pg. 30	

Information Only

Table 3-33 Measured boron molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7 \cdot 10H_2O$ and $MgCl_2$ interaction

	[B] (M)						
Set-up ID	**704 Days**	**994 Days**	**1015 Days**	**1307 Days**	**1883 Days**	**1986 Days**	**Average**
Nd(OH)3-B-0.01 Mg-1	5.46E-01	5.49E-01	4.84E-01	6.55E-01	5.61E-01	5.03E-01	5.50E-01
Nd(OH)3-B-0.01 Mg-2	5.50E-01	5.74E-01	5.34E-01	6.44E-01	5.60E-01	4.94E-01	5.59E-01
Nd(OH)3-B-0.1 Mg-1	4.75E-01	5.07E-01	4.69E-01	5.73E-01	4.97E-01	4.44E-01	4.94E-01
Nd(OH)3-B-0.1 Mg-2	4.86E-01	4.93E-01	4.86E-01	5.96E-01	5.16E-01	4.43E-01	5.03E-01
Nd(OH)3-B-1.0 Mg-1	4.02E-01	4.27E-01	4.21E-01	4.49E-01	4.15E-01	3.91E-01	4.18E-01
Nd(OH)3-B-1.0 Mg-2	3.96E-01	3.85E-01	3.56E-01	3.81E-01	3.56E-01	3.45E-01	3.70E-01
Nd(OH)3-B-1.5 Mg-1	5.34E-01	5.76E-01	5.54E-01	4.39E-01	4.02E-01	3.79E-01	4.81E-01
Nd(OH)3-B-1.5 Mg-2	5.33E-01	6.14E-01	5.76E-01	4.84E-01	4.03E-01	3.83E-01	4.99E-01
Nd(OH)3-B-2.0 Mg-1	2.80E-01	2.86E-01	3.02E-01	3.08E-01	3.13E-01	3.33E-01	3.04E-01
Nd(OH)3-B-2.0 Mg-2	2.71E-01	2.77E-01	2.97E-01	2.89E-01	3.02E-01	3.34E-01	2.95E-01
Nd(OH)3-B-2.5 Mg-1	3.22E-01	3.77E-01	4.17E-01	4.29E-01	4.09E-01	3.96E-01	3.92E-01
Nd(OH)3-B-2.5 Mg-2	3.26E-01	3.69E-01	3.63E-01	4.24E-01	4.19E-01	3.83E-01	3.81E-01
Reference	WIPP-Nd-Borate-5 Pg. 92	WIPP-Nd-Borate-5 Pg. 92-93	WIPP-Nd-Borate-5 Pg. 94	WIPP-Nd-Borate-6 Pg. 42	WIPP-Nd-Borate-6 Pg. 69	WIPP-Nd-Borate-7 Pg. 27	

3.3 Task 3: Experimental determination of psi parameters (Ψ) for $NdHB_4O_7^{2+}$—Na^+—Cl^- and $NdHB_4O_7^{2+}$—Mg^{2+}—Cl^-

Undersaturation experiments were set-up with the addition of $Nd(OH)_3$ as the solid phase and both NaCl and $MgCl_2$ as the aqueous phase ranging from 0.5 m to 5.0 m and 0.5 m to 1.64 m respectively. Table 3-34 shows the experimental set-up and Tables 3-35 to 3-38 show the collected data to date. Identified outliers for neodymium data:

Day 334: Nd-MgCl2-F-2

Day 1544: Nd-MgCl2-B-1

A second set of undersaturation experiments were set-up with the addition of $Nd(OH)_3$ and $Na_2B_4O_7 \cdot 10H_2O$ together as the solid phases and both NaCl and $MgCl_2$ as the aqueous phase ranging from 0.5 m to 5.0 m and 0.5 m to 1.64 m respectively. Table 3-39 shows the experimental set-up and Tables 3-40 to 3-45 show the collected data to date. Identified outliers for neodymium data:

Day 657: Nd-B4-MgCl2-D-1

Day 1524: Nd-B4-MgCl2-A-1

Information Only

Table 3-34 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$ and $NaCl+MgCl_2$ interaction

Set-up ID	$Nd(OH)_3$ (s) (g)	NaCl (m)	NaCl (M)	$MgCl_2$ (m)	$MgCl_2$ (M)	Reference	Density g/mL	Reference
Nd-MgCl2-A-1	0.34	5.00	4.53	0.47	0.47	WIPP-Nd-Borate-4 Pg. 18	1.189	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-A-2	0.35	5.00	4.53	0.47	0.47	WIPP-Nd-Borate-4 Pg. 18	1.189	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-B-1	0.35	3.50	3.26	0.74	0.72	WIPP-Nd-Borate-4 Pg. 18	1.159	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-B-2	0.36	3.50	3.26	0.74	0.72	WIPP-Nd-Borate-4 Pg. 18	1.159	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-C-1	0.35	3.00	2.82	1.10	1.08	WIPP-Nd-Borate-4 Pg. 18	1.164	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-C-2	0.36	3.00	2.82	1.10	1.08	WIPP-Nd-Borate-4 Pg. 18	1.164	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-D-1	0.35	2.00	1.92	1.29	1.26	WIPP-Nd-Borate-4 Pg. 18	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-D-2	0.35	2.00	1.92	1.29	1.26	WIPP-Nd-Borate-4 Pg. 18	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-E-1	0.36	1.50	1.45	1.47	1.43	WIPP-Nd-Borate-4 Pg. 18	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-E-2	0.35	1.50	1.45	1.47	1.43	WIPP-Nd-Borate-4 Pg. 18	1.145	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-F-1	0.35	0.50	0.50	1.64	1.59	WIPP-Nd-Borate-4 Pg. 18	1.126	WIPP-Nd-Borate-8 Pg. 14
Nd-MgCl2-F-2	0.35	0.50	0.50	1.64	1.59	WIPP-Nd-Borate-4 Pg. 18	1.126	WIPP-Nd-Borate-8 Pg. 14

Note: Densities used to convert starting solutions from molality to molarity can be found in Appendix C. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-35 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$ and $NaCl+MgCl_2$ interaction

	pH					
Set-up ID	334 Days	893 Days	1441 Days	1544 Days	1631 Days	AVG
Nd-MgCl2-A-1	7.65	7.60	7.87	7.94	7.95	7.80
Nd-MgCl2-A-2	7.79	7.78	7.88	7.92	7.99	7.87
Nd-MgCl2-B-1	7.60	7.54	7.67	7.76	7.82	7.68
Nd-MgCl2-B-2	7.63	7.65	7.70	7.76	7.81	7.71
Nd-MgCl2-C-1	7.41	7.46	7.50	7.54	7.55	7.49
Nd-MgCl2-C-2	7.38	7.31	7.47	7.54	7.55	7.45
Nd-MgCl2-D-1	7.24	7.31	7.35	7.38	7.40	7.34
Nd-MgCl2-D-2	7.20	7.24	7.32	7.35	7.43	7.31
Nd-MgCl2-E-1	7.15	7.21	7.28	7.29	7.27	7.24
Nd-MgCl2-E-2	7.15	7.19	7.30	7.32	7.30	7.25
Nd-MgCl2-F-1	7.42	7.43	7.55	7.59	7.54	7.51
Nd-MgCl2-F-2	7.39	7.40	7.50	7.53	7.52	7.47

