THE CONFORMATIONS OF BUTAN-2,3-DIOL BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

J. P. I. HEARN and B. J. HOWARD, *Physical and Theoretical Chemistry, South Parks Road, Oxford, OX1 3QZ, UK.*.

The conformational landscape of butan-2,3-diol is dominated by the presence of two adjacent chiral centres and by the stabilisation from intramolecular hydrogen bonding; different conformational preferences are observed depending on whether the molecule is homo (R,R or S,S) or hetero (R,S) chiral. For instance, only the homochiral molecule may form an intramolecular hydrogen bond if the two methyl groups are anti to one another.

The microwave spectrum of a conformer of (R,S) butan-2,3-diol has been recorded in a supersonic jet Fourier transform microwave spectrometer between 5 and 18 GHz. A Kraitchman analysis and evidence from an *ab intio* study suggest that the observed conformer is the global minimum of (R,S) butan-2,3-diol, and that it displays an intramolecular hydrogen bond.

The spectrum of R,R and S,S butan-2,3,diol is believed to perturbed by a large amplitude motion, similar to that in the g'Ga conformer of ethylene glycol [a], caused by a concerted tunnelling of the two hydroxyl groups. The spectrum of the homochiral molecule was located by studying a deuterated sample. The rotational constants of the two possible monodeuterated species, where the tunnelling is quenched, have been extracted. We believe that the observed conformer is the global minimum of (R,R) and (S,S) butan-2,3-diol.

[a] D. Christen, L. H. Coudert, R. D. Suenram and F. J. Lovas, *J. molec. Spectrosc.* **172**, 57-77 (1995).