
Abstract

The structural stabilities of CF3-SF, CF3-SCI, CCl3-SF, and CCl3-SCI were investigated by DFT-B3LYP and ab initio MP2 calcns. using 6-311 + G** basis set. Full energy optimizations were carried out from which the three-fold barrier about C-S bond was calc. to be about 3 kcal mol⁻¹ in (trifluoromethyl)sulfenyl fluoride and (trifluoromethyl)sulfenyl chloride and about 6 kcal mol⁻¹ in (trichloromethyl)sulfenyl fluoride and (trichloromethyl)sulfenyl chloride. The vibrational frequencies of the four mols. were computed at the DFT-B3LYP level and the vibrational assignments for the normal modes of the compds. in their ground state structure were made on the basis of normal coordinate calcns. and reported exptl. data.