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Theoretical Investigation of Hydrogen Bonding in the $\text{H}_2\text{SO}_4\cdots\text{HNO}_3$ System

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Abstract

Molecular clusters of two acidic species, H_2SO_4 and HNO_3 , were investigated using ab initio methods to observe intermolecular interactions. Geometric optimizations were conducted at the MP2 level using aug-cc-pVDZ and aug-cc-pVTZ basis sets. Eleven different stable geometries were detected on the intermolecular potential energy surface. Two main theories, atoms in molecules (AIM) and non-covalent interactions (NCI), were used to analyze the nature of hydrogen bonds in the $\text{H}_2\text{SO}_4\cdots\text{HNO}_3$ system. The results are discussed in terms of structural, energetic, spectroscopic and topological perspectives.

Keywords: hydrogen bonds, ab initio calculations, intermolecular interaction, electron density

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