

## ROTATIONAL SPECTRUM OF HEXAFLUOROISOPROPANOL AND COMAPRISION TO HEXAFLUOROISOBUTENE

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Last year<sup>a</sup>, the rotational spectra of hexafluoroisopropanol(HFIP) and its OD species was presented. Microwave spectra of three more isotopologues of HFIP (two <sup>13</sup>C and one CD-OD) have now been recorded and fitted within experimental uncertainty. Many new lines for the parent species have also been observed (making it to total 111 transitions for the parent species). Previous IR studies<sup>b</sup> show that the molecule exists in two conformers: antiperiplanar (AP) and synclinal (SC). Ab initio calculations show that the AP conformer is more stable than the SC conformer. Moreover, AP conformer has *bc*-plane of symmetry and thus has no *a*-dipole moment. The fitted rotational constants and absence of any *a*-type transition confirm that the observed spectra correspond to the AP-conformer. Kraitchman's analysis further support this observation. There was no signature for the SC conformer however, nearly 35 lines still remain unassigned. Unlike the similar molecule hexafluoroisobutene<sup>c</sup>, HFIP does not show any doubling in transitions though both the molecules have very similar frequency for the puckering mode. Moreover, HFIP offers different possibilities for H-bonding and search for its water complex is in progress. Details will be presented in the talk.

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<sup>a</sup>A. Shahi, D. Mani and E. Arunan, Talk RH08, 67th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, OH (2012).

<sup>b</sup>H. Schaal, T. Häber, M. A. Suhm, *J. Phys. Chem. A* 104, 265 (2000).

<sup>c</sup>G. S. Grubbs, S. E. Novick, W. C. Pringle, E. J. Ocola and S. A. Cooke, *J. Phys. Chem. A* 116, 8169 (2012).