COMPARATIVE STUDY OF THE LANTHANIDE (Ln) AND ACTINIDE (An) TRIFLATE COMPLEXES $M(OTf)_n$

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Theoretical studies on the lanthanide and actinide triflate complexes $M(OTf)_n$ where M = La, Ce, Gd, Yb, Lu, Th, U, Np, Pu, Am, Cm, Bk, and No; $n = 3$ and 4, are carried out using functional density theory (DFT). The study of $An(OTf)_3$ complexes showed that the three OTf groups are bidentate, generating a trigonal prism (TP). Two limiting structures of TP are observed; the most distorted is the thorium triflate $Th(OTf)_3$ and the ideal one is $U(OTf)_3$. The highest population contribution of 5*d* orbital compared to 5*f* orbital in Th–O bond of $Th(OTf)_3$ explains the distortion. The intramolecular rearrangement of the OTf ligands in $Ln(OTf)_3$ generates two conformers. In $Yb(OTf)_3$, the pseudo-eclipsed and the staggered conformations are stable and can be isolated.

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