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 complex[3] and PA-dimer[4] have been studied using microwave spectroscopy. More recently, there have been matrix-isolation infrared spectroscopic studies on PA-water[5] and PA-acetylene[6] 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 D_2O for the experiments since our laser sources at Bochum do not cover the IR spectral region of H_2O. IR spectra of PA-D_2O complex were recorded in the region of symmetric and antisymmetric stretches of the bound D_2O. Multiple signals were found in these regions which were dependent on the concentration of PA as well as D_2O. Using pickup curves most of these signals could be assigned to 1:1 PA:D_2O clusters. The ab-initio calculations helped in a definitive assignment of the spectra to the different conformers of PA-D_2O 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).