Vibrational assignments and derived potential energy distributions for tri- and difluoromethyl ketene by density functional calculations. Forner, Wolfgang; Badawi, Hassan M.; Al-Saadi, Abdulaziz A.; Ali, Sk. Asrof. Dep. Chem., King Fahd Univ. Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of Molecular Modeling [online computer file] (2001), 7(9), 343-353.

Abstract

The structures of 3,3,3-trifluoromethyl ketene (I) and 3,3-difluoromethyl ketene (II) were studied by utilizing ab initio calcns. with the 6-311++G** basis set at the (B3LYP) D. Functional level. Full optimization was performed for both mols. in their ground and transition states. Energy optimization of the systems under investigation shows that I exists only in the cis conformation (fluorine atom eclipses the ketene group). II was predicted to have two stable conformations: the cis (hydrogen at-om eclipses the ketene group) and the gauche (fluorine atom eclipses the ketene group) form. The conformational stability of the mols. was found to be governed mainly by electrostatic and MO interactions. The vibrational frequencies were computed and complete assignments were provided on the basis of normal coordinate calcns. and comparison with similar mols. The potential energy distributions (PED) among symmetry coordinates were derived for the stable conformations of the two mols.