Structural stability and vibrational analysis of aminoethylene CH2 CH-NH2 and aminoketene OCCH-NH2. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Peteroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2005), 726(1-3), 253-260.

Abstract

The structural stability of vinylamine (aminoethylene) CH2 =CH-NH2 and keteneamine (aminoketene) O=C=CH-NH2 were investigated by DFT-B3LYP and ab initio MP2 calcns. with 6-311+G** basis set. From the calcns. vinylamine was predicted to exist predominantly in a non-planar structure consistent with an earlier microwave results, while keteneamine in a mixt. of anti and syn conformations, with the anti being the low energy conformer at ambient temp. The equil. const. for the anti<=>syn interconversion in keteneamine was estd. to be 0.4456 at 300 K. From the calcns. the NH2 inversion barrier was estd. to be about 0.5 and 1.6 kcal/mol for vinylamine and about 2.3 and 3.3 for keteneamine at DFT-B3LYP/6-311+G** and MP2/6-311+G** levels, resp. as compared to about 1.0 kcal/mol (356 cm-1) obtained from a microwave data of vinylamine. The vibrational frequencies were computed at the DFT-B3LYP level and the IR and Raman spectra for each mol. and its deuterated species. Complete vibrational assignments were made on the basis of normal coordinate analyses and isotopic substitution for vinylamine and keteneamine.