CONFORMATION-SPECIFIC ELECTRONIC SPECTROSCOPY OF JET-COOLED BIS(2-HYDROXYPHENYL)METHANE

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The electronic and infrared spectroscopy of jet-cooled bis(2-hydroxyphenyl)methane was studied using laser induced fluorescence (LIF) and a series of double resonance methods. UV-UV hole-burning (UVHB) spectroscopy was used to prove the existence of two conformations, with S_0-S_1origins at 35667.8 (conformer A) and 35811.5 cm^{-1} (conformer B). Fluorescence-dip infrared (FDIR) spectroscopy was used to record infrared spectra of these two conformers in the hydride stretch region. Conformer A was found to have a free OH (3657 cm^{-1}) and a H-bonded OH stretch fundamental (3531 cm^{-1}), consistent with *ab initio* calculations for an OH$\cdots$OH inter-ring H-bond structure. Conformer B exhibits only a single OH stretch fundamental at 3560 cm^{-1}, indicative of a C2 symmetry structure in which the OH groups on each ring H-bond to the π cloud of the opposing ring. S_1-state FDIR spectra were also recorded, showing dramatic changes in the strengths of the H-bonding upon electronic excitation. In addition, the π-bound conformer has two resolved S_1-state OH stretch fundamentals, both of which possess long progressions in the OH stretch – torsion combination bands. Ground state vibrational frequencies for each conformer were also obtained using dispersed fluorescence (DF). Finally, rotationally resolved UV spectra have also been taken to determine the rotational constants and transition moment direction in the excited state, providing more detailed insight to the structural changes that accompany electronic excitation in this model bichromophore.