

Analyses of vibrational spectra of nitroso- and nitroethylenes. Badawi, H. M.; Foerner, W..

Abstract

The conformational and structural stability of nitrosoethylene $\text{CH}_2\text{:CH-N:O}$ and nitroethylene $\text{CH}_2\text{:CH-NO}_2$ were studied by DFT-B3LYP and ab initio MP2 calcns. with 6-311+G basis set. From the calcns. nitrosoethylene was predicted to exist predominantly in the planar trans structure (C:C and N:O bonds are trans to each other) with high trans-cis rotational barrier of .apprx.9 kcal/mol as a result of pronounced conjugation between C:C and N:O bonds. The NO_2 rotational barrier in nitroethylene is of .apprx.4 kcal/mol. The vibrational frequencies were computed at the DFT-B3LYP level and the IR and Raman spectra plotted for both mols. and their -d₃ deuterated species. Complete vibrational assignments were made from normal coordinate analyses and isotopic substitution for the two mols.