Theoretical study of the structure and vibrational spectra of formyl and methyl azides.
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Abstract

The structure and conformational stability of formyl azide CHO-NNN and Me azide CH3-NNN were investigated using DFT-B3LYP and ab initio MP2 calcns. The calcns. were carried out using 6-311++G** basis set. From the calcn. formyl azide was predicted to exist predominantly in the planar cis conformation. The potential functions for internal rotation in each of the mols. were detd. at the two levels. The three-fold barrier of the Me group in Me azide was calcd. at MP/6-311++G** level to be of about 0.7 kcal/mol in good agreement with exptl. value obtained from microwave study. The vibrational wavenumbers were computed at B3LYP/6-311++G** level for the two mols. Normal coordinate calcns. were carried out and potential energy distributions (PED) among symmetry coordinates of the normal modes were calcd. for the mols.