Vibrational spectra and normal coordinate analyses of vinyl cyanamide in the planar conformation. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2002), 584 201-210.

Abstract

The conformational and structural stability of vinyl cyanamide CH2:CH-NHCN were investigated by DFT-B3LYP and MP2 calcns. with 6-311+G** basis set. The mol. was predicted to have the planar structure as a result of conjugation effects. The mol. was predicted to exist in the cis (-NCN moiety eclipses the vinyl C:C- group) and the trans conformations with the cis being the lower energy form. The cis-trans barrier was calcd. to be of about 7 kcal mol-1. The vibrational frequencies were computed at the DFT-B3LYP level and the calcd. IR and Raman spectra of the cis-trans mixt. of the mol. were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for both stable conformers of vinyl cyanamide.