

Theoretical potential functions and vibrational analysis for halocarbonyl azides CXO-NNN (X = F, Cl and Br). Badawi, Hassan M.; Foerner, Wolfgang; Al-Ghamdi, Khalid S. Dep. Chem., King Fahd Univ. Petroleum and Minerals, Dhahran, Saudi Arabia. *Journal of Molecular Modeling* (2003), 9(2), 124-133.

Abstract

The structural stability of halocarbonyl azides CXO-NNN (X = F, Cl and Br) was investigated by DFT and MP2 calcns. using the 6-311++G** basis set. From the calcns., the mols. were found to have and S-cis.tautm.s-trans conformational equil. with cis being the lower-energy form. Full energy optimizations were carried out for the transition states and the min. at the B3LYP/6-311++G** and MP2/6-311++G** levels, from which the rotational barriers were calcd. to be o the order 8-10 kcal mol⁻¹. The vibrational frequencies were computed at the DFT-B3LYP level and the vibrational assignments for the normal modes of the stable conformers were made on the basis of normal coordinate calcns.