Three-fold barrier and normal coordinate analyses of (trihalomethyl)sulfenyl halides CX3-SX (X = F and Cl). Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2005), 61A(5), 967-974.

Abstract

The structural stabilities of CF3-SF, CF3-SCl, CCl3-SF, and CCl3-SCl 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 calcd. 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.