Conformational And Vibrational Analyses For 2,2-Dihalovinyl Azides

CX2=CH-NNN (X Is F And CI)

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Summary

The conformational behavior of 2,2-dihalovinyl aizdes CX2=CH-NNN (X is F and Cl) were investigated by DFT-B3LYP and ab initio MP2 calculations with 6-311+ +G** basis set. The two molecules 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 calculated to decrease in the order: dichloride > difluoride. Full optimization was performed at the ground and transition states in the molecules at both MP2 and B3LYP levels. The barrier to internal rotation around the C-N single bond was calculated to be 3.719 and 5.171 kcal/mol in the difluoride and the dichloride, respectively. The vibrational frequencies were computed at the DFT-B3LYP level and the calculated infrared and Raman spectra of the cis-trans mixture of the two molecules were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the two molecules. (C) 2003 Elsevier B.V. All rights reserved.

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