Information Only

Reference	WIPP-Nd-Borate-4 Pg. 58-60	WIPP-Nd-Borate-6 Pg. 50	WIPP-Nd-Borate-6 Pg. 64	WIPP-Nd-Borate-7 Pg. 32	WIPP-Nd-Borate-7 Pg. 81

Table 3-36 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $NaCl+MgCl_2$ interaction

	[Nd(III)] (M)					
Set-up ID	**334 Days**	**1441 Days**	**1544 Days**	**$\tilde{x}$**	**MAD**	**AVG**
Nd-MgCl2-A-1	3.91E-07	7.72E-07	4.38E-07	4.38E-07	4.69E-08	5.33E-07
Nd-MgCl2-A-2	4.77E-07	7.10E-07	4.33E-07	4.77E-07	4.39E-08	5.40E-07
Nd-MgCl2-B-1	4.14E-06	4.04E-06	3.42E-06	4.04E-06	9.59E-08	4.09E-06
Nd-MgCl2-B-2	3.70E-06	4.40E-06	3.90E-06	3.90E-06	2.02E-07	4.00E-06
Nd-MgCl2-C-1	1.76E-05	1.26E-05	1.02E-05	1.26E-05	2.35E-06	1.35E-05
Nd-MgCl2-C-2	1.68E-05	1.54E-05	1.35E-05	1.54E-05	1.43E-06	1.52E-05
Nd-MgCl2-D-1	3.78E-05	3.54E-05	3.64E-05	3.64E-05	1.06E-06	3.65E-05
Nd-MgCl2-D-2	4.17E-05	4.20E-05	NA	4.19E-05	1.05E-07	4.19E-05
Nd-MgCl2-E-1	5.63E-05	6.03E-05	4.96E-05	5.63E-05	3.97E-06	5.54E-05
Nd-MgCl2-E-2	4.83E-05	5.45E-05	4.56E-05	4.83E-05	2.66E-06	4.95E-05
Nd-MgCl2-F-1	2.05E-05	1.85E-05	1.56E-05	1.85E-05	1.94E-06	1.82E-05
Nd-MgCl2-F-2	2.16E-05	1.91E-05	1.90E-05	1.91E-05	1.20E-07	1.90E-05
Reference	WIPP-Nd-Borate-4 Pg. 60-61	WIPP-Nd-Borate-6 Pg. 71	WIPP-Nd-Borate-7 Pg. 47	Note: Average does not contain outliers		

Note: Days 893 and 1631 have not been analyzed for Nd to date

Modified Z-Score for the Nd(III) concentrations shown in Table 3-36			
Set-up ID	**334 Days**	**1441 Days**	**1544 Days**
Nd-MgCl2-A-1	0.67	4.80	0.00
Nd-MgCl2-A-2	0.00	3.58	0.67
Nd-MgCl2-B-1	0.67	0.00	4.43
Nd-MgCl2-B-2	0.67	1.68	0.00
Nd-MgCl2-C-1	1.44	0.00	0.67
Nd-MgCl2-C-2	0.67	0.00	0.89
Nd-MgCl2-D-1	0.89	0.67	0.00
Nd-MgCl2-D-2	0.67	0.67	NA
Nd-MgCl2-E-1	0.00	0.67	1.15
Nd-MgCl2-E-2	0.00	1.59	0.67
Nd-MgCl2-F-1	0.67	0.00	1.03
Nd-MgCl2-F-2	14.36	0.00	0.67

Table 3-37 Measured magnesium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $NaCl+MgCl_2$ interaction

[Mg(II)] (M)

Information Only

Set-up ID	334 Days	893 Days	1441 Days	1544 Days	1631 Days	AVG
Nd-MgCl2-A-1	4.77E-01	4.01E-01	4.42E-01	4.27E-01	4.47E-01	4.39E-01
Nd-MgCl2-A-2	4.64E-01	3.98E-01	4.71E-01	4.22E-01	4.46E-01	4.40E-01
Nd-MgCl2-B-1	7.17E-01	6.14E-01	7.21E-01	6.55E-01	6.76E-01	6.76E-01
Nd-MgCl2-B-2	7.31E-01	6.12E-01	7.13E-01	6.53E-01	6.55E-01	6.73E-01
Nd-MgCl2-C-1	1.14E+00	8.97E-01	1.06E+00	1.01E+00	1.08E+00	1.04E+00
Nd-MgCl2-C-2	1.08E+00	8.98E-01	1.06E+00	1.02E+00	1.02E+00	1.02E+00
Nd-MgCl2-D-1	1.29E+00	1.22E+00	1.21E+00	1.15E+00	1.13E+00	1.20E+00
Nd-MgCl2-D-2	1.28E+00	1.05E+00	1.21E+00	1.09E+00	1.13E+00	1.15E+00
Nd-MgCl2-E-1	1.54E+00	1.37E+00	1.40E+00	1.29E+00	1.24E+00	1.37E+00
Nd-MgCl2-E-2	1.48E+00	1.20E+00	1.39E+00	1.29E+00	1.21E+00	1.31E+00
Nd-MgCl2-F-1	1.57E+00	1.46E+00	1.55E+00	1.43E+00	1.38E+00	1.48E+00
Nd-MgCl2-F-2	1.63E+00	1.43E+00	1.81E+00	1.43E+00	1.33E+00	1.53E+00
Reference	WIPP-Nd-Borate-5 pg. 94-95	WIPP-Nd-Borate-7 Pg. 74	WIPP-Nd-Borate-6 Pg. 77	WIPP-Nd-Borate-7 Pg. 35	WIPP-Nd-Borate-8 Pg. 23	

Table 3-38 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$ and $NaCl+MgCl_2$ interaction

