VIBRONIC COUPLING IN A FLEXIBLE BICHROMOPHORE: 1,2-DIPHENOXYETHANE

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Investigations of isolated flexible bichromophores through single conformation spectrocopy have provided tremendous insights into the intrinsic properties of close lying, vibronically coupled electronic states. However, the S_2 origin is often elusive, requiring a gambit of experimental techniques aided by high level calculations to pin down its location and the excitonic splitting. Here, we expand our studies on flexible bichromophores to 1,2-diphenoxyethane (C_6H_5-O-CH_2-CH_2-O-C_6H_5, DPOE). Ultraviolet hole-burning identified two confomrers present in the supersonic jet expansion with C_{2h} and C_2 symmetry. Both experimental and computational results suggest a small excitonic splitting of no more than a few cm^{-1}. The vibrationally and rotationally resolved spectra of DPOE conformational isomers will be discussed with regard to the vibronic coupling and excitonic splitting. Finally, the perturbation to the DPOE excited states due to a single water molecule will be discussed.