THE MOLECULAR STRUCTURE OF PHENETOLE STUDIED BY MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

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A pulsed molecular beam Fourier transform microwave spectrometer operating in the frequency range 2 - 26.5 GHz was used to measure the spectrum of phenetole (ethyl phenyl ether or ethoxybenzene, $C_6H_5OC_2H_5$). The conformational landscape is completely determined by the orientations of the phenyl ring and the ethyl group. A two-dimensional potential energy surface was calculated at the MP2/6-311++G(d,p) level of theory. Two conformers were found: The trans conformer has a C_s symmetry, and the gauche conformer has the ethyl group tilted out of the phenyl plane by about 70°.

Totally 186 rotational transitions were assigned to the more stable planar trans conformer, and fitted using a semi-rigid rotor model to measurement accuracy of 2 kHz. Highly accurate rotational and centrifugal distortion constants were determined. Several method and basis set combinations were applied to check for convergence and to compare with the experimentally deduced molecular parameters. The inertial defect of the observed conformer Δ_c = (I_c - I_a - I_b) = -6.718 u$\mathrm{\AA}^2$ confirms that the heavy atom skeleton is planar with two pairs of hydrogen atoms out of plane. All lines in the spectrum could be assigned to the trans conformer, which confirms that the gauche conformer cannot be observed under our measurement conditions. In agreement with the rather high torsional barrier of the methyl group (V_3 = 1168 cm^{-1}) calculated by quantum chemical methods, all assigned lines appeared sharp and no signs of splittings were observed for the methyl internal rotation.