Potential energy distributions and potential scans for the internal rotation of two rotors in 3,3-dichloro and 3,3,3-trichloropropanals

Author(s): Badawi HM, Forner W

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Abstract: The conformational behavior and structural stability of 3,3-dichloropropanal and 3,3,3-trichloropropanal were investigated by ab initio calculations. The 6-311 + + G** basis set was employed to include polarization and diffuse functions in the calculations at B3LYP level. From the calculation, the trans conformer of 3,3,3-trichloropropanal was predicted to be the predominant conformer with about 2 kcal mol(-1) of energy lower than the tis form. Additionally, 3,3 dichloro-propanal was predicted to exist as a mixture of three stable conformers. The potential function scans were calculated for the two molecules from which the rotational barriers could be estimated. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calculations for the conformers of the two molecules. Vibrational Raman and infrared spectra of the mixture of the stable conformers were computed at 300 K.