539304 Yongliang Xiong

Xiong, Yongliang

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 (μ^o/RT) of $Th(OH)_4$ (aq) recommended by Nowak (2005) has been adopted. Therefore, the value of μ^o/RT of $Th(OH)_4$ (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 $EDTA^{-4}$ is $C_{10}H_{12}N_2O_8^{-4}$. Therefore, the molecular weight of $EDTA^{-4}$ 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 $EDTA^{-4}$ 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.

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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 $Th(OH)_4$ (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 $Th(OH)_4$ (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.

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Hammond, C.R., 2005. "Section 4, Properties of the Elements and Inorganic Compounds." In Lide, R.D., ed., *CRC Handbook of Chemistry and Physics, 84th Edition, 2004–2005*, 4-1–4-36. Boca Raton, FL: CRC Press.

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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: QA-L: 210790

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

compare.txt (5 KB)

XIONG Yongliang, Ph.D.
Sandia National Laboratories
4100 National Parks Highway
Carlsbad, NM 88220
Telephone: 505-234-0054

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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

*****

***** 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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