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Theoretical Investigation of Hydrogen Bonding in the H<sub>2</sub>SO<sub>4</sub>...HNO<sub>3</sub> System

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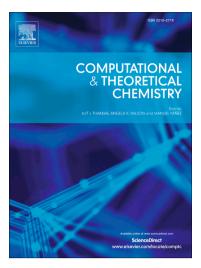
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## **ACCEPTED MANUSCRIPT**

Theoretical Investigation of Hydrogen Bonding in the H<sub>2</sub>SO<sub>4</sub>...HNO<sub>3</sub> 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

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