

**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

**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<sup>-1</sup>. 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.