HIGH RESOLUTION INFRARED SPECTRA OF JET-COOLED FORMAMIDE AND FORMAMIDE DIMER IN THE C=O STRETCH REGION

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Formamide (FA) is the simplest molecule with a peptide bond. It has attracted considerable theoretical and spectroscopic attention as a model peptide. The structure of the FA monomer in the ground state was determined to be planar by rotational spectral analyses of several isotopic species.[a] Its high resolution FIR spectrum and IR spectrum in the symmetric N-H stretching region were reported previously.[b] Both matrix isolation[c] and jet-cooled FTIR[d] studies of FA dimer reported spectral evidence for the cyclic C_{2h} symmetric FA dimer bonded by two NH—O bonds, which was predicted to be the most stable structure by ab initio calculations. No high-resolution spectrum of FA dimer, however, has been recorded so far. Our aim in the present study is to study high-resolution IR absorption spectra of both FA and its dimer in the C=O stretching region in order to gain information about the peptide-peptide interactions.

IR spectrum of the FA monomer was measured using a rapid scan infrared laser spectrometer equipped with an astigmatic multipass cell. While the monomer band centers at 1754 cm^{-1}, the lines most likely belonging to FA dimer were observed around 1740 cm^{-1}. The spectral assignment of the C=O stretching band of the monomer was made by the means of ground state combination differences. Further data collection and spectral analysis of FA dimer are currently underway. The results will be updated at the conference.

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