

Theoretical potential scans and vibrational spectra of vinyl selenonyl halides $\text{CH}_2=\text{CH}-\text{SeO}_2\text{X}$ (X is F, Cl and Br). Badawi, Hassan M.; Foerner, Wolfgang; Seddigi, Zaki S. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. *Journal of Molecular Modeling* (2004), 10(4), 250-258

Abstract

The structure and conformational stability of vinyl selenonyl fluoride, chloride and bromide $\text{CH}_2=\text{CH}-\text{SeO}_2\text{X}$ (X is F, Cl and Br) were investigated using d. functional B3LYP/6-311+G** and ab initio MP2/6-311+G** calcns. From the calcns. the mols. were predicted to exist only in the non-planar gauche conformation with the vinyl C=C group almost eclipsing one of the selenonyl Se=O bonds as a result of conjugation between the two moieties. Single-min. potential scans were calcd. at the DFT level for the mols. The vibrational frequencies were computed using B3LYP/6-311+G**. Normal coordinate calcns. were then carried out and potential energy distributions were calcd. for the three mols. in the gauche conformation.