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subject: A Correction of the Dimensionless Standard Chemical Potential of $NpO_2Ac(aq)$ in FMT_041116.CHEMDAT

The release of the FMT thermodynamic database FMT_041116.CHEMDAT (Xiong, 2004) was motivated by the recent finding by Nathalie Wall that there was an inconsistency regarding the dimensionless standard chemical potential (μ°/RT) of $NpO_2Ac(aq)$ in FMT_021120.CHEMDAT. In FMT_021120.CHEMDAT, the μ°/RT of $NpO_2Ac(aq)$ was recorded as -519.615 (Table 1), whereas the recommended value by Giambalvo (2002) is -526.061, which was from Choppin et al. (2001) (Table 1). However, that recommended value was rejected when FMT_021120.CHEMDAT was released (Giambalvo, 2003) because of poor fitting of the experimental data of Choppin et al. (2001). Giambalvo (2003) obtained a value of -519.615 for the μ°/RT of $NpO_2Ac(aq)$ by NONLIN fitting of the experimental data of Choppin et al. (2001). The value of -519.615 fits the experimental data better, is close to the value of the μ°/RT of $NpO_2Ac(aq)$ in the FMT database used for the PAVT (Novak, 1997) (Table 1), and was adopted in FMT_021120.CHEMDAT (Giambalvo, 2003). Therefore, in the new version of FMT CHEMDAT to be released following this correction, the μ°/RT of $NpO_2Ac(aq)$ will be changed back to -519.615.

References

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Table 1. The dimensionless standard chemical potential (μ^o/RT) of NpO_2Ac(aq) from different sources

Sources	μ^o/RT	Remarks
PAVT	–519.809	From FMT_970407.CHEMDAT, the version developed by Novak (1997) for the 1997 PAVT. Cited in Giambalvo (2002) and close to the value adopted in FMT_021120.CHEMDAT
Choppin et al. (2001)	-526.061	Recommended in Giambalvo (2002), but rejected by Giambalvo (2003)
Giambalvo (2002)	-526.061	Recommended based on a poor NONLIN fit of the experimental data in Choppin et al. (2001); rejected by Giambalvo (2003)
Giambalvo (2003)	–519.615	Obtained by NONLIN fitting of the experimental data, and adopted in FMT_021120.CHEMDAT, and to be adopted in the version of FMT CHEMDAT to be released following this correction

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