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ERRATUM

Erratum to: Computational study of Th^{4+} and Np^{4+} hydration and hydrolysis of Th^{4+} from first principles

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Erratum to: **J Mol Model (2017) 23:69**
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As originally published, the article contained a few minor errors. In order to avoid any confusion or misunderstanding, we would like to make the following corrections:

1) The correct temperature for entropy calculations was 298.15 k and not 198.15 K; the correct grid quadrature employed for the numerical XC term was m3 and not m5.
2) The last line in abstract should be: "Finally, this methodology has the advantage…" instead of "Finally, our methodology has the advantage…".
3) On page 69-4, before the equations (7) and (8) should be: "The values were calculated according the equations [44]," instead of "The values were calculated according the equations,".
4) On page 69-4, after equations (7) and (8) should be: "We had to approximate $\Delta H_H{}^0$ by ΔE_H since $An_{(g)}{}^{4+}H^0$ data were not available, as done by Wiebke et al [44].".
5) On page 69-4, The $\Delta G\ Solv^0$ instead of "ΔG 0 Solv".
6) On page 69-2, should be: "…the recommended values [47,48] of 172 and 130 pm were used." instead of "the recommended values [47, 48] of r of 172 and…".

These corrections do not affect any results or conclusions of the published work.

The online version of the original article can be found at http://dx.doi.org/10.1007/s00894-017-3252-9.

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