

**Theoretical potential scans and vibrational spectra of vinyl selenonyl halides CH<sub>2</sub>=CH-SeO<sub>2</sub>X (X is F, Cl and Br).** Badawi, Hassan M.; Foerner, Wolfgang; Seddigi, Zaki S

**Abstract**

The structure and conformational stability of vinyl selenonyl fluoride, chloride and bromide CH<sub>2</sub>=CH-SeO<sub>2</sub>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.