	[Cl-] (M)					
Set-up ID	334 Days	893 Days	1441 Days	1544 Days	1631 Days	AVG
Nd-MgCl2-A-1	5.40E+00	4.27E+00	5.40E+00	5.51E+00	5.21E+00	5.16E+00
Nd-MgCl2-A-2	5.55E+00	4.98E+00	5.41E+00	5.79E+00	5.36E+00	5.42E+00
Nd-MgCl2-B-1	4.75E+00	3.76E+00	4.51E+00	4.62E+00	4.63E+00	4.45E+00
Nd-MgCl2-B-2	4.78E+00	4.16E+00	4.54E+00	4.71E+00	4.72E+00	4.58E+00
Nd-MgCl2-C-1	4.84E+00	4.48E+00	4.61E+00	4.49E+00	4.88E+00	4.66E+00
Nd-MgCl2-C-2	4.82E+00	4.65E+00	4.72E+00	4.50E+00	4.86E+00	4.71E+00
Nd-MgCl2-D-1	4.48E+00	4.82E+00	4.15E+00	4.24E+00	4.29E+00	4.40E+00
Nd-MgCl2-D-2	4.42E+00	4.28E+00	4.17E+00	4.22E+00	4.26E+00	4.27E+00
Nd-MgCl2-E-1	4.42E+00	4.83E+00	4.04E+00	4.03E+00	4.20E+00	4.30E+00
Nd-MgCl2-E-2	4.36E+00	4.03E+00	4.08E+00	4.22E+00	4.05E+00	4.15E+00
Nd-MgCl2-F-1	3.83E+00	4.18E+00	3.71E+00	3.64E+00	3.73E+00	3.82E+00
Nd-MgCl2-F-2	3.75E+00	4.28E+00	3.54E+00	3.61E+00	3.82E+00	3.80E+00
Reference	WIPP-Nd-Borate-5 Pg. 83-84	WIPP-Nd-Borate-7 Pg. 87-88	WIPP-Nd-Borate-6 Pg. 78	WIPP-Nd-Borate-7 Pg. 87	WIPP-Nd-Borate-8 Pg. 17, 26	

Table 3-39 Experimental set-up for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7 \cdot 10H_2O$ and $NaCl+MgCl_2$ interaction

Set-up ID	$Nd(OH)_3$ (s) (g)	$Na_2B_4O_7$ (s) (g)	NaCl (m)	NaCl (M)	$MgCl_2$ (m)	$MgCl_2$ (M)	Reference	Density g/mL	Reference
Nd-B4-MgCl2-A-1	0.35	10.04	5.00	4.53	0.47	0.47	WIPP-Nd-Borate-4 Pg. 11-12	1.199	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-	0.35	10.01	5.00	4.53	0.47	0.47	WIPP-Nd-	1.199	WIPP-Nd-

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MgCl2-A-2							Borate-4 Pg. 11-12		Borate-8 Pg. 14
Nd-B4-MgCl2-B-1	0.36	10.10	3.50	3.26	0.74	0.72	WIPP-Nd-Borate-4 Pg. 11-12	1.171	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-B-2	0.35	10.03	3.50	3.26	0.74	0.72	WIPP-Nd-Borate-4 Pg. 11-12	1.171	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-C-1	0.35	10.20	3.00	2.82	1.10	1.08	WIPP-Nd-Borate-4 Pg. 11-12	1.172	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-C-2	0.35	10.07	3.00	2.82	1.10	1.08	WIPP-Nd-Borate-4 Pg. 11-12	1.172	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-D-1	0.35	10.09	2.00	1.92	1.29	1.26	WIPP-Nd-Borate-4 Pg. 11-12	1.157	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-D-2	0.35	10.11	2.00	1.92	1.29	1.26	WIPP-Nd-Borate-4 Pg. 11-12	1.157	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-E-1	0.34	10.05	1.50	1.45	1.47	1.43	WIPP-Nd-Borate-4 Pg. 11-12	1.155	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-E-2	0.35	10.13	1.50	1.45	1.47	1.43	WIPP-Nd-Borate-4 Pg. 11-12	1.155	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-F-1	0.38	10.20	0.50	0.50	1.64	1.59	WIPP-Nd-Borate-4 Pg. 11-12	1.137	WIPP-Nd-Borate-8 Pg. 14
Nd-B4-MgCl2-F-2	0.36	10.90	0.50	0.50	1.64	1.59	WIPP-Nd-Borate-4 Pg. 11-12	1.137	WIPP-Nd-Borate-8 Pg. 14

Note: Densities used to convert starting solutions from molality to molarity can be found in Appendix C. The numbers in the Table represent the respective read-out of the instrument used for the measurement.

Table 3-40 Measured pH data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $NaCl+MgCl_2$ interaction

	pH						
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	**AVG**
Nd-B4-MgCl2-A-1	7.47	7.29	7.30	7.22	7.13	7.07	7.25
Nd-B4-MgCl2-A-2	7.69	7.36	7.35	7.21	7.13	7.04	7.30
Nd-B4-MgCl2-B-1	6.86	6.92	6.93	6.99	7.02	6.97	6.95
Nd-B4-MgCl2-B-2	7.65	7.70	7.71	6.90	6.74	6.67	7.23
Nd-B4-MgCl2-C-1	7.50	7.54	7.52	6.58	6.49	6.41	7.01
Nd-B4-MgCl2-C-2	7.45	7.50	7.48	7.00	6.70	6.61	7.12
Nd-B4-MgCl2-D-1	6.79	6.74	6.72	6.66	6.50	6.43	6.64
Nd-B4-MgCl2-D-2	7.40	7.43	7.36	6.81	6.63	6.54	7.03
Nd-B4-MgCl2-E-1	7.02	6.86	6.83	6.69	6.55	6.47	6.74
Nd-B4-MgCl2-E-2	6.48	6.53	6.53	6.57	6.62	6.53	6.54
Nd-B4-MgCl2-F-1	6.68	6.65	6.64	6.58	6.50	6.40	6.58

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Nd-B4-MgCl2-F-2	6.92	6.81	6.79	6.70	6.57	6.47	6.71
Reference	WIPP-Nd-Borate-4 Pg. 61-62	WIPP-Nd-Borate-4 Pg. 75-76	WIPP-Nd-Borate-4 Pg. 93-94	WIPP-Nd-Borate-6 Pg. 38	WIPP-Nd-Borate-6 Pg. 72	WIPP-Nd-Borate-7 Pg. 37	

Table 3-41 Measured neodymium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $NaCl+MgCl_2$ interaction

