

THEORETICAL INVESTIGATION OF YTTERBIUM TRI-CHELATES COMPOUNDS

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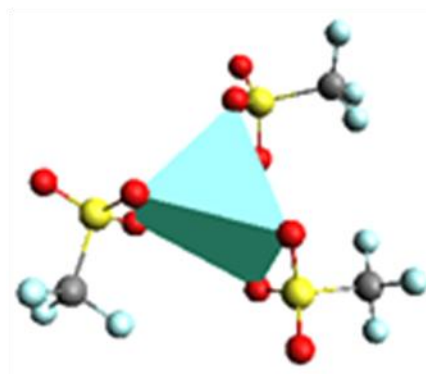
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Abstract

Theoretical studies on ytterbium tri-chelates, $\text{Yb}(\text{L})_3$ (L= **trifluoromethanesulfonate (OTF)**, **perchlorate (ClO_4)**, **p-toluenesulfonic (TOS)**, **nitrobenzenesulfonic (NBSA)**, and **dodecylsulfate (DOS)**), are carried out using density functional theory (DFT) method at the PW91/TZP level, for the first time. All ligands are bidentate and the compounds exhibit a distorted trigonal prismatic structure, with a maximum twist angle obtained for ytterbium p-toluenesulfonic compound $\text{Yb}(\text{TOS})_3$. The quantum theory of atoms in molecules (AIM) and energy decomposition analysis reveal the dominant ionic character in ytterbium–oxygen bonding with a little covalent character. According to the Pearson terminology, the $\text{Yb}(\text{NBSA})_3$ complex reveals the higher acidity.



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