Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Seminar

Conformations and Hydrogen Bonded Interactions in Propargyl Systems: A Matrix Isolation Infrared and Computational Study

Jyoti Saini

IISER, Mohali

This work presents the study of molecular conformations and hydrogen bonding interactions in the two propargyl systems, (1) propargyl alcohol, PA and (2) propargyl amine, PAm, using the matrix isolation infrared spectroscopy and computations. Firstly, the reason for conformational ordering in PA and PAm has been understood through Natural bond orbital NBO analysis. Being multifunctional molecules, they provide multiple sites for hydrogen bonded interaction with H_2O molecule. In the complex having dual interactions, cooperativity effects have been explored. Further, the possibility of CH interactions of methyl group in methanol MeOH, have been studied. A common thread, linking PA-H_2O and PA-MeOH complexes to systematically derive structures of different PA homodimers, has been discussed.

Thursday, Apr 4th 2019

11:30 AM (Tea/Coffee at 11:00 AM)

Seminar Hall, TIFR-H