MICROWAVE SPECTRAL STUDIES OF BENZYL ALCOHOL AND SEC-PHENETHANOL

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Benzyl compounds ($C_6H_5C_\alpha H_2X$), generally fall into two conformational classes. With X=CH_3, C_2H_5, F, or Cl, the C-C-C_α-X dihedral angle is 90°; with X=CN and CCH, the dihedral angle is 0°; however, benzyl alcohol ($C_6H_5CH_2OH$) and benzyl amine ($C_6H_5CH_2NH_2$) have asymmetric structures. Two conformers of benzyl amine have been observed, [a] one with a dihedral angle approximately 50° and a higher energy form with dihedral angle 90°. Benzyl alcohol has a single asymmetric conformation with dihedral, C-C-C_α-O about 60° [b]. The microwave rotational spectrum displays tunneling doublets for all transitions indicating a low barrier path between two of the four equivalent energy minima. These splittings are significantly smaller in the $C_6H_5CH_2OD$ spectrum. The rotational spectrum of sec-phenethanol, ($C_6H_5C_\alpha H(C_\beta H_3)OH$), displays a single conformation with C-C-C_α-C_β dihedral angle approximately 90° and the C-C-C_α-O dihedral angle approximately 30°, and no tunneling split transitions. ab initio calculations on sec-phenethanol and benzyl alcohol will also be discussed.

[a] S. Melandri, A. Maris, P.G. Favero, W. Caminati, CHEMPHYSCHEM 2(3), 172-177 (2001).
[b] M. Trætteberg, H. Østensen, R. Seip, Acta Chemica Scandinavica A 34, 449-454 (1980).