	[Nd(III)] (M)								
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	$\tilde{x}$	**MAD**	**AVG**
Nd-B4-MgCl2-A-1	1.89E-06	3.39E-06	4.05E-06	1.74E-06	3.24E-05	8.54E-06	3.72E-06	1.91E-06	3.92E-06
Nd-B4-MgCl2-A-2	1.55E-06	3.96E-06	4.21E-06	3.19E-06	1.43E-06	2.12E-06	2.66E-06	1.17E-06	2.74E-06
Nd-B4-MgCl2-B-1	1.77E-06	9.02E-07	1.75E-06	4.17E-07	7.43E-07	4.80E-07	8.23E-07	3.74E-07	1.01E-06
Nd-B4-MgCl2-B-2	2.09E-06	2.35E-06	2.88E-06	1.47E-06	6.02E-07	3.04E-07	1.78E-06	8.33E-07	1.62E-06
Nd-B4-MgCl2-C-1	1.70E-06	4.43E-06	2.28E-06	2.07E-06	8.10E-07	3.36E-07	1.89E-06	7.36E-07	1.94E-06
Nd-B4-MgCl2-C-2	1.96E-06	1.93E-06	2.18E-06	6.93E-07	8.02E-07	3.41E-07	1.37E-06	6.31E-07	1.32E-06
Nd-B4-MgCl2-D-1	6.80E-07	6.42E-07	2.01E-06	3.24E-07	6.40E-07	2.84E-07	6.41E-07	1.78E-07	5.14E-07
Nd-B4-MgCl2-D-2	1.41E-06	1.41E-06	1.61E-06	5.28E-07	6.79E-07	3.24E-07	1.04E-06	4.42E-07	9.94E-07
Nd-B4-MgCl2-E-1	9.79E-07	6.75E-07	1.29E-06	3.29E-07	7.92E-07	1.29E-06	8.86E-07	3.05E-07	8.93E-07
Nd-B4-MgCl2-E-2	6.34E-07	4.49E-07	1.49E-06	3.58E-07	8.72E-07	2.83E-07	5.42E-07	2.21E-07	6.81E-07
Nd-B4-MgCl2-F-1	1.49E-06	4.75E-07	1.02E-06	2.49E-07	9.42E-07	2.56E-07	7.09E-07	3.83E-07	7.39E-07
Nd-B4-MgCl2-F-2	1.09E-06	6.91E-07	1.69E-06	2.51E-07	7.97E-07	3.26E-07	7.44E-07	3.83E-07	8.09E-07
Reference	WIPP-Nd-Borate-7 Pg. 7-8, 10	WIPP-Nd-Borate-7 Pg. 7-8, 10	WIPP-Nd-Borate-7 Pg. 7-8, 10	WIPP-Nd-Borate-7 Pg. 7-8	WIPP-Nd-Borate-6 Pg. 76, 81	WIPP-Nd-Borate-7 Pg. 41	Note: Average does not contain outliers		

Modified Z-Score for the Nd(III) concentrations shown in Table 3-41

Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**
Nd-B4-MgCl2-A-1	0.65	0.12	0.12	0.70	10.15	1.70
Nd-B4-MgCl2-A-2	0.64	0.75	0.90	0.31	0.71	0.31
Nd-B4-MgCl2-B-1	1.70	0.14	1.68	0.73	0.14	0.62
Nd-B4-MgCl2-B-2	0.25	0.46	0.89	0.25	0.95	1.20
Nd-B4-MgCl2-C-1	0.17	2.33	0.36	0.17	0.98	1.42
Nd-B4-MgCl2-C-2	0.63	0.61	0.87	0.72	0.61	1.10

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Nd-B4-MgCl2-D-1	0.15	0.00	5.20	1.20	0.00	1.36
Nd-B4-MgCl2-D-2	0.56	0.55	0.87	0.79	0.55	1.10
Nd-B4-MgCl2-E-1	0.21	0.46	0.91	1.23	0.21	0.88
Nd-B4-MgCl2-E-2	0.28	0.28	2.90	0.56	1.01	0.79
Nd-B4-MgCl2-F-1	1.38	0.41	0.55	0.81	0.41	0.80
Nd-B4-MgCl2-F-2	0.61	0.09	1.68	0.87	0.09	0.74

Table 3-42 Measured sodium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7 \cdot 10H_2O$ and $NaCl+MgCl_2$ interaction

	[Na(I)] (M)						
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	**AVG**
Nd-B4-MgCl2-A-1	4.53E+00	4.65E+00	4.36E+00	4.68E+00	4.81E+00	4.19E+00	4.61E+00
Nd-B4-MgCl2-A-2	4.43E+00	4.54E+00	4.28E+00	4.69E+00	4.80E+00	4.21E+00	4.55E+00
Nd-B4-MgCl2-B-1	3.57E+00	3.57E+00	3.43E+00	3.53E+00	3.63E+00	3.23E+00	3.55E+00
Nd-B4-MgCl2-B-2	3.14E+00	4.11E+00	3.15E+00	3.51E+00	3.58E+00	3.15E+00	3.50E+00
Nd-B4-MgCl2-C-1	3.06E+00	2.93E+00	2.87E+00	3.11E+00	3.27E+00	2.85E+00	3.05E+00
Nd-B4-MgCl2-C-2	3.08E+00	2.98E+00	2.98E+00	3.02E+00	3.09E+00	2.80E+00	3.03E+00
Nd-B4-MgCl2-D-1	2.30E+00	2.21E+00	2.18E+00	2.21E+00	2.44E+00	1.92E+00	2.27E+00
Nd-B4-MgCl2-D-2	2.23E+00	2.29E+00	2.15E+00	2.20E+00	2.45E+00	1.92E+00	2.26E+00
Nd-B4-MgCl2-E-1	1.81E+00	1.74E+00	1.74E+00	1.72E+00	1.80E+00	1.51E+00	1.76E+00
Nd-B4-MgCl2-E-2	1.84E+00	1.81E+00	1.77E+00	1.70E+00	1.85E+00	1.56E+00	1.80E+00
Nd-B4-MgCl2-F-1	1.00E+00	1.01E+00	1.01E+00	1.05E+00	1.03E+00	8.66E-01	1.02E+00
Nd-B4-MgCl2-F-2	1.15E+00	1.09E+00	1.09E+00	1.14E+00	1.13E+00	9.55E-01	1.12E+00
Reference	WIPP-Nd-Borate-5 Pg. 88	WIPP-Nd-Borate-5 Pg. 88-89	WIPP-Nd-Borate-5 Pg. 90	WIPP-Nd-Borate-8 Pg. 7	WIPP-Nd-Borate-6 Pg. 79	WIPP-Nd-Borate-7 Pg. 45	

Table 3-43 Measured magnesium molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7 \cdot 10H_2O$ and $NaCl+MgCl_2$ interaction

