

Potential scans for X-MO₂-NCO (M=S and Se and X=F and Cl) and vibrational assignments of haloselenonyl isocyanates. Badawi, H. M.; Seddigi, Z. S.; Forner, W

Abstract

The structural stability of halosulfonyl isocyanate X-SO₂-NCO and haloselenonyl isocyanate X-SeO₂-NCO (X is F and Cl) was investigated by d. functional DFT-B3LYP/6-311+G and ab initio MP2/6-311+G calcns. The potential scans for the rotation of the -NCO rotor were calcd. and found to be consistent with a single min. that corresponds to a gauche conformation (-NCO moiety nearly eclipses one of the two M:O bonds). The vibrational frequencies, IR intensities as well as depolarization ratios were calcd. at DFT-B3LYP/6-311+G level for the two selenides at their gauche conformation. The potential energy distributions among symmetry coordinates of the normal modes of both F-SeO₂-NCO and Cl-SeO₂-NCO in their gauche conformation were then computed from normal coordinate analyses.