Vibrational analyses of vinylsulfonamide CH2=CH-SO2NH2. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals (KFUPM), Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2005), 61A(7), 1445-1451.

Abstract

The structure and conformational stability of vinylsulfonamide CH2:CH-SO2NH2 were investigated by DFT-B3LYP/6-311 + G** and ab initio MP2/6-311 + G** calcns. From the calcns. the mol. was predicted to exist predominantly in the gauche-syn (vinyl group nearly eclipses one of the S=O bonds and the NH2 and the SO2 moieties eclipse each other) conformation with the possibility of low abundance of the cis-syn and the gauche-anti forms. The asym. potential function for the internal rotation about C-S bond was detd. for the mol. The vibrational frequencies were computed at DFT-B3LYP level for the gauche-syn conformer of the mol. and its d2(C2H3-SO2ND2) and d3(C2D3-SO2NH2) deuterated species. Normal coordinate calcns. were then carried out and the potential energy distributions were calcd. for the mol.