

MP2 C-N barrier and vibrational spectra and assignments for CH₂:CH-N:C:X (X=O, S and Se). Badawi, H. M.; Forner, W.; Seddigi, Z. S

Abstract

The structure of the CH₂:CH-N:C:X (X = O, S and Se) series of compds. was optimized at ab initio MP2/6-311+G level of calcn. Vinyl isocyanate, vinyl isothiocyanate and vinyl isoselenocyanate were predicted to exist in a mixt. of the cis (the NCX group eclipses the vinyl group) and the trans conformations with the latter being the predominant form at ambient temp. The size of the rotational barrier of the internal rotations around C-N bond was predicted to decrease in the order: isocyanate>isothiocyanate>isoselenocyanate. The vibrational wavenumbers, IR intensities, and Raman activities were calcd. at MP2/6-311+G** level for the mols. in their cis and trans conformations. Normal coordinate calcns. were then carried out and potential energy distributions were calcd. for each of the three mols. in their stable forms. The vibrational IR and Raman spectra were plotted for the mixt. of two stable conformations of the mols.