	[Mg(II)] (M)						
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	**AVG**
Nd-B4-MgCl2-A-1	3.97E-01	2.99E-01	2.78E-01	2.27E-01	1.81E-01	1.83E-01	2.76E-01
Nd-B4-MgCl2-A-2	4.73E-01	3.33E-01	3.18E-01	2.32E-01	1.87E-01	1.86E-01	3.09E-01
Nd-B4-MgCl2-B-1	4.85E-01	4.54E-01	4.58E-01	4.50E-01	4.59E-01	4.94E-01	4.61E-01
Nd-B4-MgCl2-B-2	7.67E-01	6.37E-01	6.98E-01	4.40E-01	4.29E-01	4.48E-01	5.94E-01
Nd-B4-MgCl2-C-1	1.09E+00	1.04E+00	1.01E+00	7.55E-01	7.53E-01	7.72E-01	9.29E-01
Nd-B4-MgCl2-C-2	8.82E-01	8.11E-01	8.35E-01	8.06E-01	7.91E-01	8.49E-01	8.25E-01
Nd-B4-MgCl2-D-1	1.02E+00	9.62E-01	9.96E-01	9.71E-01	9.50E-01	9.59E-01	9.80E-01
Nd-B4-MgCl2-D-2	9.79E-01	9.92E-01	9.58E-01	9.47E-01	9.40E-01	9.59E-01	9.63E-01
Nd-B4-MgCl2-E-1	1.19E+00	1.15E+00	1.19E+00	1.20E+00	1.13E+00	1.16E+00	1.17E+00
Nd-B4-MgCl2-E-2	1.21E+00	1.32E+00	1.17E+00	1.11E+00	1.10E+00	1.15E+00	1.18E+00
Nd-B4-MgCl2-F-1	1.34E+00	1.36E+00	1.35E+00	1.26E+00	1.29E+00	1.24E+00	1.32E+00
Nd-B4-MgCl2-F-2	1.31E+00	1.28E+00	1.31E+00	1.21E+00	1.21E+00	1.19E+00	1.27E+00

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Reference	WIPP-Nd-Borate-5 Pg. 91	WIPP-Nd-Borate-5 Pg. 89-90	WIPP-Nd-Borate-5 Pg. 91	WIPP-Nd-Borate-6 Pg. 47	WIPP-Nd-Borate-6 Pg. 77	WIPP-Nd-Borate-7 Pg. 40

Table 3-44 Measured chloride molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $NaCl+MgCl_2$ interaction.

	[Cl-] (M)						
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	**AVG**
Nd-B4-MgCl2-A-1	5.35E+00	5.19E+00	5.58E+00	4.47E+00	5.04E+00	5.18E+00	5.13E+00
Nd-B4-MgCl2-A-2	5.44E+00	5.48E+00	5.05E+00	4.49E+00	5.25E+00	5.50E+00	5.14E+00
Nd-B4-MgCl2-B-1	4.59E+00	4.21E+00	4.55E+00	4.25E+00	4.46E+00	4.57E+00	4.42E+00
Nd-B4-MgCl2-B-2	4.48E+00	4.42E+00	4.52E+00	4.12E+00	4.43E+00	4.63E+00	4.39E+00
Nd-B4-MgCl2-C-1	4.58E+00	4.40E+00	4.52E+00	3.38E+00	4.60E+00	4.76E+00	4.30E+00
Nd-B4-MgCl2-C-2	4.63E+00	4.55E+00	4.69E+00	3.75E+00	4.37E+00	4.75E+00	4.40E+00
Nd-B4-MgCl2-D-1	4.28E+00	4.16E+00	4.56E+00	4.24E+00	4.07E+00	4.10E+00	4.26E+00
Nd-B4-MgCl2-D-2	4.04E+00	4.19E+00	3.54E+00	4.36E+00	4.03E+00	4.23E+00	4.03E+00
Nd-B4-MgCl2-E-1	4.10E+00	4.00E+00	4.01E+00	3.33E+00	3.98E+00	4.15E+00	3.88E+00
Nd-B4-MgCl2-E-2	4.19E+00	3.99E+00	4.06E+00	3.61E+00	4.03E+00	4.18E+00	3.98E+00
Nd-B4-MgCl2-F-1	3.56E+00	3.53E+00	3.43E+00	3.51E+00	3.55E+00	3.68E+00	3.52E+00
Nd-B4-MgCl2-F-2	3.63E+00	3.59E+00	3.73E+00	3.23E+00	3.53E+00	3.68E+00	3.54E+00
Reference	WIPP-Nd-Borate-5 Pg. 83-84	WIPP-Nd-Borate-5 Pg. 83-84	WIPP-Nd-Borate-5 Pg. 83-84	WIPP-Nd-Borate-7 Pg. 89	WIPP-Nd-Borate-6 Pg. 78	WIPP-Nd-Borate-7 Pg. 43, 89	

Table 3-45 Measured boron molar concentration data for undersaturation experiment investigating $Nd(OH)_3$, $Na_2B_4O_7{\cdot}10H_2O$ and $NaCl+MgCl_2$ interaction

	[B] (M)						
Set-up ID	**417 Days**	**627 Days**	**657 Days**	**950 Days**	**1524 Days**	**1622 Days**	**AVG**
Nd-B4-MgCl2-A-1	3.84E-01	4.55E-01	4.20E-01	5.20E-01	5.76E-01	5.39E-01	4.71E-01
Nd-B4-MgCl2-A-2	3.88E-01	4.52E-01	4.49E-01	4.98E-01	5.99E-01	5.31E-01	4.77E-01
Nd-B4-MgCl2-B-1	5.04E-01	5.33E-01	5.00E-01	5.25E-01	5.93E-01	5.33E-01	5.31E-01
Nd-B4-MgCl2-B-2	5.82E-01	5.18E-01	5.72E-01	4.88E-01	4.86E-01	4.42E-01	5.29E-01
Nd-B4-MgCl2-C-1	9.63E-01	9.32E-01	9.88E-01	4.98E-01	4.91E-01	4.53E-01	7.75E-01
Nd-B4-MgCl2-C-2	3.77E-01	3.65E-01	3.58E-01	3.93E-01	5.51E-01	5.14E-01	4.09E-01
Nd-B4-MgCl2-D-1	3.79E-01	4.18E-01	4.21E-01	4.50E-01	5.09E-01	4.57E-01	4.35E-01
Nd-B4-MgCl2-D-2	3.40E-01	3.35E-01	3.04E-01	3.97E-01	5.11E-01	4.95E-01	3.78E-01
Nd-B4-MgCl2-E-1	3.14E-01	3.42E-01	3.67E-01	4.21E-01	4.93E-01	4.76E-01	3.88E-01
Nd-B4-MgCl2-E-2	5.12E-01	4.72E-01	4.90E-01	4.88E-01	4.93E-01	4.49E-01	4.91E-01
Nd-B4-MgCl2-F-1	3.34E-01	3.76E-01	3.94E-01	3.93E-01	4.64E-01	4.15E-01	3.92E-01
Nd-B4-MgCl2-F-2	3.18E-01	3.42E-01	3.66E-01	3.75E-01	4.37E-01	3.96E-01	3.67E-01

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Reference	WIPP-Nd-Borate-5 Pg. 93	WIPP-Nd-Borate-5 Pg. 97	WIPP-Nd-Borate-5 Pg. 97	WIPP-Nd-Borate-6 Pg. 46	WIPP-Nd-Borate-6 Pg. 80	WIPP-Nd-Borate-7 Pg. 39

3.4 Task 4: Experimental validation of determined Pitzer parameters for $NdHB_4O_7^{2+}$ in GWB and ERDA-6 brine

The objective of this set of experiments is to validate the determined Pitzer parameters for the neodymium-borate system. In these experiments, synthetic GWB and ERDA-6 brines (Xiong, 2008) will be used. These brines will be mixed with known quantities of $Mg(OH)_2$, $Nd(OH)_3$ and $Na_2B_4O_7{\cdot}10H_2O$. These experiments have not yet been started.

