

HIGH RESOLUTION INFRARED SPECTROSCOPY OF PROPARGYL ALCOHOL-WATER COMPLEX EMBEDDED IN HELIUM NANODROPLETS

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Propargyl alcohol (hereafter abbreviated as PA) is a molecule of astrophysical interest and has been probed extensively using microwave spectroscopy.^{1,2} It is a multifunctional molecule and offers multiple sites for hydrogen bonding interactions. Therefore, it has also attracted the attention of groups interested in weak intermolecular interactions. Recently, the Ar...PA complex³ and PA-dimer⁴ have been studied using microwave spectroscopy. More recently, there have been matrix-isolation infrared spectroscopic studies on PA-water⁵ and PA-acetylene⁶ complexes.

In the present work, clusters of PA and water were formed in the helium nanodroplets and probed using a combination of infrared spectroscopy and mass spectrometry. Using ab-initio quantum mechanical calculations, PA-water clusters were optimised and five minimum structures were found on the potential energy hypersurface, which were used as a guidance to the experiments. We used D₂O for the experiments since our laser sources at Bochum do not cover the IR spectral region of H₂O. IR spectra of PA-D₂O complex were recorded in the region of symmetric and antisymmetric stretches of the bound D₂O. Multiple signals were found in these regions which were dependent on the concentration of PA as well as D₂O. Using pickup curves most of these signals could be assigned to 1:1 PA:D₂O clusters. The ab-initio calculations helped in a definitive assignment of the spectra to the different conformers of PA-D₂O complex. The details will be presented in the talk.

References: 1. E. Hirota, *J. Mol. Spec.* 26, 335 (1968). 2. J.C. Pearson and B.J. Drouin, *J. Mol. Spectrosc.* 234, 149 (2005). 3. D. Mani and E. Arunan, *ChemPhysChem* 14, 754 (2013). 4. D. Mani and E. Arunan, *J. Chem. Phys.* 141, 164311 (2014). 5. J. Saini, K.S. Vishwanathan, *J. Mol. Struct.* 1118, 147 (2016). 6. K. Sundararajan et al., *J. Mol. Struct.* 1121, 26 (2016).