VAPOR-PHASE INFRARED AND RAMAN SPECTRA AND THEORETICAL INVESTIGATIONS OF π-TYPE INTRAMOLECULAR HYDROGEN BONDING IN 3-CYCLOPENTEN-1-OL AND 3-CYCLOPENTEN-1-AMINE

ESTHER JULIANA OCOLA, JAAN LAANE, *Department of Chemistry, Texas A & M University, College Station, TX, USA*.

The vapor-phase and Raman spectra of 3-cyclopenten-1-ol (3CPOL) and 3-cyclopenten-1-amine (3CPAM) have been recorded and analyzed. The spectra demonstrate the existence of six conformers for each molecule, two pairs of which are mirror images of each other and with equivalent vibrational modes. The conformational minima are achieved for selected values of the ring-puckering coordinate and the internal rotation coordinate of either the -OH or -NH2 group. Theoretical CCSD/cc-pVTZ computations for both molecules were carried out and their two-dimensional potential energy surfaces (PEFs) were calculated. The PEFs confirm the existence of all conformers and provide the relative energies for these. The structures with the π-type intramolecular hydrogen bonding are at the lowest calculated energies and 301 to 411 cm^{-1}lower than the other conformations for 3CPOL, and 165 to 197 cm^{-1}lower for 3CPAM.