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**Valérie Vallet,\* Henry Moll, Ulf Wahlgren, Zoltán Szabó, and Ingmar Grenthe\***: Structure and Bonding in Solution of Dioxouranium(VI) Oxalate Complexes: Isomers and Intramolecular Ligand Exchange

Pages 1982–1993. We have discovered a computing error in isomer 2 of  $[\text{UO}_2(\text{oxalate})_2\text{F}]^{3-}$  that affects the calculated values of the electronic energy and the Gibbs energy of reaction, but not the geometry and bond distances. The total energies in hartrees corresponding to the structure optimized in the gas phase and in a CPCM solvent at the Hartree–Fock level reported in Table S4 in the Supporting Information should be changed to  $-679.222914434$  and  $-679.778345880$ , respectively. This results in a change of the entries in the last line of Table 2 on p 1986 that should read:  $\Delta U(\text{MP2, CPCM geometry})$ , 34.0 kJ/mol;  $\Delta G^\circ(\text{MP2, CPCM geometry})$ , 30.3 kJ/mol;  $\Delta U(\text{MP2, gas-phase geometry})$ , 30.0 kJ/mol;  $\Delta G^\circ(\text{MP2, gas-phase geometry})$ , 26.4 kJ/mol. These values are close to those for the corresponding isomer of  $[\text{UO}_2(\text{oxalate})_2(\text{H}_2\text{O})]^{2-}$ . In the statement on p 1986, second column, we suggested that the isomers 1 and 2 may exist in equilibrium in solution; with the revised value of the relative stability of the two isomers this is less likely, suggesting that isomer 1 is the one present in solution for both  $[\text{UO}_2(\text{oxalate})_2\text{F}]^{3-}$  and  $[\text{UO}_2(\text{oxalate})_2(\text{H}_2\text{O})]^{2-}$ .

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