Influence of fluorine substitution in nitrosoethylene and their vibrational spectra, calculated with Moller-Plesset perturbation theory of second order. Badawi, Hassan M.; Foerner, Wolfgang. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2005), 725(1-3), 183-189.

## Abstract

The conformational and structural stability of monofluoro-nitrosoethylene $CH_2=CF-N=O$, and difluoro-nitrosoethylene $CF_2=CH-N=O$ were investigated by ab initio Moller-Plesset Perturbation Theory of second order (MP2) calcns. using the 6-311+G** basis set to include electron correlation. From the calcns. the two mols. were predicted to exist predominantly in the planar trans structure with high trans-cis rotational barriers of about 10-11 kcal/mol as a result of pronounced conjugation between C=C and N=O bonds. The differences in the rotational barriers when going from the parent mol., nitrosoethylene, to its fluorinated derivs. are explained on the basis of electronegativity. The vibrational frequencies were computed for the two mols. at the MP2 level. Normal coordinate analyses were carried out and the potential energy distributions, PED, among the symmetry coordinates of the normal modes of the mols. were computed. Complete vibrational assignments were made on the basis of normal coordinate analyses for the mols. As expected we find there low Raman and appreciable IR intensities in all modes which contain a high content of fluorine movements because vibrations of C-F bonds lead to a small change in polarizability, but to a large change in dipole moment. However, also modes involving double bonds have quite large intensities in both spectra. An appreciable no. of modes in these mols. are composed of relatively large nos. of symmetry coordinates, i.e. they are highly mixed.