SPECTROSCOPY AND STRUCTURE OF A HYDROGEN BONDED CIS AMIDE DIMER

A. V. FEDOROV, J. R. CABLE, Department of Chemistry and Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH 43403.

Electronic spectra of the dimer of the cis amide oxindole and the complex of oxindole and formamide have been obtained in a supersonic jet expansion using mass-resolved resonant two-photon ionization spectroscopy. The experimental results are supportive of cyclic hydrogen bonded structures for both complexes. The oxindole chromophores in the dimer are equivalent and statistical deuteration reveals a small exciton splitting, indicative of an essentially localized excitation. Spectra of the oxindole dimer hydrated with one and two water molecules have also been obtained and have been interpreted by comparison to the dimer spectrum in conjunction with ab initio Hartree-Fock calculations.