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**Spectroscopic and Theoretical Investigations of the Intramolecular $\pi$-Type Hydrogen Bonding and Conformations of 3-Cyclopentene-1-amine** ESTHER J. OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX 77843-3255, USA — Ab initio MP2/cc-pVTZ computations show that 3-cyclopentene-1-amine (3CPAM) can exist in six different conformers, two pairs of which are mirror images of each other. These are labeled **A1**, **A2** and **C1**, **C2**. Conformers **A1** and **A2**, which have the lowest conformational energy, show a weak intramolecular $\pi$-type hydrogen bonding, where one hydrogen atom of the $NH_2$ group is interacting with the C=C double bond. The other four conformers **B**, **C1**, **C2**, and **D** have calculated conformational energies 284, 315, 315 and 336 $cm^{-1}$ higher in energy. The six conformers can interconvert through ring-puckering vibrations or by torsional rotation of the $–NH_2$ bond. A two-dimensional potential energy surface in terms of these vibrational coordinates has been calculated. Vapor-phase infrared spectra of 3CPAM have been analyzed and these show the existence of the six conformers of this molecule. The observed vibrational frequencies are in excellent agreement with the theoretical calculations for each of the conformers. The liquid-phase infrared spectra of 3CPAM, which show evidence for four different conformers, have also been recorded.

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