

Vibrational assignments and barrier to internal rotation in formyl isocyanate by ab initio and normal coordinate calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The structure and conformational stability of formyl isocyanate were investigated using ab initio calcns. The calcns. were carried out at RHF/6-311++G** and DFT B3LYP/6-311++G** levels. From the calcn. the mol. was predicted to exist predominantly in the planar cis and trans conformations with the former being the lowest energy conformer. The asym. potential function for the internal rotation was detd. for the mol. The vibrational frequencies were computed at both levels. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the two conformers of the mol.