

Potential scans for X-MO₂-NCO (M = S and Se and X = F and Cl) and vibrational assignments of haloselenonyl isocyanates

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Abstract: The structural stability of halosulfonyl isocyanate X-SO₂-NCO and haloselenonyl isocyanate X-SeO₂-NCO (X is F and Cl) was investigated by density functional DFT-B3LYP/6-311 + G** and ab initio MP2/6-311 + G** calculations. The potential scans for the rotation of the -NCO rotor were calculated and found to be consistent with a single minimum that corresponds to a gauche conformation (-NCO moiety nearly eclipses one of the two M=O bonds). The vibrational frequencies, infrared intensities as well as depolarization ratios were calculated 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.