3.5 Task 5: Experimental determination of speciation of Nd (III) and solubility of $Nd(OH)_3$ in the alkaline region

Two types of solubility experiments of $Nd(OH)_3$ in the alkaline region are being conducted at room temperature and elevated temperatures (up to 90°C). The first type of experiments are set up with $Nd(OH)_3$ solid in NaCl solutions varying from 0.01 m-4.0 m. The solutions were pH adjusted to 10, 11, 12 and 13 with NaOH.

A second type of alkaline region experiments will be set up at room temperature, with $Nd(OH)_3$ solid in varying mixtures of $Ba(OH)_2.8H_2O$ in 50% w/w NaOH and de-aerated water, and $Nd(OH)_3$ solid in varying mixtures of BaCl in 50% w/w NaOH and DDI water. The barium in these experiments will be used to adsorb the potential trace CO_2 within the experiments.

All data that has been produced for this task was published in the Second Milestone Report on Test Plan TP 12-02, "Experimental Investigation of Borate Interactions with Rare Earth Elements Under the WIPP Relevant Conditions at Sandia National Laboratories Carlsbad Facility" (Kirkes et al. 2017a). There are no new data to report for these experiments.

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4.0 ACKNOWLEDGEMENTS

Authors are grateful to Jandi Knox, Cassandra Marrs, Heather Burton, Chase Kicker, Yoni Xiong and William Sullivan for laboratory assistance.

Information Only

Appendix A. Calculations in "TP 12-02_092820"

Appendix A provides a guide to the calculations in the "TP 12-02_092820" spreadsheet accompanying the 3rd Milestone TP 12-02 report. The appendix is structured by spreadsheet tab, proceeding in order from left to right. Terms that have been defined and calculations that have been explained in preceding tabs are not repeated for subsequent tabs unless there is a variation that warrants additional comment.

The data presented in each spreadsheet tab from "Neodymium NEW" to "Sulfate" is sub-divided by brine component and further organized by experiment start date (in descending order down the column) and then experiment collection date/day of experiment followed by sample number as described in tab "Sample Guide" (in ascending order across the rows from left to right).

Tab: "Neodymium NEW"

- "Average ppb":
  - Average measured neodymium (Nd) concentration – expressed in units of parts per billion (ppb) – calculated as the average concentration of the measured concentrations of two abundant Nd isotopes, ^{142}Nd and ^{144}Nd, in samples:

$$Average\ ppb = \frac{[^{142}Nd] + [^{144}Nd]}{2}$$

  - Note: for task 2: Nd(OH)3…NaCl, Nd isotope concentrations are average values of duplicate runs. Footnote in cell O58 to see Neodymium(2) tab for individual runs.

- "Sample Wt.":
  - Sample weight in units of grams (g). Weight of specific volume of undiluted aqueous sample in a tared volumetric flask.

- "Dilution":
  - Final sample dilution factors. The sample weight and density are for the undiluted sample solutions.

$$Dilution = \frac{Final\ volume\ (mL)}{\left(\frac{Sample\ wt.\ (g)}{Density\ \left(\frac{g}{mL}\right)}\right)} \times dilution\ factor_2$$

$$Dilution = \frac{Final\ volume\ (mL)}{(sample\ volume\ (mL))} \times dilution\ factor_2$$

  - Example calculation derived from WIPP-Nd-Borate-1. On page 14, initial sampling takes place: 3 mL of sample removed from bottle and pipetted into a tared 10 mL grade A volumetric flask which was filled to the line

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(dilution factor$_1$ ≈ 3.33). On page 38, for ICP-MS analysis, the sample is further diluted: 0.2 mL of the diluted sample is pipetted into a 10 mL grade A volumetric flask which was filled to the line (dilution factor$_2$ = 50). Thus, Dilution = (10 mL/3 mL) × 50. Or, Dilution = dilution factor$_1$ × dilution factor$_2$.

- "ppm" (g solute/10^6 g sample solution):
  - Converting average Nd concentration in Column G from ppb (g solute/10^9 g sample solution) to parts per million (ppm) while also factoring in that the sample was diluted for analysis and "Average ppb" is the diluted measured concentration in the samples:

$$ppm = (Average\ ppb \times Dilution) \times \left(\frac{1\ ppm}{1000\ ppb}\right)$$

- "CV":
  - Coefficient of variation (CV) or relative standard deviation for duplicate ppm measurements (e.g., for Nd(OH)3-0.01 SO4-1 and Nd(OH)3-0.01 SO4-2). Ratio of the sample standard deviation to the sample mean.

$$CV = \frac{Standard\ deviation(ppm_1, ppm_2)}{Mean(ppm_1, ppm_2)}$$

- "Molarity" (mole solute/L of sample solution)
  - Converting from concentration in ppm to molarity (M) using the [isotope averaged] molar mass of Nd (144.24 g/mol) referred to as MW_{solute}
  - Samples were diluted prior to analysis. It is assumed for these dilute solutions that the mass of the sample solution is comparable to the mass of the solvent, which is water. Thus, sample solution density ($\rho_{sample\ solution}$) is assumed to be the density of water (i.e., $\rho_{sample\ solution} \approx 1$ g/mL).

$$Molarity = \frac{ppm \times 10^{-3} \times \rho_{sample\ solution}}{MW_{solute}}$$

  - Derivation:

$$\frac{ppm\left(\frac{g\ solute}{10^6\ g\ sample\ solution}\right) \times 10^{-6} \times \rho_{sample\ solution}\left(\frac{g\ sample\ solution}{mL\ sample\ solution}\right) \times}{MW_{solute}\left(\frac{g\ solute}{mol\ solute}\right)}$$

$$\frac{ppm\left(\frac{g\ solute}{10^6\ g\ sample\ solution}\right) \times \rho_{sample\ solution}\left(\frac{g\ sample\ solution}{L\ sample\ solution}\right) \times 10^{-3}}{MW_{solute}\left(\frac{g\ solute}{mol\ solute}\right)}$$

