Vibrational analyses of sulfamoyl halides NH2SO2X (X is F, Cl and Br). Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2006), 65A(2), 453-458.

Abstract

The structural stability of sulfamoyl halides NH2-SO2X (X is F, Cl and Br) were investigated by DFT-B3LYP/6-311 + G** and ab initio MP2/6-311 + G** calcns. From the calcns. the mols. were predicted to exist only in the anti (X-S bond is anti with respect to nitrogen lone pair) conformation with the possibility of very low abundance of the syn (SO2 and NH2 groups eclipse each other) form of only the fluoride. The equil. const. for the syn .dblarw. anti conformational conversion of sulfamoyl fluoride was calcd. to be 0.0172 that corresponds to an equil. mixt. of about 2% syn and 98% anti at 298.15 K. The vibrational frequencies were computed at DFT-B3LYP level for the stable anti conformer of the d0 and d2 (ND2-SO2X) deuterated species of the three mols. Normal coordinate calcns. were then carried out and the potential energy distributions were calcd. for the mols.