

MICROWAVE SPECTRUM OF HYDROGEN BONDED HEXAFLUOROISOPROPANOL•••WATER COMPLEX

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Stabilizing α -helical structure of protein and dissolving a hard to dissolve polymer, polythene terphthalate, are some of the unique properties of the organic solvent Hexafluoroisopropanol (HFIP). After determining the complete microwave spectrum of HFIP monomer^a, we have recorded the spectrum of HFIP•••H₂O complex. Ab initio calculations were used to optimize three different possible structures. The global minimum, structure 1, had HFIP as proton donor. Another promising structure, Structure 2, has been obtained from a molecular dynamic study^b. A total of 46 observed lines have been fitted well for obtaining the rotational and distortion constants within experimental uncertainty. The observed rotational constants are $A = 1134.53898(77)$ MHz, $B = 989.67594(44)$ MHz and $C = 705.26602(20)$ MHz. Interestingly, the rotational constants of structure 1, structure 2 and experiments were very close. Experimentally observed distortion constants were close to structure 1. *b* – *type* transitions were stronger than *c* – *type* which is also consistent with the calculated dipole moment components of structure 1. Calculations predict a non-zero *a*-dipole moment but experimentally *a* – *type* transitions were absent. Microwave spectra of two of the deuterium isotopologues of this complex i.e. HFIP•••D₂O (30 transitions) and HFIP•••HOD (33 transitions) have been also observed. Search for other isotopologues are in progress. To characterize the nature of hydrogen bonding, Atoms in Molecules and Natural Bond Orbital theoretical analysis have been done. Experimental structure and these theoretical analyses indicate that the hydrogen bonding in HFIP•••H₂O complex is stronger than that in water dimer.

^aA. Shahi and E. Arunan, Talk number RK16, 68th International Symposium on Molecular Spectroscopy 2013, Ohio, USA.

^bYamaguchi, T.; Imura, S.; Kai, T.; Yoshida, K. *Zeitschrift für Naturforsch.* A 2013, 68a, 145.