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$$= \left(\frac{g\ solute}{g\ sample\ solution}\right) \times \left(\frac{mol\ solute}{g\ solute}\right) \times \frac{g\ sample\ solution}{L\ sample\ solution}$$

$$= \left(\frac{mol\ solute}{L\ sample\ solution}\right)$$

- "Density g/mL"
  - The densities in this column are from the "Density-pCH" tab. In turn, the densities reported in the "Density-pCH" tab derive from the "Density Measurements" tab and the referenced scientific notebook pages contain replicates of the tables therein as well as a description of how the densities were measured.
    - E.g., from WIPP-Nd-Borate-7 pg. 75 entry dated 4/17/2020: "…recorded the weights for density measurements by taring the weight of a 10 mL class A volumetric flask and then using a disposable pipette I filled with solution to the 10 mL line… repeated that 3 times per each sample… used balance… in glovebox…" Weights (Wts) are recorded in grams (g).
    - Generally, the weight of 10 mL of solution was measured in triplicate. The weights were averaged and divided by the solution volume to determine density in g/mL.

$$\frac{Average\ Sample\ Weight\ (g)}{Flask\ Volume\ (mL)}$$

      - Presumably, the brine/matrix solution was prepared in batch and thus there are no differences between duplicate sample solutions (i.e., Nd(OH)3-0.01 SO4-1 and Nd(OH)3-0.01 SO4-2 are from the same solution and will have the same density).
      - All measurements were conducted at room temperature

- **Tab: "Boron"**
  - "Raw ppm"
    - Boron (B) concentration measured in diluted samples on ICP-AES.
  - "Actual ppm"
    - Boron concentration in undiluted solution. See above (Tab: "Neodymium NEW") for discussion on the "Dilution" term.

$$Actual\ ppm = (Raw\ ppm \times Dilution)$$

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- "Molarity" (mole solute/L of sample solution) Converting from concentration in ppm to molarity (M) using the molar mass of B (10.811 g/mol).

- "Density g/mL"
  - Same as Neodymium NEW tab

- **Tab: "Sodium"**
  - "Dilution":
    - Final sample dilution factors.
      - Density is referenced from tab "Density-pcH" .Values reported in "Density g/mL" column are copied from the "Density-pcH" tab.

$$Dilution = \frac{Final\ volume\ (mL)}{\left(\frac{Sample\ wt.\ (g)}{Density\ \left(\frac{g}{mL}\right)}\right)} \times dilution\ factor_2$$

$$Dilution = \frac{Final\ volume\ (mL)}{(sample\ volume\ (mL))} \times dilution\ factor_2$$

  - "Molarity" (mole solute/L of sample solution)
    - Converting from concentration in ppm to molarity (M) using the molar mass of Na (22.99 g/mol).

- **Tab: "Magnesium"**
  - "Molarity" (mole solute/L of sample solution)
    - Converting from concentration in ppm to molarity (M) using the molar mass of Mg (24.305 g/mol).

- **Tab: "Chloride"**
  - "Molarity" (mole solute/L of sample solution)
    - Converting from concentration in ppm to molarity (M) using the molar mass of Cl (35.453 g/mol).

- **Tab: "Sulfate"**
  - "Molarity" (mole solute/L of sample solution)
    - Converting from concentration in ppm to molarity (M) using the molar mass of SO_4^{2-} (96.061 g/mol).

- **Tab: "Density-pcH"**
  - This tab presents the average measured densities for each background solution as tabulated in the next tab "Density Measurements".
  - pCH values (corrected pH values) are not yet presented in this tab.

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- **Tab: "Density Measurements"**
  - Measured weights of solutions and calculated density are presented in this tab
    - Density = weight (wt., g)/volume (mL)
  - From WIPP-Nd-Borate-7 pg. 75: "4/17/2020…recorded the weights for density measurements by taring the weight of a 10 mL class A volumetric flask and then using a disposable pipette I filled with solution to the 10 mL line… repeated that 3 times per each sample… used balance… in glovebox…"
    - Weights reported out to the thousandth place (up to 5 significant figures)
    - Densities are reported up to 4 significant figures
  - A summary of the average densities is tabulated in the preceding tab "Density-pcH"

- **Tab: "Sample Guide"**
  - Column B, "Originally Prepared" refers to the initial samples. The description of the set up of the original samples is found in the referenced lab notebook (i.e., WIPP-Nd-Borate-1, page 50)
  - Column C, "1F" refers to the first sampling and analysis event in the experimental set. The subsequent columns refer to subsequent sampling. (From WIPP-Nd-Borate-7 pg. 54, which is referenced in column J (8F): "2/25/2020 The following experiments were sampled. All the original samples were set up on page 50 of WIPP-Nd-Borate-1.")

- **Tab: "Neodymium (2)"**
  - In the "Neodymium NEW" tab: for task 2, ND(OH)3…NaCl, Nd isotope concentrations are average values of duplicate runs. Footnote in cell O58 to see Neodymium(2) tab for individual runs.
  - This tab presents replicate ICP-MS measurements for Nd(OH)3 and Nd(OH)3 SO4 samples collected on various dates/sampling periods. Averages of the replicates are presented in the "Neodymium NEW" tab with a brief explanation.

- **Tab: "MgCl2 Solution Corrections"**
  - This tab includes calculations to correct the previously reported $MgCl_2$ concentrations to account for the 6 waters of hydration in the salt ($MgCl_2 \cdot 6H_2O$, molecular weight = 203.3 g/mol).
    - Starting at Row 2: the calculations are for solutions of Nd in $MgCl_2$
      - Column A is the desired molal concentration in solution
      - Column G is the calculated molal concentration based on:

$$m = \frac{g\ MgCl_2 \cdot 6H_2O\ added}{MW_{MgCl_2 \cdot 6H_2O} \times kg\ total\ H_2O}$$

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Where $kg\ total\ H_2O = [g\ H_2O\ from\ salt + g\ H_2O\ added] \times \frac{1\ kg}{1000\ g}$

$$kg\ total\ H_2O = \left[\frac{(g\ MgCl_2 \cdot 6H_2O\ added) \times (6\ mol\ H_2O \times MW_{H_2O})}{(1\ mol\ MgCl_2 \cdot 6H_2O \times MW_{MgCl_2 \cdot 6H_2O})} + g\ H_2O\ added\right] \times \frac{1\ kg}{1000\ g}$$

- The conversion from molal to molar in column I is described in the report by equation 4 using the densities reported in column H (from "Density Measurements" tab rows 28-33 or "Density-pcH" tab rows 40-45) and the molecular weight of $MgCl_2$ (95.211 g/mol).

- Starting at Row 12: the calculations are for solutions of Nd in varying mixtures of $MgCl_2$ and NaCl
  - Column A is the ID for the solution and Column B is the desired molal $MgCl_2$ concentration in solution
  - Column H is the calculated molal concentration based on the equation above.
  - The conversion from molal to molar in column J is described in the report by equation 4 using the densities reported in column I (from the $MgCl_2$ densities calculated in Table 4 of the "Solutions Corrections" tab) and the molecular weight of $MgCl_2$.

