

MP2 C-N barrier and vibrational spectra and assignments for $\text{CH}_2 = \text{CH} - \text{N} = \text{C} = \text{X}$ (X = O, S and Se)

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Abstract: The structure of the $\text{CH}_2=\text{CH}-\text{N}=\text{C}=\text{X}$ (X = O, S and Se) series of compounds was optimized at ab initio MP2/6-311+G** level of calculation. Vinyl isocyanate, vinyl isothiocyanate and vinyl isoselenocyanate were predicted to exist in a mixture of the cis (the NCX group eclipses the vinyl group) and the trans conformations with the latter being the predominant form at ambient temperature. 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 calculated at MP2/6-311 + G** level for the molecules in their cis and trans conformations. Normal coordinate calculations were then carried out and potential energy distributions were calculated for each of the three molecules in their stable forms. The vibrational infrared and Raman spectra were plotted for the mixture of two stable conformations of the molecules.