Study of structural stability and vibrational spectra of nitroso and nitroketenes

Author(s): Badawi HM, Forner W

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 542 **Pages:** 7-20

Abstract: The structural stability of nitrosoketene and nitroketene was investigated using ab initio calculations. The calculations were carried out. at DFT-B3LYP/6-311++G** level. From the calculation the molecules were predicted to exist predominantly in the planar conformations. Nitrosoketene was predicted to exist predominantly in the trans conformation with high ti-ans-cis rotational barrier. The rotational barrier of the NO group in nitrosoketene was calculated to be about 18 kcal/mol, while that of the NO2 group in nitroketene to be about 10 kcal/mol. The vibrational frequencies were computed, normal coordinate calculations were carried out and potential energy distributions were calculated for both molecules.