HYDROGEN BONDING AND TUNNELING IN TROPOLONE AND THE TROPOLONE-WATER COMPLEX STUDIED BY ROTATIONALLY RESOLVED MW AND UV SPECTROSCPOPY.

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Hydrogen bonding and intramolecular proton transfer are being investigated in jet cooled tropolone and tropolone-water complexes by high-resolution MW and UV spectroscopies. Tropolone is a seven-member ring compound with an OH..O moiety that undergoes tautomerization across a symmetric double minimum potential surface. The two isoenergetic configurations of the molecule are separated by a small barrier that results in facile tunneling of the hydrogen atom. Analysis of the spectra reveals nearly a 20 fold increase in the tunneling splitting from the S_0 to S_1 levels. Most remarkably, with the addition of one water molecule to tropolone the observed tunneling splitting vanishes. This is likely due to the destruction of the symmetric potential by the addition the water molecule. Only one possible ab initio structure of the tropolone-water complex is consistent with the experimental results.