C-S barrier and vibrational analyses of (halocarbonyl)sulfenyl halides XCO-SX (X = F, Cl, and Br). Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2004), 60A(11), 2573-2580.

Abstract

The structural stability of (halocarbonyl)sulfenyl halides XCO-SX (X is F, Cl, and Br) was investigated by DFT-B3LYP and ab initio MP2 calcns. using 6-311 + G** basis set. From the calcns. the mols. were found to exist predominantly in the trans conformation (two halogen atoms are trans to each other). Full energy optimizations were carried out for the min. and the transition states (TS) at the two levels, from which the rotational barriers about C-S bond in the three mols. were calcd. to be about 12-13 kcal mol-1. The vibrational frequencies of (fluorocarbonyl)sulfenyl fluoride (FCO-SF), (chlorocarbonyl)-sulfenyl chloride (ClCO-SCl), and (bromocarbonyl)-sulfenyl bromide (BrCO-SBr) were computed at the DFT-B3LYP level and the vibrational assignments for the normal modes of the stable forms of the compds. were made on the basis of normal coordinate calcns. and exptl. data of the chloride.