DENSITY FUNCTIONAL THEORY OF ACTINIDE COMPLEXES

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Density functional theory (DFT) in combination with relativistic effective core potentials provides a useful computational technique for the study of the ionic complexes of actinides. We have been studying the carbonate, nitrate, fluoride, chloride, acetate, hydroxide, and water solvated complexes of uranium and uranyl as well as thorium and thoranyl. In addition, calculations on MO_2^{n+} for Th through Am have also been done. Molecular structures, vibrational frequencies and charge distributions in these species will be presented and compared to experiment. Both local and gradient-corrected DFT methods have been used for a number of structures and the results of the different computational approaches will be compared.

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