

Structural stability and vibrational analyses of haloselenonyl azides, XSeO₂-NNN, where X is F, Cl, Br. Forner, Wolfgang; Badawi, Hassan M.; Seddigi, Zaki S

Abstract

The structural stability of haloselenonyl azides was investigated by quantum mech. Moller-Plesset perturbation theory of second order and d. functional theory calcns. The 6-311+G** basis set was used to include polarization and diffuse functions in the calcns. at the DFT-B3LYP level. The potential scans for the rotation of the -NNN rotor were calcd. and found to be consistent with a single min. that corresponds to a gauche conformation (-NNN moiety nearly eclipses one of the two selenonyl Se=O bonds) for the three halogens at ambient temp. The structural parameters for the min. calcd. by MP2 and DFT turned out to be very similar. The vibrational modes, IR and Raman intensities as well as depolarization ratios were calcd. at DFT-B3LYP/6-311+G** level for the three mols. in their gauche conformations. The potential energy distributions among symmetry coordinates of the normal modes of the mols. in their gauche conformation were then computed from normal coordinate analyses.