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Localized Charge Distributions. II. An Interpretation of the Barriers to Internal Rotation in H₂O₂

Walter Bernard England
Iowa State University

Mark S. Gordon
Iowa State University, mgordon@iastate.edu

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Abstract

The INDO geometry optimized H₂O₂ barriers are analyzed with localized molecular orbitals and findings from an earlier study of CzH₆. Emphasis is placed on the slight delocalization of an orbital onto bonds coplanar with its largest amplitude and accompanying nodal properties. The cis barrier is found to arise from HH interferences in the OH orbitals. The trans barrier is found to arise from OO interferences in lone pairs roughly trans to OH bonds in the equilibrium molecule. An explanation for the incorrect INDO H₂O₂ frozen frame barrier is also offered.

Keywords

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Comments

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