

Structural stability and derived potential energy distributions for fluoro and chloromethyl ketene. Badawi, Hassan M.; Forner, W.; Al-Saadi, A.

Abstract

D. functional calcns. 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 mols. 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 calcd. to be 102° and 103.3° in the fluoro and chloro derivs., resp. The vibrational frequencies were computed at the DFT-B3LYP/6-311++G** level and the calcd. vibrational IR and Raman spectra of the two mols. were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for the stable conformer of the two mols.