LOW BARRIER QUANTUM TUNNELING IN THE CIS-CONFORMER OF 3-METHYLSTYRENE PROBED USING FT-MICROWAVE SPECTROSCOPY

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We recorded the first pure rotational spectrum of 3-methylstyrene (3MS) to study quantum tunneling effects and how they differ between the cis- and trans-conformations of the molecule. The rotational spectrum (10 - 22 GHz) was recorded using the cavity molecular beam FT-microwave spectrometer at Kent State University. We used computational geometry optimizations at the B3LYP-GD3BJ/Def2TZVP level to differentiate between the cis- and trans-conformers. The combination of low dipole moment (μ_a= -0.51 D, μ_b= - 0.16 D, μ_c= 0.00 D) and low methyl torsional barrier resulted in weak and widely split rotational lines for cis-3MS. We used BELGI-Cs and XIAM internal rotor fitting programs to fit 115 transition frequencies of cis-3MS, up to J=11, to obtain its torsional and rotational parameters. Our fits show a low barrier to methyl torsion in cis-3MS, V_3= 30.35 (5) cm^{-1}, aligning with the behavior observed in toluene and its derivatives lacking significant steric hindrance.