SPECTROSCOPY OF 1,2-DIPHENYLETHANE-$(H_2O)_n$ (n=1-3) CLUSTERS

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1,2-diphenylethane (DPE) is a prototypical flexible bichromophore which forms two conformers in the gas phase having close lying S_1 and S_2 states. Resonant ion-dip infrared (RIDIR) spectroscopy in the alkyl CH stretch region, 2800-3000 cm^{-1}, was used to assign the two observed isomers to *gauche* and *anti* structures having C_2 and C_{2h} symmetry similar to those in butane.[a] In the present work, the ultraviolet and infrared spectroscopy of DPE-$(H_2O)_n$ (n=1-3) clusters has been studied to understand how the 'solvent' water molecules bind to this molecule with two phenyl rings, and how the solvent binding perturbs the excited state behavior. RIDIR spectra in the OH stretch region (3350-3750 cm^{-1}) show that DPE-$(H_2O)_1$ adopts a single conformation in which the water molecule bridges the two phenyl rings of the *gauche* conformer, forming π H-bonds with both rings. DPE-$(H_2O)_2$ forms two structures, in which a water dimer is bound to either the *gauche* or *anti* DPE conformer. In the *anti* DPE-$(H_2O)_2$ structure, the water dimer interacts primarily with one phenyl ring, disrupting the symmetry of DPE enough that the S_1 and S_2 origins are localized, splitting the origins by approximately 50 cm^{-1}. The development of these cluster structures with additional H_2O molecules, and the OH stretch spectra of the clusters in the excited state(s) will also be discussed.

[a] E. G. Buchanan, J. C. Dean, T. S. Zwier and E. L. Sibert, III *J. Chem. Phys* 2013, **138**.