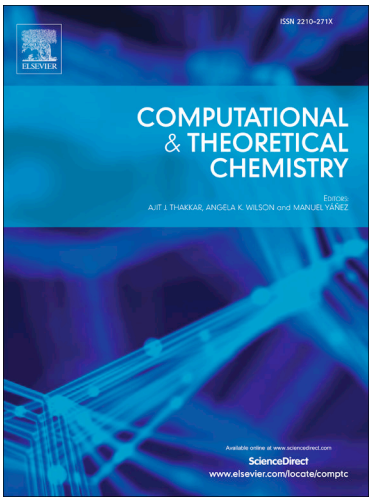


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# Theoretical Investigation of Hydrogen Bonding in the $H_2SO_4$…$HNO_3$ System

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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 $H_2SO_4$…$HNO_3$ system. The results are discussed in terms of structural, energetic, spectroscopic and topological perspectives.



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