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

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Abstract
The INDO geometry optimized H20 2 barriers are analyzed with localized molecular orbitals and findings from an earlier study of CzH 6• 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 00 interferences in lone pairs roughly trans to OH bonds in the equilibrium molecule. An explanation for the incorrect INDO H 202 frozen frame barrier is also offered.

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