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Sandia National Laboratories

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4100 National Parks Highway
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date: November 11, 2004

to: Larry Brush, Repository Performance Dept. 6822 (MS-1395)
Carlsbad Programs Group

from: Yongliang Xiong, Repository Performance Dept. 6822 (MS-1395)
Carlsbad Programs Group

A handwritten signature in black ink, appearing to read 'Yongliang Xiong'.

subject: A Update on the Dimensionless Standard Chemical Potential of $\text{NpO}_2\text{Ac (aq)}$ in FMT
CHEMDAT

Recently, Nathalie Wall found an inconsistency regarding the dimensionless standard chemical potential (μ°/RT) of $\text{NpO}_2\text{Ac (aq)}$ in the FMT database, FMT_021120.CHEMDAT (Giambalvo, 2003). In the FMT_021120.CHEMDAT, the μ°/RT of $\text{NpO}_2\text{Ac (aq)}$ was recorded as -519.615, which is close to the value of PAVT (-519.809) (Giambalvo, 2002). However, the recommended value by Giambalvo (2002) should be -526.061. This recommended value is from Choppin et al. (2001). The recommended value will be recorded in the revised FMT CHEMDAT to be released soon. This revised FMT CHEMDAT will be based on the FMT_040628.CHEMDAT in which the error of the molecular weight of oxalate in FMT_021120.CHEMDAT was corrected and calcium oxalate monohydrate (whewellite) was incorporated (Xiong, 2004).

WIPP:1.4.2.2:SFT:QA-L:210790

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References

- Choppin, G.R., A.H. Bond, M. Borkowski, M.G. Bronikowski, J.F. Chen, S. Lis, J. Mizera, O. Pokrovsky, N.A. Wall, Y.X. Xia, and R.C. Moore. 2001. *Waste Isolation Pilot Plant Actinide Source Term Test Program: Solubility Studies and Development of Modeling Parameters*. SAND99-0943. Albuquerque, NM: Sandia National Laboratories.
- Giambalvo, E.R. 2002a. "Recommended Parameter Values for Modeling Organic Ligands in WIPP Brines." Unpublished memorandum to L.H. Brush, July 25, 2002. Carlsbad, NM: Sandia National Laboratories. ERMS 522981.
- Giambalvo, E.R. 2003. "Release of FMT Database FMT_021120.CHEMDAT." Memorandum to L.H. Brush, March 10, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 526372.
- Xiong, Y.-L. 2004. A Correction of the Molecular Weight of Oxalate in FMT_021120.CHEMDAT, and Incorporation of Calcium Oxalate Monohydrate (Whewellite) into CHEMDAT with Its Recommended Dimensionless Standard Chemical Potential Value. Unpublished memorandum to L.H. Brush, June 8, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 535813.