The Computational Approach for Uranyl-ligand Complexes

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Abstract

Spectral analyses of the uranyl-ligand complexes are essential part for the remote detection of leaking of radioactive stream. However, there is riskiness that caused radioactivity during experimental approaches to obtain radioisotope spectra, therefore the virtual screening using advanced simulation techniques has been proposed and extensively used to reduce the chance of exposure to radioactive materials. The recent improvement of computer performance and the relativistic quantum chemistry pave the way to attack multi-electron system with computational chemistry. Here, we perform the computational investigations for uranyl-ligand complexes, especially uranyl-hydrate, and uranyl-oxalate complexes. All of simulations are accomplished using Gaussian 09 program package with B3LYP functional and the levels of basis set are 6-311++G(3df,3pd) for H, C, O and the MWB60, a Wood-Boring quasi-relativistic method, for U. We optimized some complex structures that are each $[U(C_2O_4)_3(H_2O)_2]^{2-}$, $[U(C_2O_4)_4]^{4-}$, and $[U(C_2O_4)_4(H_2O)]^{2-}$, simulated their IR and UV-Vis spectra. The U-O bond lengths of $[U(C_2O_4)_3(H_2O)_2]^{2-}$ and $[U(C_2O_4)_4]^{4-}$ are approximately 2.40 angstrom and the other one has 2.46 angstrom for U-O bond distance. This difference is explained by the number of coordination bond. Through the IR spectrum simulation, we could assign their peaks on the spectra to their vibrational normal mode and analyzed the thermochemical properties like bonding formation energy.