An investigation of structural stability and internal rotation in 3-cyclopropenecarboxaldehyde and 3-cyclopropenecarboxylic acid fluoride by ab initio calculations. Badawi, Hassan M.; Forner, Wolfgang; Al-Rayyes, Ali A

Abstract

The structural stability and internal rotation in 3-cyclopropenecarboxaldehyde and 3-cyclo-propenecarboxylic acid fluoride were investigated by ab initio calcns. with a 6-31G* at. basis in the latter and a 6-311G* at. basis set in the former case. For the sake of comparison also results obtained with a 3-21G basis are given in the paper. As expected, it turned out that this basis set is not large enough for three-membered rings. The calcns. were carried out both at the RHF (HF) and the second order Moller-Plesset (MP2) levels. The trans-form is predicted to be the lower energy conformer for both mols. However, in case of the fluoride the two conformers have nearly the same energy. Full optimization was performed at the transition states and the asym. potential function for the CXO internal rotations was predicted for both mols.