HYDROGEN-BOUND COMPLEXES OF TROPOLONE: GATEWAYS FOR THE INTERROGATION OF MULTIPLE PROTON-TRANSFER EVENTS

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Tropolone (TrOH) serves as a model system for the study of coherent proton-transfer processes, where a potential barrier of finite height hinders the symmetric exchange of a lone hydron between hydroxylic (proton-donating) and ketonic (proton-accepting) oxygen centers. This talk will discuss ongoing efforts to build upon the known structural and dynamical properties of tropolone so as to explore related multiple proton-transfer events that are mediated by successive formation and breaking of several hydrogen bonds. Of particular interest are weakly-bound complexes created *in situ* under "cold" molecular-beam conditions by docking amphoteric ligands (*e.g.*, HF and HCOOH) into the reaction cleft of the TrOH substrate. Such species have the tantalizing possibility of undergoing double proton transfer,[a] with resulting tunneling-induced bifurcation of rovibronic features reflecting the intrinsic vibrational and/or electronic specificity of the attendant unimolecular transformation. Spectroscopic studies of several hydrogen-bound TrOH complexes through use of the richly structured $\tilde{A}^1\mathrm{B}_2 - \tilde{\mathrm{X}}^1\mathrm{A}_1(\pi^* \leftarrow \pi)$ absorption system will be presented, with complementary quantum-chemical calculations serving to guide the assignment and interpretation of observed spectral patterns.

[a] L. A. Burns, D. Murdock, and P. H. Vaccaro, *Mol. Phys.*, **108**, 1171 (2010).