Propargyl Alcohol and its Rich Hydrogen Bonded Chemistry: Matrix Isolation Infrared and *Ab initio* Studies.

Jyoti Saini, and K.S. Viswanathan*
Department of Chemical Sciences, IISER Mohali, Punjab, INDIA
(E-mail: jyotisaini@iisermohali.ac.in)

Abstract:
Propargyl alcohol (PA), which is a multifunctional molecule with O-H group and π-electron cloud, has important implications in combustion and astrochemical processes. The first infrared spectroscopic study of different hydrogen bonded systems of this molecule has been investigated, which includes PA-H_2O, PA-CH_3OH and PA-dimer systems. All these systems were studied experimentally using matrix isolation infrared spectroscopy, supported by quantum chemical computations performed at M06-2X, MP2 and CCSD(T) level using 6-311++G(d,p), aug-cc-pVDZ and CBS basis sets. A 1:1 PA-H_2O complex in which PA was in gauche conformation was identified as the global minimum, with n-σ interaction between O-H group of PA and the oxygen atom of H_2O, and another H-π contact between O-H group of H_2O and π system of PA, thus forming a ring structure with these two contacts operating antagonistically[1]. In addition to this experimentally observed structure, computations also indicated three other local minima. Similar ring-structured global minimum was also observed for PA-CH_3OH system.

Rotational spectroscopic studies on PA-dimer by Mani and Arunan[2], showed the presence of only one structure with an O-H···O, an O-H···π and a C-H···π contact. In our work[3], the presence of two isomers for PA-dimers which were nearly isoergic, have been experimentally observed in which both PA submolecules were in gauche conformation. In addition to the reported structure with three contacts, another isomer having an O-H···O and an O-H···π interaction was trapped in the matrix. The experimental observation of the nearly isoergic local minima may have important implications in the understanding of the astrochemically important propargyl alcohol ices[4]. Computations indicate a multitude of local minima for the dimer system. All our results will be presented in the poster.

References and Notes:

1. Saini, J.; Viswanathan, K. S. *J. Mol. Struct.* 2016, *1118*, 147-156.
2. Mani, D.; Arunan, E. *J. Chem. Phys.* 2014, *141*, 164311.
3. Unpublished results.
4. Sivaraman, B.; Mukherjee, R.; Subramanian, K. P.; Banerjee, S. B. *ApJL* 2015, *798*, 1-4.