CONFORMATIONS AND HYDROGEN BONDED INTERACTIONS IN PROPARGYL SYSTEMS:

A Matrix Isolation Infrared and Computational Study

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ABSTRACT

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 has been understood through Natural bond orbital NBO analysis. Being multifunctional molecule with O-H group and acetylenic π cloud, it provides multiple sites for hydrogen bonded interaction with H_2O molecule, forming 1:1 PA-H_2O complexes. 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, through studies on PA-MeOH complexes. A common thread linking PA-H_2O and PA-MeOH complexes led to systematically derive structures of different PA homodimers. Propargyl amine studies further provide a logical extension to PA conformational work.

Thus, the antagonism, where the optimum conditions when individual interactions were present, were sacrificed in forming dual interaction complex, have been highlighted. In addition, an interesting correlation between the PA-H_2O, PA-MeOH and PA homodimers; useful in predicting the structures for PA-PAm complexes and PAm homodimers, has been discussed.