Rotational barriers in monomeric CH2 = CX-COOH and CH2 = CX-CONH2 (X is H or CH3) and vibrational analysis of methacrylic acid and methacrylamide

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Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 68 **Issue:** 3 **Pages:** 432-442

Abstract: The internal rotations in acrylic and methacrylic acids CH2=CX-COOH and their amides CH2=CX-CONH2 (X is H or CH3) were investigated by DFT-B3LYP calculations with 6-31 I+G** basis set. The potential energy curves were consistent with two minima that correspond to planar cis and trans conformation in the case of the acids (or cis and near-trans forms in the case of the amides). Acrylic acid and acrylamide were predicted to have the cis form as the low and predominant conformation of the molecules. In the case of the methacrylic acid and methacrylamide, the conformational relative stability was predicted to reverse as going from the acrylic to the metha compounds. The trans conformer in methacrylic acid or the near-trans in methacrylamide were predicted to be thermodynamically low energy structures of the molecules. The CCCO rotational barrier was calculated to vary from 4 to 6 kcal/mol in the four molecules. The OCOH and OCNH torsional barriers were calculated to be about 13 and 22 kcal/mol in the acids and the amides, respectively. The vibrational frequencies of methacrylic acid and methacrylamide were computed at the DFr-B3LYP/6-31 I+G** level and reliable vibrational assignments were made on the basis of normal coordinate analyses and comparison with experimental data of both molecules in their low energy conformations.