Conformational and vibrational analyses for 2,2-dihalovinyl azides CX2:CH-NNN (X is F and Cl). Badawi, Hassan M.; Forner, Wolfgang; Al-Ghamidi, Khalid S. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2003), 638 147-156.

Abstract

The conformational behavior of 2,2-dihalovinyl azides CX2:CH-NNN (X is F and Cl) were investigated by DFT-B3LYP and ab initio MP2 calcns. with 6-311++G basis set. The two mols. were predicted to exist predominantly in the trans (the vinyl CX2:CH- and the azide -NNN groups are trans to each other) conformation. The relative energy between cis and trans were calcd. to decrease in the order: dichloride > difluoride. Full optimization was performed at the ground and transition states in the mols. at both MP2 and B3LYP levels. The barrier to internal rotation around the C-N single bond was calcd. to be 3.719 and 5.171 kcal/mol in the difluoride and the dichloride, resp. The vibrational frequencies were computed at the DFT-B3LYP level and the calcd. IR and Raman spectra of the cis-trans mixt. of the two mols. were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for both stable conformers of the two mols.