

Structural stability and vibrational assignments of halosulfonyl azides. Badawi, H. M.;
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Abstract

The structural stability of fluoro- and chlorosulfonyl azides was investigated by quantum mech. DFT and ab initio MP2 calcns. The 6-311++G** basis set was employed to include polarization and diffuse functions in the calcn. at DFT-B3LYP and MP2 levels. The potential scans for the rotation of the -NNN rotor were calcd. and found to be consistent with single min. that corresponds to gauche conformation (-NNN moiety nearly eclipse one of the two sulfonyl S=O bonds) for both the fluoride and the chloride at ambient temp. The vibrational frequencies, IR intensities as well as depolarization ratios were calcd. at DFT-B3LYP/6-311++G** level for the two mols. at their gauche conformation. 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.