STRUCTURAL STABILITY AND DERIVED POTENTIAL ENERGY DISTRIBUTIONS FOR FLUORO- AND CHLOROMETHYL KETENE

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ABSTRACT

Density Functional calculations with the extended 6-311++G** basis set were employed to study the structural stability and the conformational behavior of fluoromethyl ketene and chloromethyl ketene. Both molecules were predicted to be stable only in the *gauche* form (halogen atom is in staggered configuration with respect to the ketenic hydrogen), while the *cis* and the *trans* conformations represented the two energy maxima on the potential surface scans. Full geometrical optimization was performed at the ground state in the two systems. The optimized dihedral angles XCCC in the stable conformers were calculated to be 102° and 103.3^{o} in the fluoro and chloro derivatives, respectively. The vibrational frequencies were computed at the DFT-B3LYP/6-311++G** level and the calculated vibrational infrared and Raman spectra of the two molecules were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for the stable conformer of the two molecules.

Keywords: Vibrational spectra and assignments; Normal coordinate analysis; Fluoromethyl ketene; Chloromethyl ketene.