A COMPARISON OF BARRIER TO METHYL INTERNAL ROTATION OF METHYLSTYRENES: MICROWAVE SPECTROSCOPIC STUDY

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Rotational spectra of α-Methylstyrene, cis-β-Methylstyrene, and trans-β-Methylstyrene were examined to investigate their intrinsic tunneling properties. Theoretical calculations at wB97XD/6-311++G(d,p) level predict only one stable conformer for each molecular system. Spectra were recorded in the frequency range of 10.5 - 22.0 GHz using a cavity based Fourier transform microwave spectrometer.

A relaxed potential scan for the methyl torsion at wB97XD/6-311++G(d,p) level of theory was used to estimate the associated barrier for the hindered internal rotation. The program XIAM was used to fit the rotational constants, distortion constants and barrier to methyl internal rotation to the measured transition frequencies of the A and E internal rotation states.