Conformational stability and normal coordinate analyses for 1-halovinyl azides CH2=CX-NNN (X is F, Cl and Br). Badawi, Hassan M.; Foerner, Wolfgang; Al-Ghamdi, Khalid S. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of Molecular Modeling (2003), 9(6), 355-364.

Abstract

The conformational behavior of 1-halovinyl azides $CH_2=CX-NNN$ (X=F, Cl and Br) were investigated by DFT-B3LYP and ab initio MP2 calcns. with the 6-311++G** basis set. The mols. were predicted to exist predominantly in the trans (the vinyl $CH_2=CH-$ and the azide -NNN groups are trans to each other) conformation. The relative energy between cis and trans were calcd. to decrease in order: bromide>chloride>fluoride. Full optimization was performed at the ground and transition states in the mol. at both MP2 and B3LYP levels. The barrier to internal rotation around the C-N single bond in the three mols. was calcd. to be about 4-5 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 three mols. were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for both stable conformers of the three mols.