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Spectroscopic and Theoretical Investigations of the Potential Energy Surfaces of Molecules with Intramolecular π-type Hydrogen Bonding[1] ESTHER OCOLA, HEE-WON SHIN, ABDULAZIZ AL-SAADI, JAAN LAANE, Texas A&M University — Spectroscopic methods and theoretical calculations have been utilized to investigate the conformations of several cyclic organic molecules. The laser induced fluorescence (LIF) spectra of 2-indanol show the presence of four conformations. The one with intramolecular hydrogen bonding between the –OH group and the benzene ring is of lowest energy. The potential energy surface (PES) in terms of the ring puckering and internal rotational vibrations, which govern the conformational changes, was determined. 3-Cyclopenten-1-ol possesses a similar PES as established from its infrared and Raman spectra and theoretical calculations. This PES also shows the presence of four conformations. The π-bonding conformer lies at lowest energy. LIF has been used to study the conformational energies of 2-hydroxytetralin, and 2-cyclohexenol has been investigated by infrared and Raman techniques. The analyses of the hydrogen bonding in these molecules as well as in a dozen others were supported by both *ab initio* and DFT calculations.

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