date: December 6, 2004

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subject: A Correction of the Dimensionless Standard Chemical Potential of NpO₂Ac(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 ($\mu^{\circ}/RT$) of NpO₂Ac(aq) in FMT_021120.CHEMDAT. In
FMT_021120.CHEMDAT, the $\mu^{\circ}/RT$ of NpO₂Ac(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 $\mu^{\circ}/RT$ of NpO₂Ac(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 $\mu^{\circ}/RT$ of NpO₂Ac(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 $\mu^{\circ}/RT$ of NpO₂Ac(aq) will be
changed back to -519.615.

References

Choppin, G.R., A.H. Bond, M. Borkowski, M.G. Bronikowski, J.F. Chen, S. Lis, J. Mizera,
Actinide Source Term Test Program: Solubility Studies and Development of Modeling


Table 1. The dimensionless standard chemical potential (µ°/RT) of NpO₂Ac(aq) from different sources

<table>
<thead>
<tr>
<th>Sources</th>
<th>µ°/RT</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAVT</td>
<td>-519.809</td>
<td>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</td>
</tr>
<tr>
<td>Giambalvo (2003)</td>
<td>-519.615</td>
<td>Obtained by NONLIN fitting of the experimental data, and adopted in FMT CHEMDAT, and to be adopted in the version of FMT CHEMDAT to be released following this correction</td>
</tr>
</tbody>
</table>
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