Vibrational Analyses and C-N Rotational Barrier in N-Vinyl and N-(2,2-Dichlorovinyl)nitrones

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ABSTRACT

The conformational and structural stability of N-vinyl nitrone CH2:CH-N(O):CH2 and N-(2,2-dichlorovinyl)nitrone CCl2:CH-N(O):CH2 were investigated by DFT-B3LYP and MP2 calcns. with 6-311+G** basis set. The mols. were predicted to have the planar structure as a result of pronounced conjugation between C:C and N:C bonds. N-vinyl nitrone was predicted to exist predominantly in the trans (C:C and N:C moieties are trans to each other) conformation, while the dichloride to exist in a mixt. of the gauche and the trans conformations with the former being the lower energy form. The trans to gauche barrier was calcd. to be about 6 kcal/mol in N-vinyl nitrone, while the gauche to trans barrier to be about 2 kcal/mol in N-(2,2-dichlorovinyl)nitrone. The vibrational frequencies were computed at the DFT-B3LYP level and the calcd. IR and Raman spectra of the two mols. were plotted. Complete vibrational assignments were made on the basis of normal coordinate analyses for both mols.