

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 π 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 π 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.

^aI. Dauster, C. A. Rice, P. Zielke, and M. A. Suhm *Phys. Chem. Chem. Phys.* **10**, 2827 (2008)

^bC. Pfaffen, D. Infanger, P. Ottiger, H. M. Frey, and S. Leutwyler *Phys. Chem. Chem. Phys.* **13**, 14110 (2011)