

C-N barriers to internal rotations and vibrational analyses of carbamoyl azide NNN-CONH₂. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia. Asian Journal of Spectroscopy (2006), 10(1&2), 7-14.

Abstract

The internal rotations around two C-N bonds in carbamoyl azide NNN-CONH₂ were investigated by D. Functional B3LYP and ab initio second-order Moller Plesset MP2 calcns. with the 6-311+G** basis set. Carbamoyl azide was predicted at both levels to exist predominantly as the cis conformation (C=O and NNN moieties eclipse each other) with a cis-trans barrier of about 8 kcal/mol. The sym. NH₂ torsional barrier was estd. to be about 20 kcal/mol by DFT and MP2 methods of calcns. The vibrational frequencies for the d0 and d2 isotopic species of the mol. in the cis conformation were computed at the B3LYP/6-311+G** level and compared to exptl. data. Normal coordinate calcns. were then carried out and the potential energy distributions (PEDs) among the symmetry coordinates of the normal vibrational modes of the mol. were calcd. Complete vibrational assignments were provided on the basis of normal coordinate calcns., isotopic substitution and comparison with reported exptl. data of the mol.