C-S Barrier And Vibrational Analyses Of (Halocarbonyl)Sulfenyl Halides

XCO-SX (X = F, Cl, And Br)

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Summary

The structural stability of (halocarbonyl)sulfenyl halides XCO-SX (X is F, Cl, and Br) was investigated by DFT-B3LYP and ab initio MP2 calculations using 6-311 + G** basis set. From the calculations the molecules 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 minima and the transition states (TS) at the two levels, from which the rotational barriers about C-S bond in the three molecules were calculated to be about 12-13 kcal mol(-1). The vibrational frequencies of (fluorocarbonyl)sulfenyl fluoride (FCO-SF), (chlorocarbonyl)-sulfenyl chloride (CICO-SCI), 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 compounds were made on the basis of normal coordinate calculations and experimental data of the chloride. (C) 2004 Elsevier B.V. All rights reserved.

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