Vibrational spectra and analysis of acetohydrazide CH3-CO-NH-NH2. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2007), 67A(3-4), 592-597.

Abstract

The structural stability of acetohydrazide CH3-CO-NH-NH2 was investigated by DFT-B3LYP and ab initio MP2 calcns. with 6-311+G** basis set. The C-N rotational barrier in the mol. was calcd. to be about 26 kcal/mol that suggested the planar sp2 nature of the nitrogen atom of the central NH moiety. The N atom of the terminal NH2 group was predicted to highly prefer the pyramidal sp3 structure with an inversion barrier of about 7-8 kcal/mol. The mol. was predicted to have a trans-syn (N-H bond is trans with respect to C=O bond and NH2 moiety is syn to C-N bond) conformation as the lowest energy structure. The vibrational frequencies were computed at B3LYP level of theory and normal coordinate calcns. were carried out for the trans-syn acetohydrazide. Complete vibrational assignments were made on the basis of normal coordinate analyses and exptl. IR and Raman data.