Analyses of vibrational spectra of nitroso- and nitroethylenes

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Abstract: The conformational and structural stability of nitrosoethylene CH2=CH-N=O and nitroethylene CH2=CH-NO2 were investigated by DTF-B3LYP and ab initio MP2 calculations with 6-311 + G** basis set. From the calculations 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 about 9 kcal/mol as a result of pronounced conjugation between C-C and N=O bonds. The NO2 rotational barrier in nitroethylene was calculated to be of about 4 kcal/mol. The vibrational frequencies were computed at the DFT-B3LYP level and the infrared and Raman spectra plotted for both molecules and their -d(3) deuterated species. Complete vibrational assignments were made on the basis of normal coordinate analyses and isotopic substitution for the two molecules.