STUDIES ON THE CONFORMATIONAL LANDSCAPE OF TERT-BUTYL ACETATE USING MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

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The tert-Butyl acetate molecule was studied using a combination of quantum chemical calculations and molecular beam Fourier transform microwave spectroscopy in the 9 to 14 GHz range. Due to its rather rigid frame, the molecule possesses only two different conformers: one of C_s and one of C_1 symmetry. According to ab initio calculations, the C_s conformer is 46 kJ/mol lower in energy and is the one observed in the supersonic jet. We report on the structure and dynamics of the most abundant conformer of tert-butyl acetate, with accurate rotational and centrifugal distortion constants. Additionally, the barrier to internal rotation of the acetyl methyl group was determined. Splittings due to the internal rotation of the methyl group of up to 1.3 GHz were observed in the spectrum. Using the programs XIAM and BELGI-Cs, we determine the barrier height to be about 113 cm^{-1} and compare the molecular parameters obtained from these two codes. Additionally, the experimental rotational constants were used to validate numerous quantum chemical calculations.

This study is part of a larger project which aims at determining the lowest energy conformers of organic esters and ketones which are of interest for flavor or perfume synthetic applications[a].

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