STRUCTURAL STUDIES OF PYRROLE-BENZENE COMPLEXES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

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Non-covalent intermolecular interactions are important in structural biology. The N-H $\cdots \pi$ hydrogen bond between amino acid side chains is an important structural determinant and highly affects the secondary structure of proteins. The pyrrole-benzene complex can be viewed as a model system for studying these fundamental interactions. Previous IR and UV spectroscopic studies of the pyrrole-benzene complex by Dauster *et al.*[a] and Pfaffen *et al.*[b] support a T-shaped structure with an N-H $\cdots \pi$ hydrogen bond to the benzene ring.
In order to obtain accurate structural information we have investigated the broadband rotational spectrum of the supersonic-jet cooled complexes of pyrrole with benzene and benzene-d_1 in the 2-18 GHz frequency range. In addition to the hetero dimer we have also observed the two cyclic mixed trimers (pyrrole)$_2$-benzene and pyrrole-(benzene)$_2$.

[a] I. Dauster, C. A. Rice, P. Zielke, and M. A. Suhm *Phys. Chem. Chem. Phys.* **10**, 2827 (2008)
[b] C. Pfaffen, D. Infanger, P. Ottiger, H. M. Frey, and S. Leutwyler *Phys. Chem. Chem. Phys.* **13**, 14110 (2011)