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Localized Charge Distributions. I. General Theory, Energy Partitioning, and the Internal Rotation Barrier in Ethane

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Abstract

Energy-localized orbitals are used to define localized distributions of positive charge and an energy partitioning of ab initio molecular orbital wave functions in the localized representation is derived. This partitioning is specialized to the INDO approximation using results from Ruedenberg's theory of chemical bonding. An interpretation is given for the internal rotation barrier in ethane with particular emphasis on the effects of geometry optimization. It is found that the origin of the barrier can be ascribed to one-electron interference energy differences among vicinal hydrogens, and that these are related to hyperconjugate effects.

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