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subject: Calculations of Thermodynamic Parameters for Experimental Data Generated at Los Alamos National Laboratory Carlsbad Operation (LANL-CO)

This memo documents calculations of thermodynamic parameters for experimental data produced by Los Alamos National Laboratory Carlsbad Operation (LANL-CO) (Table 1).

LANL-CO performs experimental studies on stability constants of $NdHB_4O_7^{2+}$ as a function of ionic strengths in NaCl and Na_2SO_4 media. The experimental work in NaCl medium has been completed. Therefore, this memo records calculations of Pitzer interaction parameters in NaCl medium. In the future, when experimental data in Na_2SO_4 medium become available, a separate memo will be released to document calculations of Pitzer interaction parameters in Na_2SO_4 medium.

Stability constants refer to the following formation reaction,

$$Nd^{3+} + HB_4O_7^- = NdHB_4O_7^{2+} \quad (1)$$

Based on the experimental results listed in Table 1, input files for NONLIN runs were generated. These input files were constructed according to suggestions in the NONLIN user's manuals (Babb, 1996; Ismail, 2008). Then, these input files were run and archived in the CMS library LIBAP134_NL. The Pitzer interaction parameters obtained are listed in Table 2. It should be mentioned that $\beta^{(1)}$ and $\beta^{(2)}$ are set to 1.74 and 0, respectively. Setting $\beta^{(1)}$ to 1.74 follows the strategy of Choppin et al. (2001), and $\beta^{(2)}$ is generally set to zero for most electrolytes. NONLIN returns C_{MX} instead of C^{ϕ}_{MX}. A C^{ϕ}_{MX} parameter is calculated from the following general equation,

$$C_{MX} = \frac{C^{\phi}_{MX}}{2|Z_M Z_X|^{1/2}} \quad (2)$$

where Z_M is the charge of species *M*, and Z_X is the charge of species *X*. As C_{MX} is returned as -0.0046130962, C^{ϕ}_{MX} is calculated as

$$C^{\phi}_{MX} = -0.0046130962 \times 2 \times |2 \times (-1)|^{1/2} = -0.013047806 \quad (3)$$

Then, it is rounded to three significant numbers, -0.0130.

In Table 3, the standard dimensionless chemical potential of $NdHB_4O_7^{2+}$ obtained in this study is listed. Also listed in Table 3 is the formation constant of $NdHB_4O_7^{2+}$ at infinite dilution, which is 4.99 in logarithmic units. This value is calculated from the standard dimensionless chemical potential of $NdHB_4O_7^{2+}$ in combination with those for Nd^{3+} and $HB_4O_7^-$ from Wagman et al. (1982).

References

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Table 1. Stability Constants of $NdHB_4O_7^{2+}$ in NaCl Medium from LANL-CO*

NaCl, molal	log β_1^I (molar scale)	log β_1^I (molal scale)
1.0	3.57±0.21	3.52±0.21
2.1	3.62±0.14	3.61±0.14
3.2	3.68±0.07	3.66±0.07
4.4	3.82±0.21	3.76±0.21
5.6	4.16±0.15	4.06±0.15

* From LANL-CO Scientific Notebook #ACP-07/1 Pages 117-121. These data are not subject to the SNL QA requirements.

Table 2. A set of Pitzer parameters for interaction of $NdHB_4O_7^{2+}$ with Cl^- obtained in this study

Binary Pitzer Parameters						
Species *i*	Species *j*	$\beta^{(0)}_{ij}$	$\beta^{(1)}_{ij}$	$\beta^{(2)}_{ij}$	c^{ϕ}_{ij}	Reference
$NdHB_4O_7^{2+}$	Cl^-	–0.0352	1.74	0	–0.0130	Present Work

Table 3. Standard dimensionless chemical potential and formation constant of $NdHB_4O_7^{2+}$ at infinite dilution and 25 °C.

Species or Formation Reaction	**μ^o/RT for Species or log β_1 for Formation Reaction**
$NdHB_4O_7^{2+}$	–1365.508
$Nd^{3+} + HB_4O_7^{1-} \leftrightarrows NdHB_4O_7^{2+}$	4.99