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Localized Charge Distributions. V. Internal Rotation Barriers in Methylamine, Methyl Alcohol, Propene, and Acetaldehyde

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Abstract

The internal rotation barriers of methylamine, methyl alcohol, propene, and acetaldehyde are investigated within the context of localized charge distributions defined in earlier papers. It is shown that, as for ethane, hydrogen peroxide, and borazane, the barriers can be understood in terms of changes in vicinal interference interactions within those orbitals adjacent to the axial bond. These vicinal interactions are compared with those in molecules studied previously. Such a comparison leads to a straightforward explanation of the observed trends in the barriers.

Disciplines

Chemistry

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