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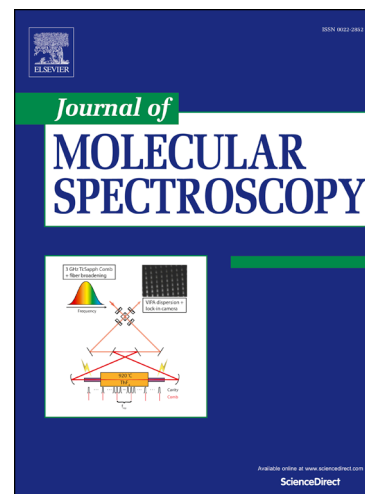
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Structure and Dynamics of Succinic, Methylsuccinic and Itaconic Anhydrides in the Gas Phase

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Abstract.

The pure rotational spectra of succinic, itaconic, and methylsuccinic anhydrides were collected in the region of 7-18 GHz using Fourier transform microwave spectroscopy. Each molecule shows varying degrees of puckering, demonstrating the effects of substitution on torsional and bond angle strain. The spectra of all three molecules exhibit perturbations consistent with internal motion; succinic and itaconic anhydride display pseudorotational motion ($\Delta E = 0.1 \text{ cm}^{-1}$ and 0.2 cm^{-1} , respectively), while methylsuccinic anhydride shows two uncoupled vibrations ($\Delta E_{01} = 0.4 \text{ cm}^{-1}$ and $\Delta E_{02} = 1.2 \text{ cm}^{-1}$). Analyses of similar five-membered rings demonstrate the relationship between the planarity of the ring and the barrier to pseudorotation.

Introduction.

The degree of planarity of five and pseudo-four membered rings is governed by the competition of two opposing forces. For some rings, the heavy-atom planar form is preferred due to its ability to maximize the already constrained bond angles of sp^3 -hybridized carbons, which conversely increases the torsional strain of eclipsed hydrogens. Other rings prefer the puckered form which reduces torsional strain but increases the bond angle strain. Thus, any substitution, such as an oxygen atom or a sp^2 -carbon atom, would reduce the number sp^3 -carbons, and quench

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