CONFORMATION SPECIFIC ELECTRONIC AND INFRARED SPECTROSCOPY OF JET-COOLED CONIFERYL ALCOHOL

CHIRANTHA P. RODRIGO and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084*.

The conformational specific electronic and infrared spectroscopy of jet-cooled coniferyl alcohol, a monomer of the natural biopolymer lignin, was studied using a series of single and double resonance methods. Fluorescence excitation spectroscopy (FES) and resonance two photon ionization (R2PI) were utilized along with UV-UV hole-burning (UVHB) spectroscopy to determine the existence of two conformations in the supersonic jet beam. The spectrum is dominated by a conformational isomer (A) with S_0–S_1 origin at 32644 cm^{-1}, while a second, minor conformer (B) appears at 33446 cm^{-1}. Single vibronic level fluorescence (SVLF) of the origin of the conformer A and several vibronic bands were recorded, leading to assignments of several of the low-frequency torsional modes of the molecule. Resonant ion-dip infrared (RIDIR) spectroscopy was used to record infrared spectra of these two conformers in the hydroxyl stretch region. Conformer A was found to have a free OH (3635 cm^{-1}) and hydrogen bonded OH (3583 cm^{-1}) indicative of a H–bond from the OH group on the ring to the adjacent methoxy oxygen. In arriving at conformational assignments for coniferyl alcohol, analogous results on the simpler analog 2-methoxy-4-vinylphenol (mvp) will also be presented. Comparison with DFT B3LYP calculations will be used in arriving at conformational assignments for the two conformers of coniferyl alcohol