

INTERNAL ROTATION OF INTRAMOLECULAR HYDROGEN BONDING OF OH OR NH₂ GROUPS ATTACHED TO THREE-MEMBERED RING MOLECULES^a

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

The internal rotations about the single bonds connecting OH or NH₂ groups to cyclopropyl or cyclopropene rings were investigated. The experimental fits to the infrared data of the one-dimensional torsional potential energy functions were compared to theoretical calculations. MP2/cc-pVTZ and CCSD/cc-pVTZ computations were found to be in good agreement with the experimental results for cyclopropanol and cyclopropylamine. Calculations were also carried out on the internal rotations of 1-cyclopropen-1-ol and 2-cyclopropen-1-amine. Each of these molecules has a calculated energy minimum corresponding to a conformation with an intramolecular π -type hydrogen bond. The π -bonding stabilization is 2.3 kcal/mol for the alcohol and 2.5 kcal/mol for the amine. The calculated O-H, N-H, and C=C stretching frequencies are lower for the hydrogen bonded conformers than for the conformations without the π -type hydrogen bonds. The C=C bond stretching frequencies show the largest decreases resulting from the hydrogen bonding.

^aThe authors wish to thank the Robert A. Welch Foundation (Grant A-0396) for financial support.