JET-FTIR-SPECTROSCOPY OF PYRROLE CLUSTERS

<u>INGO DAUSTER</u>, COREY A. RICE and MARTIN A. SUHM, *Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany.*

Jet-FTIR spectroscopy is a powerful technique to investigate small hydrogen bonded clusters^a. The filet-jet-spectrometer combines a $600 \times 0.2 \text{ mm}^2$ slit nozzle with a commercial FTIR-instrument^b.

Pyrrole is a five-membered heterocyclic aromat with hydrogen bond donor (N–H) and acceptor (π -system) functionalities. Weak N–H··· π hydrogen bonds^c play an important role in biological systems. Therefore, weakly bound aggregates of pyrrole and some of its methylated derivatives have been systematically characterised by the filet-jet-spectroscopy.

In pyrrole-2-carboxaldehyde, the additional carbonyl group offers a better hydrogen bond acceptor site and leads to the formation of more conventional $N-H\cdots O$ hydrogen bonds. Its dimer has therefore been investigated as a small model system for hydrogen bonding in peptides.

^aT. Häber, U. Schmitt, C. Emmeluth and M. A. Suhm Faraday Discuss. 118, 2001, 331–359.

^bC. A. Rice, N. Borho and M. A. Suhm Z. Phys. Chem. **219**, 2005, 379–388.

^c A. Gómez-Zavagalia and R. Fausto J. Phys. Chem. A 108, 2004, 6953–6967.