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Spectroscopic and Ab-Initio Studies of π -Type Hydrogen Bonding in Cyclic Alcohols and Amines ESTHER OCOLA, JAAN LAANE, Texas A&M University — Infrared and Raman spectroscopy have been used to investigate several molecules capable of intramolecular π-type hydrogen bonding. Ab-initio calculations have been utilized to complement the experimental work. The cyclic alcohols, 3-cyclopenten-1-ol (3CYPO), 2-cyclopenten-1-ol, 2-cyclohexen-1-ol, and the cyclic amines, 3-cyclopenten-1-amine, 2-aminoindan, 2-cyclopenten-1-amine, 1-aminoindan, and 2-hydroxytetralin have been studied. 3CYPO can exist in four different conformational forms and all were observed in the infrared and Raman spectra. The conformer with the weak π-type intramolecular hydrogen bonding is about 400 cm^{-1} (1.1 kcal/mole) lower in energy than the other three conformations to which the lowest energy form can interconvert through ring-puckering or internal rotation vibrations. The interconversions and relative energies of all the other molecules were also investigated. In each case the conformation with the lowest energy had a π-type hydrogen bonding.

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