

Normal coordinate analyses, vibrational assignments and barrier to internal rotation in isocyanatoacetaldehyde based on ab initio calculations. Forner, Wolfgang; Badawi, Hassan M.

Abstract

The structure and conformational stability of OCNCH₂CHO were studied using ab initio calcns. The calcns. were carried out at RHF/6-311G* and MP2/6-311G* levels. The mol. was predicted by the calcns. to exist predominantly in the cis-cis conformation. The potential function for the internal rotation of the CHO group was detd. for the mol. The inclusion of electron correlation into the calcns. had a very small effect on the calcd. potential coeffs. The vibrational frequencies were computed at the Hartree-Fock level. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the cis-cis conformer of the mol. The calcd. vibrational frequencies for the two conformers were scaled and compared to those obsd. exptl. for similar mols.