Study of structural stability and vibrational spectra of nitroso and nitroketenes. Badawi, H. M.; Forner, W

Abstract

The structural stability of nitrosoketene and nitroketene was investigated using ab initio calcns. The calcns. were carried out at DFT-B3LYP/6-311++G** level. From the calcn. the mols. were predicted to exist predominantly in the planar conformations. Nitrosoketene was predicted to exist predominantly in the trans conformation with high trans-cis rotational barrier. The rotational barrier of the NO group in nitrosoketene was calcd. 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 calcns. were carried out and potential energy distributions were calcd. for both mols.