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DFT and QTAIM study of the tetra-*tert*-butyltetraoxa[8]circulene regioisomers structure

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Abstract

The recently synthesized tetra-*tert*-butyltetraoxa[8]circulene regioisomers characterized by unusual solution-state aggregation behavior are calculated at the density functional theory (DFT) level with the quantum theory of atoms in molecules (QTAIMs) approach to the electron density distribution analysis. The presence of stabilizing intramolecular hydrogen bonds and hydrogen–hydrogen interactions in the studied molecules is predicted and the energies of these interactions are estimated with QTAIM. Occurrence of the CH^{δ+}–O^{δ-} bonds is detected by the single-crystal X-ray analysis for two regioisomers, obtained in high purity.

Highlights

– Tetra-*tert*-butyltetraoxa[8]circulene regioisomers were studied by DFT method. –

Electronic density distribution was calculated by the QTAIM method. The presence of stabilizing non-valence bonds is detected by X-ray experiment. The H \cdots H contacts are dynamically unstable due to high ellipticity. The energy of the H \cdots H and CH \cdots O contacts was estimated by the Espinosa equation.



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Keywords

Tetraoxa[8]circulene; Density functional theory; Bader method; Hydrogen bond; Critical point; Binding energy

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