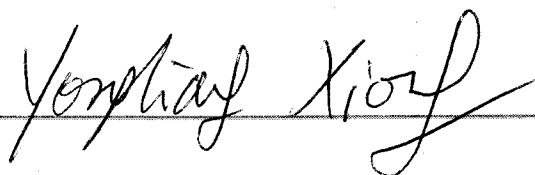


551706

Xiong, Yongliang

From: Xiong, Yongliang
Sent: Wednesday, July 22, 2009 9:04 AM
To: Long, Jennifer J
Cc: Brush, Laurence H; Chavez, Mario Joseph
Subject: Release of FMT_090720.CHEMDAT
Attachments: compare_090720_050405.txt

Jennifer,

Could you please copy FMT_090720.CHEMDAT from my directory to FMT library. The path is U1: [YXIONG.FMT.DB]FMT_090720.CHEMDAT.

In FMT_090720.CHEMDAT, the dimensionless standard chemical potential (μ^0/RT , -1365.166) of phase 5 ($Mg_3Cl(OH)_5 \cdot 4H_2O$) is incorporated. The dimensionless standard chemical potential of phase 5 is obtained by dividing the Gibbs free energy of formation of phase 5 ($-3384,000 \text{ J mol}^{-1}$) from Xiong et al. (2009) by 8.314×298.15 . Phase 5 takes the space of $PuPO_4(c)$, a deactivated species in FMT_050405.CHEMDAT.

Attached is a comparison file (COMPARE_090720_050405.TXT) between FMT_050405.CHEMDAT and FMT_090720.CHEMDAT. Two sections have differences. The first difference is the statement of my update of FMT_050405.CHEMDAT. The second difference is the addition of the dimensionless standard chemical potential of phase 5 in FMT_090720.CHEMDAT in the space previously occupied by $PuPO_4(c)$ in FMT_050405.CHEMDAT.

Reference

Xiong, Y.-L., H.-R. Deng, M.B. Nemer, S. Johnsen, 2009. Thermodynamic Data for Phase 5 ($Mg_3Cl(OH)_5 \cdot 4H_2O$) Determined from Solubility Experiments. Unpublished memorandum to L.H. Brush, May 18, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS 551294.

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WIPP: 1.4.1.1: PA: QA-L: 210790

Comparing files FMT_090720.CHEMDAT and FMT_050405.CHEMDAT

***** FMT_090720.CHEMDAT

'FMT_090720.chemdat'

'Xiong, Yongliang update of FMT_050405.chemdat'

***** FMT_050405.CHEMDAT

'FMT_050405.chemdat'

'Xiong, Yongliang update of FMT_041210.chemdat'

***** FMT_090720.CHEMDAT

'NaPu(CO3)2.6H2O(c)_____deactivated' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 2
999.999

'Mg3Cl(OH)5.4H2O(c)_____Phase_5' 13 9 0 0 3 0 1 0 2 -
1365.166 Xiong09_Phase5

***** FMT_050405.CHEMDAT

'NaPu(CO3)2.6H2O(c)_____deactivated' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 2
999.999

'PuPO4(c)_____deactivated' 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0 2
999.999
