Octahedral complexes of the series of actinides hexafluorides AnF 6

Pérez-Villa, Andrea

David, Jorge

Fuentealba, Patricio

Restrepo, Albeiro

Non-relativistic DFT (PW91, PBE, PB86) geometry optimizations followed by relativistic ZORA single point energy calculations on the neutral hexafluoride complexes of the series of actinides U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr in octahedral symmetry are presented. Bond lengths are in good agreement with available experimental data. Actinide bond length contraction as a function of the atomic number of the central metal atom of up to ?4% is observed. An approximate inverse relationship is predicted for the bonding energies as a function of the atomic number of the central cation at the two component ZORA//DFT level; pure DFT bonding energies do not exhibit the same pattern.