

539304  
Xiong, Yongliang

Yongliang Xiong

**From:** Xiong, Yongliang  
**Sent:** Tuesday, April 05, 2005 5:20 PM  
**To:** Kanney, Joseph F; Long, Jennifer J  
**Cc:** Chavez, Mario Joseph; Brush, Laurence H; 'Jim Nowak'; Nowak, E James  
**Subject:** Release of FMT\_050405.CHEMDAT

**Attachments:** compare.txt

Joe, Jennifer,

Please copy FMT\_050405.CHEMDAT from my directory to FMT library. The path is U1:  
[YXIONG.FMT.DB]FMT\_050405.CHEMDAT. FMT\_050405.CHEMDAT supersedes FMT\_041210.CHEMDAT.

In FMT\_050405.CHEMDAT, the dimensionless standard chemical potential ( $\mu^\circ/RT$ ) of  $\text{Th}(\text{OH})_4$  (aq) recommended by Nowak (2005) has been adopted. Therefore, the value of  $\mu^\circ/RT$  of  $\text{Th}(\text{OH})_4$  (aq),  $-622.47$  in FMT\_041210.CHEMDAT, originated from the FMT database, FMT\_021120.CHEMDAT (Giambalvo, 2003), has been changed to  $-626.5853$  in FMT\_050405.CHEMDAT.

In addition, errors in molecular weight for Pu, U and EDTA in FMT\_041210.CHEMDAT, identified by Don Wall and me, have also been corrected in FMT\_050405.CHEMDAT. The molecular weight of Pu has been corrected from 238.029 g to 244 g, U from 242 g to 238.0289 g, respectively; all are from Hammond (2005). The formula of  $\text{EDTA}^{4-}$  is  $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8^{4-}$ . Therefore, the molecular weight of  $\text{EDTA}^{4-}$  is summed as

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$$10 \times 12.011 + 12 \times 1.0079 + 2 \times 14.00674 + 8 \times 15.9994 = 288.213$$

In the above summation, the molecular weight of H, O and C are from FMT\_041210.CHEMDAT. The molecular weight of N (14.00674 g) is from Hammond (2005). Therefore, the molecular weight of  $\text{EDTA}^{4-}$  is corrected from 888.888 g to 288.213 g. Although these errors were inherited from FMT\_021120.CHEMDAT, they have NO impact on any previous calculations.

Attached is a comparison file (COMPARE.TXT) between FMT\_050405.CHEMDAT and FMT\_041210.CHEMDAT. Five sections have differences. The first difference is the statement of my update of FMT\_041210.CHEMDAT. The second difference is the updated molecular weights of Pu, U and EDTA. The third difference is the updated dimensionless standard chemical potential of  $\text{Th}(\text{OH})_4$  (aq) and associated references. The fourth difference is the entry of Neck et al. (2002) from which E. J. Nowak derived the recommended dimensionless standard chemical potential of  $\text{Th}(\text{OH})_4$  (aq) (Nowak, 2005). The fifth difference is the entry of the reference to E.J. Nowak's memo (Nowak, 2005).

#### References

Giambalvo, E.R. 2003. "Release of FMT Database FMT\_021120.CHEMDAT." Unpublished memorandum to L.H. Brush, March 10, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 526372.

4 YX/04/07/05  
Hammond, C.R., 2005. "Section 4, Properties of the Elements and Inorganic Compounds." In Lide, R.D., ed., *CRC Handbook of Chemistry and Physics*, 84<sup>th</sup> Edition, 2004-2005, 4-1-4-36. Boca Raton, FL: CRC Press.  
5 YX/04/07/05

Neck, V., R. Muller, M. Bouby, M. Altmaier, J. Rothe, M.A. Denecke, and J.I. Kim. 2002. "Solubility of Amorphous Thorium(IV) Hydroxide - Application of LIBD to Determine the Solubility Product and EXAFS for Aqueous Speciation," *Radiochimica Acta*. Vol. 90, 484-494.

Nowak, E.J., 2005. "Recommended Change in the FMT Thermodynamic Data Base." Unpublished

WIPP = 1.4.2.2 = SFT: OA-L: 210790

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memorandum to L. H. Brush, April 1, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS  
539227.



compare.bt (5  
KB)

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Comparing files fmt\_041210.chemdat and FMT\_050405.CHEMDAT

\*\*\*\*\* fmt\_041210.chemdat  
'FMT\_041210.chemdat'  
'Xiong, Yongliang update of FMT\_041116.chemdat'

\*\*\*\*\* FMT\_050405.CHEMDAT  
'FMT\_050405.chemdat'  
'Xiong, Yongliang update of FMT\_041210.chemdat'

\*\*\*\*\*

\*\*\*\*\* fmt\_041210.chemdat  
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 88.0196 10.81 79.904 59.044  
232.0381 243.0 238.029 237.0482 99.4506 30.974 242.0 89.07 888.888 189.1 0.0 0.0

\*\*\*\*\* FMT\_050405.CHEMDAT  
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 88.0196 10.81 79.904 59.044  
232.0381 243.0 244.000 237.0482 99.4506 30.974 238.0289 89.07 288.213 189.1 0.0 0.0

\*\*\*\*\*

\*\*\*\*\* fmt\_041210.chemdat  
7  
'Th(OH)4(aq) Th(OH)4(aq)' 4 4 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 -622.47  
ERG\_Th\_memo/RR87

\*\*\*\*\* FMT\_050405.CHEMDAT  
7  
'Th(OH)4(aq) Th(OH)4(aq)' 4 4 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 -626.5853  
EJN\_Th\_memo/NMB0

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\*\*\*\*\* fmt\_041210.chemdat  
Species in Natural Waters: A Review. J. Soln. Chem. 28:533-553 (SAND99-0340J).  
CFN960119 == Novak to Nowak, 19Jan96, "Preliminary inorganic model for thorium solubility in WIPP brines, in

\*\*\*\*\* FMT\_050405.CHEMDAT  
Species in Natural Waters: A Review. J. Soln. Chem. 28:533-553 (SAND99-0340J).  
NMB02 == Neck et al. 2002. Solubility of amorphous thorium (IV) hydroxide - Application of LIBD to determine the  
solubility product and EXAFS for aqueous speciation. RCA 90:484-494.  
CFN960119 == Novak to Nowak, 19Jan96, "Preliminary inorganic model for thorium solubility in WIPP brines, in  
\*\*\*\*\*

\*\*\*\*\* fmt\_041210.chemdat  
ERMS 522986.  
Rai96 == U(IV) Fax from Dhan Rai, 13 Mar 96

\*\*\*\*\* FMT\_050405.CHEMDAT  
ERMS 522986.  
EJN\_th\_memo == Nowak to Brush, 01April05, "Recommended Change in the FMT Thermodynamic Data Base" ERMS 539227.  
Rai96 == U(IV) Fax from Dhan Rai, 13 Mar 96

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