Structural stability and vibrational assignments of halosulfonyl azides

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Abstract: The structural stability of fluoro- and chlorosulfonyl azides was investigated by quantum mechanical DFF and ab initio MP2 calculations. The 6-311+ +G** basis set-was employed to include polarization and diffuse functions in the calculation at DFT-B3LYP and MP2 levels. The potential scans for the rotation of the -NNN rotor were calculated and found to be consistent with single minimum 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 temperature. The vibrational frequencies, infrared intensities as well as depolarization ratios were calculated at DFT-B3LYP/6-311+ + G** level for the two molecules at their gauche conformation. The potential energy distributions among symmetry coordinates of the normal modes of the molecules in their gauche conformation were then computed from normal coordinate analyses.