FLUORESCENCE-DIP INFRARED SPECTROSCOPY OF THE TROPOLONE-H_2O COMPLEX

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Fluorescence-dip infrared spectroscopy (FDIRS) is used to probe the effect of solvent binding by water on the intramolecular H-atom tunneling in tropolone. As with the bare molecule in the adjoining presentation, the FDIR spectrum of the jet-cooled tropolone-H_2O complex is recorded in the O-H and C-H regions. The spectrum possesses distinct absorptions due to the water free OH, water hydrogen-bonded OH, and tropolone OH. Extensive *ab initio* calculations on tropolone-H_2O are carried out at both the MP2 and Becke3LYP levels of theory. Two isomers for the complex are identified with binding energies and vibrational frequencies quite similar to one another. The experimental evidence does not conclusively distinguish between these two possibilities, though discussion will focus one that is more in keeping with the data as a whole.