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 (\(\mu^0/RT\)) of Th(OH)\(_4\) (aq) recommended by Nowak (2005) has been adopted. Therefore, the value of \(\mu^0/RT\) 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:

\[
10 \times 12.011 + 12 \times 1.0079 + 2 \times 14.0067 + 8 \times 15.9994 = 288.213
\]

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.

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


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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'

*****

1.0079 15.9994 22.9877 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 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

*****

1.0079 15.9994 22.9877 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 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

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CPN960119 == Novak to Nowak, 19Jan96, "Preliminary inorganic model for thorium solubility in WIPP brines, in

***** FMT_050405.CHEMDAT


CPN960119 == Novak to Nowak, 19Jan96, "Preliminary inorganic model for thorium solubility in WIPP brines, in

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ERMS 522986.

Rai96 == U(IV) Fax from Dhan Rai, 13 Mar 96

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EJN_Th_memo == Nowak to Brush, 01April105, "Recommended Change in the FMT Thermodynamic Data Base" ERMS 539227.

Rai96 == U(IV) Fax from Dhan Rai, 13 Mar 96