CONFORMATION SPECIFIC ELECTRONIC AND INFRARED SPECTROSCOPY OF ISOLATED [2,2,2]-PARA-TRICYLCLOPHANE AND ITS MONOHYDRATED CLUSTER

EVAN G. BUCHANAN, JACOB C. DEAN, BRETT M. MARSH , and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

[2,2,2]-Para-tricyclophane (TCP) is a highly symmetric macrocycle containing three para-substituted phenyl rings linked by ethyl bridges. Therefore, TCP affords a unique opportunity to explore the coupling between three electronic chromophores isolated in supersonic expansion. Furthermore, the three phenyl rings create an electron rich macrocyclic cavity capable of forming a π-hydrogen bond to a single water molecule. Resonant two-photon ionization and UV-UV hole-burning spectroscopy proved that the monomer population resides in a single conformer. Its vibronic spectrum shows unusual activity in the first 150 cm^{-1} due to the close, intermingled set of three excited states. Resonant ion-dip infrared (RIDIR) spectroscopy was carried out in the alkyl and aromatic CH stretch regions to probe the conformations of the three ethyl linkages. Dispersed fluorescence spectra served to probe the electronic energy transfer between the three phenyl rings, which is rampant already at low energies. In the TCP-H_2O complex, RIDIR spectroscopy is used to characterize the π H-bonding of H_2O in the TCP cavity.