THE ROTATIONAL SPECTRUM OF COMPLEX ORGANIC MOLECULES: 2(N)-METHYLAMINOETHANOL

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The detection of molecules in space, is based on their spectroscopic features and high resolution spectral data is needed to allow an unambiguous identification of them. Many of the molecules detected in space are complex organic molecules containing chains of carbon atoms and which therefore show a high degree of molecular flexibility. The high number of low energy conformations and the presence of large amplitude motions on shallow potential energy surfaces are peculiar to this kind of systems. The presence of a high number of stable conformers - often interconverting through small energy barriers - usually gives rise to very complex spectra, which represent a challenge for spectroscopic and computational methods. We report the rotational study of methylaminoethanol (MAE) performed by Free Jet Absorption Microwave Spectrocopy (FJAMW). For this species it has proved essential to compute the complete potential energy surfaces related to the low amplitude modes. This has been calculated at the B3LYP/6-311++G** level of theory while the stable geometries have been characterized MP2/6-311++G**. The interest in the conformational properties of MAE is twofold: in the first place, aminoethanol and thus also MAE can be considered precursors of aminoacids in the interstellar medium [a] and secondly, the MAE side chain is present in important biological molecules such as adrenaline. The conformational preferences of MAE are dominated by the intramolecular hydrogen bond between the OH and NH2 groups and its flexibility and asymmetry generate a very high number of conformers. 24 stable conformations have been predicted and two conformers were observed by FJAMW spectroscopy with our 60-72 GHz spectrometer. With respect to a previous study[b] we have extended the observed frequency range, partly reassigned the rotational spectrum of one of the conformers and determined the nuclear quadrupole constants. The search for higher energy conformers has also been undertaken.

[a] S. Charnley, in Proceedings of the workshop: The bridge between the Big Bang and Biology, CNR, Italy 1999.
[b] R. E. Penn and L. W. Buxton *J. Mol. Spectrosc.* **56** 229 1975.