Conformational stability and vibrational analyses of vinyl diazene CH2=CH-N=NH and vinyl imine CH2=CH-CH=NH. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2005), 715(1-3), 39-46.

Abstract

The conformational and structural stability of vinyl diazene and vinyl imine were studied by DFT-B3LYP and ab initio MP2 calcns. with 6-311+G** basis set. Vinyl diazene was predicted to exist only in the planar trans-anti conformation (CCNN and CNNH dihedral angles are 180°), while vinyl imine to exist in two trans (CCCN dihedral angle is 180°) conformations. The trans-anti (CCNH dihedral angles is 180°) conformation of vinyl imine was predicted to be .apprx.1 kcal/mol lower in energy than the trans-syn (CCNH dihedral angles is 0°) form that is in excellent agreement with an earlier microwave results. The vibrational frequencies were computed at the DFT-B3LYP level and the calcd. IR and Raman spectra of each mol. were plotted. Complete vibrational assignments were made from normal coordinate calcns. for the two mols.