Potential energy scans and vibrational assignments of cyclopropanecarboxylic acid and cyclopropanecarboxamide

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ABSTRACT

The structural stability and internal rotations in cylopropanecarboxylic acid and cyclopropanecarboxamide were investigated by the DFT-B3LYP and the ab initio MP2 calculations using 6-311G** and 6-311+G** basis sets. The computations were extended to the MP4//MP2/6-311G** and CCSD(T)//MP2/6-311G** single-point calculations. From the calculations the molecules were predicted to exist predominantly in the *cis* (C=O group eclipses the cyclopropane ring) with *cis*-*trans* barrier of about 4-6 kcal/mol. The OCOH torsional barrier in the acid was estimated to be about 12-13 kcal/mol while the corresponding OCNH torsional barrier in the amide was calculated to be above 20 kcal/mol. The equilibrium constant *k* for the *cis* ⇔ *trans* interconversion in cyclopropanecarboxylic acid was calculated to be 0.1729 at 298.15 K that corresponds to an equilibrium mixture of about 85% *cis* and 15% *trans*. The vibrational frequencies were computed at the DFT-B3LYP level. Normal coordinate calculations were carried out and potential energy distributions were calculated for the low energy *cis* conformer of the molecules. Complete vibrational assignments were made on the basis of normal coordinate calculations and comparison with experimental data of the molecules.

Keywords: DFT-B3LYP; ab initio MP2; MP4//MP2; CCSD(T)//MP2; rotational barriers; vibrational assignments; cyclopropanecarboxylic acid; cyclopropane-carboxamide.