- **Tab: "Solution Corrections"**
  - The information in this tab is replicated in Appendices B and C.
    - Conversions from m to M in Tables 1-4 follow equation 4 in the report and use the respective molecular weights for Na_2SO_4 (142.04 g/mol), NaCl (58.44 g/mol), $MgCl_2 \cdot 6\ H_2O$ (203.3 g/mol) and $MgCl_2$ (95.211 g/mol).
      - Densities in Tables 1-3 are from "Density Measurements" and "Density-pcH" tabs.
      - The densities in Table 4 are calculated from the linear regression of density versus molality data in Tables 2 and 3. The equation of the line is displayed on the respective graph.

- Scanned lab notebooks and binders:
  - WIPP-Nd-Borate-1 Notebook
  - WIPP-Nd-Borate-1-Binder 1
  - WIPP-Nd-Borate-2 Binder 1
  - WIPP-Nd-Borate-2
  - WIPP-Nd-Borate-4
  - WIPP-Nd-Borate-5

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Appendix B. Starting Solution Conversions of Simple Solutions

	Starting Solutions for Tables 3-1 & 3-6		
	Na_2SO_4, m	Density	Na_2SO_4, M
Table 1	0.01	0.999	0.01
	0.10	1.009	0.10
	0.50	1.057	0.49
	1.00	1.115	0.98
	1.50	1.165	1.44
	1.80	1.191	1.71
	Density Reference: WIPP-Nd-Borate-7 Pg. 75		
	Starting Solutions for Tables 3-12 & 3-23		
	NaCl, m	Density	NaCl, M
Table 2	0.01	1.000	0.01
	0.10	1.005	0.10
	1.00	1.044	0.99
	2.00	1.074	1.92
	3.00	1.106	2.82
	4.00	1.138	3.69
	5.00	1.168	4.52
	Density Reference: WIPP-Nd-Borate-7 Pg. 75		
	Starting Solutions for Tables 3-28 & 3-34		
	$MgCl_2$, m	Density	$MgCl_2$ M
Table 3	0.01	1.001	0.01
	0.10	1.006	0.10
	0.90	1.065	0.88
	1.29	1.099	1.26
	1.64	1.115	1.59
	1.97	1.138	1.89
	Density Reference: WIPP-Nd-Borate-8 Pg. 13		

The numbers in the Table represent the respective read-out of the instrument used for the measurement.

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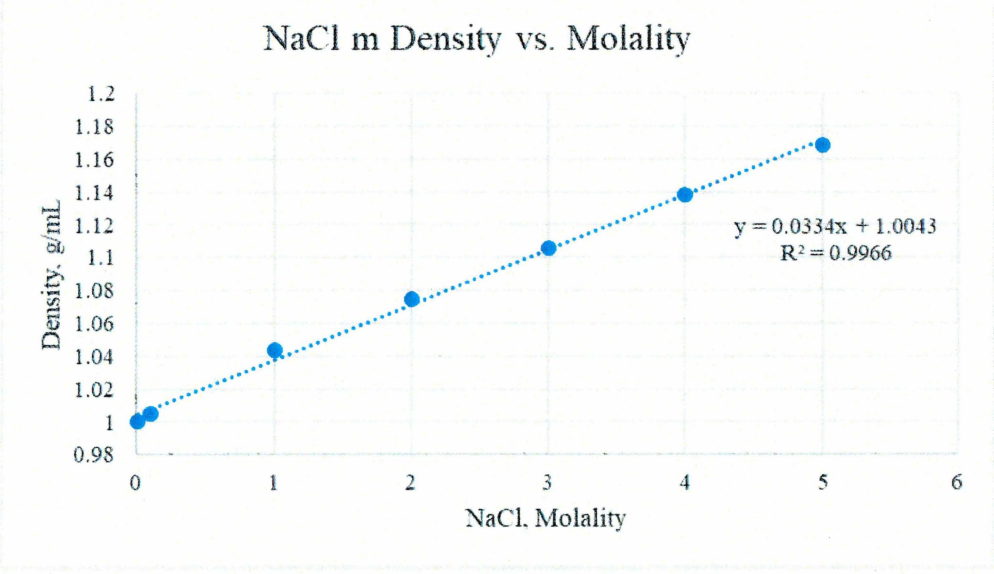
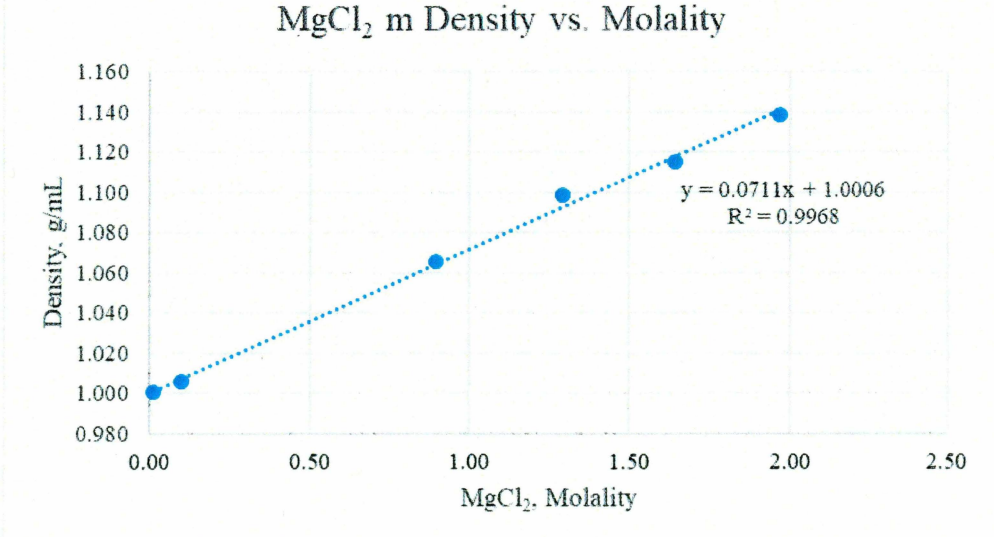
Appendix C. Starting Solution Conversion for Mixed Solutions

	Starting Solutions (Solutions A-F) for Tables 3-34 & 3-39						
		NaCl, m	NaCl, m Density calculation	NaCl, M	$MgCl_2$, m	$MgCl_2$ m Density Calculation	$MgCl_2$, M
Table 4	Solution A	5.00	1.171	4.53	0.47	1.034	0.47
	Solution B	3.50	1.121	3.26	0.74	1.053	0.72
	Solution C	3.00	1.105	2.82	1.10	1.079	1.08
	Solution D	2.00	1.071	1.92	1.29	1.092	1.26
	Solution E	1.50	1.054	1.45	1.47	1.105	1.43
	Solution F	0.50	1.021	0.50	1.64	1.118	1.59

Note: Densities were calculated for the mixed solutions by plotting density measurements from Table 2 and 3 (respectively) of Appendix 2. See Figures below for plots and equations. The numbers in the Table represent the respective read-out of the instrument used for the measurement.





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