CONFORMATIONAL PREFERENCES IN METHOXYFURAN AND METHOXYTHIOPHENE STUDIED BY ROTATIONAL SPECTROSCOPY

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Methoxy-substituted heterocycles exhibit strong conformational preferences dependent on heteroatom identity, reflecting a subtle balance of intramolecular interactions. In this study, we investigated the conformational landscapes of 2-methoxyfuran and 2-methoxythiophene by chirped-pulse Fourier transform microwave spectroscopy and quantum chemistry. We confirm that the anti-coplanar geometry of the methoxy group represents the lowest energy confirmation for both species. However, our computational results find significant differences between their second lowest energy conformations and that the barrier to methyl internal rotation is strongly modified by the orientation of the methoxy group.