STUDIES ON PLUTONIUM SPECIES

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We will report the status of our ongoing calculations on species containing plutonium. These have had a two-pronged approach: Density Functional Theory Methods (using ADF) studying the speciation of the various plutonium ions in water and multi-reference spin-orbit configuration interaction calculations (using COLUMBUS) studying the electronic structure of plutonyl ions. The speciation studies have concentrated on the comparison of coordination number and Pu-O bond lengths to experimental (from XANES and eXAFS) results. Recently, the electronic structure methods have allowed us to calculate transition spectra. The results for $PuO_2{}^{2+}$ will be reported and compared to experiment.

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