Vibrational spectra and potential energy distributions of normal modes of 3-nitroso- and 3-nitrocyclopropenes. Badawi, Hassan M.; El-Rayyes, Ali A. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2002), 588 17-27.

Abstract

The structural stability of 3-nitrosocyclopropene c-C3H3-N:O and 3-nitrocyclopropene c-C3H3-NO2 was studied by d. functional B3LYP and ab initio MP2 calcns. using 6-311+G** basis set. From the calcn., 3-nitrosocyclopropene was predicted to exist predominantly in the trans conformation (N:O bond is trans to the ring and eclipse α-H of the ring) with high trans-cis rotational barrier of .apprx.8 kcal/mol. The NO2 rotational barrier in 3-nitrocyclopropene was predicted from the sym. potential scan to be of .apprx.4.4 kcal/mol. The vibrational frequencies were computed at DFT-B3LYP/6-311+G** level for both mols. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the two mols.