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Intramolecular π-Type Hydrogen Bonding in Cyclic Molecules[1]

ESTHER OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX 77843-3255, USA — We have studied theoretically and experimentally the presence of intramolecular π-type hydrogen bonds in several cyclic molecules with attached OH, NH_2 or SH groups to the ring. The structures of the conformers of each of the molecules were calculated, and the changes of the potential energy due to the internal rotation of the attached groups were plotted. Infrared spectroscopy and Raman spectroscopy have been used to confirm the presence of different conformers. Among the molecules which we studied are 2-indanol, 3-cyclopenten-1-ol, 2-cyclohexen-1-ol, 2-cyclopropen-1-ol, 2-cyclopropen-1-thiol, 2-cyclopropen-1-amine, and 3-cyclopenten-1-amine. For all these molecules the energy minimum was found to have an intramolecular π-hydrogen bonding. The π bonding stabilizations range from about 2 to 10 kJ/mol. The calculated distances from the hydrogen bonded atom of the OH, NH_2 or SH group to the center of the C=C bond of the cyclic molecule is calculated to be in the range of 2.488 Å – 2.850 Å from CCSD/cc-pVTZ computations and in the range of 2.478 Å and 2.740 Å from MP2/cc-pVTZ computations.

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