# Conformational Stability And Normal Coordinate Analyses For 1-Halovinyl Azides CH2=CX-NNN (X Is F, Cl And Br)

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## Summary

The conformational behavior of 1-halovinyl azides CH2=CX-NNN (X=F, Cl and Br) were investigated by DFT-B3LYP and ab initio MP2 calculations with the 6-311++G** basis set. The molecules were predicted to exist predominantly in the trans (the vinyl CH2=CH- and the azide -NNN groups are trans to each other) conformation. The relative energy between cis and trans were calculated to decrease in order: bromide>chloride>fluoride. Full optimization was performed at the ground and transition states in the molecule at both MP2 and B3LYP levels. The barrier to internal rotation around the C-N single bond in the three molecules was calculated to be about 4-5 kcal mol(-1). The vibrational frequencies were computed at the DFT-B3LYP level and the calculated infrared and Raman spectra of the cis-trans mixture of the three molecules were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the three molecules.

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