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Additions and Corrections

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Valérie Vallet,* Ulf Wahlgren, Bernd Schimmelpfennig, Henry Moll, Zoltán Szabó, and Ingmar Grenthe*: Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry

Page 3519. We have discovered two computing errors in the relative energies of the bare tetrafluoride complex, $UO_2F_4^{2-}$. The first error is a result of an interchange between two energies resulting in a slight change of the computed relative stabilities with respect to structure 1, from 3.9 and 50.8 to −3.9 and 54.7 kJ/mol for structures 2 and 3, respectively. The second error results from using the density functional theory geometry instead of the Hartree−Fock geometry when making the single-point conductor-like polarizable continuum medium (CPCM) calculation of structure 1. We have made a new calculation using the proper geometry with the same *Gaussian 98* (revision A.11) version to ensure that the parameters of the CPCM solvent model are the same as those in the original calculations (note that the GePol algorithm for the generation of the cavity embedding the solute has been changed in the latest version of Gaussian (*Gaussian 03*), affecting not only the total solvation energy of each complex but also the relative energies, as indicated in the revised table). The revised numbers change the relative order of the various isomers, predicting structure 2 with a single water molecule in the second sphere to be more stable by 13.1 kJ/mol than the five-coordinated uranyl(VI) isomer. However, the inclusion of three outer-sphere water molecules in the model makes the five-coordinated uranyl(VI) isomer, $UO_2F_4(OH_2)^{2-}$, the preferred one, in agreement with the reported EXAFS data.

The corrected version of Table 3 is as follows.

Table 3. Relative Stability of the Three Isomers of $UO_2F_4(H_2O)^{2-}$ in the Gas Phase and in a Model Solvent[a]

		$UO_2F_4(H_2O)^{2-}$		
complex	method	coordinated water	water in the plane at long distance	water out of the plane at long distance
bare complex	structure no.	1	2	3
	gas phase	0.00	**−138.8**	−99.6
	B3LYP	0.00	**−149.0**	−110.0
	spherical cavity	0.00	**−3.9**	+54.7
	single point (cavity size)	(3.43 Å)	(4.47 Å)	(4.81 Å)
	CPCM single point (*Gaussian 98*)	0.00	**−13.1**	2.7
	CPCM single point (*Gaussian 03*)	0.00	**−19.5**	−3.6
	CPCM geom opt	**0.00**	+10.1	+23.6
complex + second coordination shell	structure no.	10	11	12
	gas phase	0.00	**−83.7**	−52.3
	spherical cavity	0.00	**−57.2**	−4.18
	single point (cavity size)	(5.18 Å)	(5.16 Å)	(5.42 Å)
	CPCM single point[b]	**0.00**	+9.0	+18.9

[a] All energies are in kJ/mol and are calculated at the MP2 and B3LYP levels. [b] Energies at the Hartree-Fock level as MP2 calculations could not be handled.

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