Investigation of conformational stability and vibrational spectra of halomethylsulfonyl isocyanates. Badawi, H. M.; Forner, W.; Oloriegbe, Y. S

Abstract

The conformational behavior and structural stability of chloro- and fluoromethylsulfonyl isocyanates were investigated by quantum mech. DFT and ab initio MP2 calcns. The 6-311++G** basis set was employed to include polarization and diffuse functions in the calcns. The mols. were found to exist in a mixt. of two stable gauche conformations. The potential scans were calcd. from which the rotational barriers could be estd. The vibrational frequencies and spectra were computed at B3LYP/6-311++G** level. The potential energy distributions were then calcd. to provide tentative vibrational assignment for the normal modes of the stable conformers of both mols.