HIGH RESOLUTION SPECTROSCOPY OF ACETYLENE-FURAN IN HE NANO-DROPLETS[a]

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Acetylene-furan is an interesting benchmark system for the evaluation of hydrogen bonds. Since acetylene is the smallest molecule containing two hydrogens and a π-system it is interesting to study the influence of a C-H ¨lone-pair¨ hydrogen-bond and a CH-π or even a π-π interaction.
The global and local minimum structures have been predicted in a recent study[b]. For the experiment the molecules have been embedded in superfluid helium nanodroplets. The radiation source was a singly resonant OPO with an output power of up to 2.7 W and a resolution of up to 4×10^{-5} cm^{-1}. Helium clusters, which have a temperature of 0.37 K are doped with acetylene (pick-up pressure 1.3×10^{-5} mbar) and furan (pick-up pressure 0.9×10^{-5} mbar) and are then excited with the OPO-radiation. A mass-spectrometer is used to detect the depletion of the cluster beam. With this setup measurements were carried out in the region of the asymmetric stretch vibration of the acetylene. Between 3256 cm^{-1} and 3280 cm^{-1} five acetylene-furan cluster peaks could be detected. Two of these could be assigned to the acetylene-furan dimer. We will present a detailed analysis of the data.

[a]this work was supported by FOR 618 of the German Science Foundation

[b]E. Sánchez-Garcýa, A. Mardyukov, A. Tekin, R. Crespo-Otero, L.A. Montero, W. Sander, G. Jansen, submitted