

Vibrational Spectra And Analyses Of Phenylcyanamide

Badawi, HM; Forner, W

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King Fahd University of Petroleum & Minerals

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Summary

The structure of phenylcyanamide $c\text{-C}_6\text{H}_5\text{-NHCN}$ was investigated by DFT-B3LYP and ab initio MP2 calculations with 6-311 + G** basis set. The planar to the perpendicular rotational barrier was calculated to be of about 4 kcal/mol by both levels of calculation. The stability of the planar structure of phenylcyanamide was explained on the basis of conjugation effects between the cyanamide-NHCN moiety and the phenyl C-C₆H₅ ring in agreement with earlier NMR results. The CNC and the UNC bond angles were calculated to be about 120degrees especially by MP2 calculation that is consistent with sp² (planar -NH-CN group) and not sp³ (pyramidal -NH-CN group) structure. The vibrational frequencies of the d(0)-, d(1)- and d(5)-phenylcyanamide and the potential energy distributions among symmetry coordinates of the normal modes of the parent molecule were computed at the DFT-B3LYP level. The calculated infrared and Raman spectra of the molecule were plotted. Complete vibrational assignments were made on the basis of isotopic substitution and normal coordinate calculations. (C) 2003 Elsevier B.V. All rights reserved.

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