Potential functions of N-C and C-S internal rotations and normal coordinate analyses of carbamothioic acid H2N-CO-SCl. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia. THEOCHEM (2005), 715(1-3), 33-38.

Abstract

The structural stability of carbamothioic acid NH2CO-SCl was studied by DFT-B3LYP and ab initio MP2 calcns. using 6-311+G** basis set. Full energy optimizations were carried out and the mol. was predicted to exist predominantly in the trans (C=O and S-Cl bonds are anti to each other) conformation. From the calcns., the two-fold NH2 barrier about the N-C bond is .apprx.12 kcal/mol, while, the asym. OCSCl barrier about the C-S bond to be .apprx.8 kcal/mol. The vibrational frequencies of the d0- (NH2COSCl) and d2- (ND2COSCl) deuterated species of the mol. were computed at the DFT-B3LYP level. Then vibrational assignments for the normal modes of the compd. in its stable trans conformation were made from normal coordinate calcns