MICROWAVE SPECTRUM OF FURFURYL ALCOHOL

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The rotational spectrum of furfuryl alcohol (2-furanmethanol) has been measured in the frequency range from 5 to 20 GHz using a pulsed supersonic jet Fourier transform microwave spectrometer and in the frequency range from 50 up to 250 GHz using conventional absorption spectrometers. There are two low energy conformations of furfuryl alcohol known from previous study: *skew 1* and *skew 3*[a], with *skew 3* being the most stable (ΔE=1.5(5) kJ/mol). In our conventional absorption spectra both conformers were easily assigned, whereas in FTMW experiments with Ne as a carrier gas *skew 3* was the only conformer observed. The high level ab initio calculations were carried out for the present work which have shown that the barrier height between the conformer *skew 1* and *skew 3* is about 3.3 kJ/mol. This value suggests effective relaxation of *skew 1* into *skew 3* during supersonic expansion[b]. In conventional absorption spectra besides ground states of both conformers all excited vibrational states below 300 cm^{-1} have been assigned and analyzed. The results of microwave studies and ab initio calculations will be discussed.

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[a] K. M. Marstokk and H. Møllendal, *Acta Chem. Scandinavica* **48** (1993) 25–31.
[b] R. S. Ruoff, T. D. Klots, T. Emilsson and H. S. Gutowsky, *J.Chem.Phys.* **93** (1990) 3142–3150.