

Vibrational spectra and analyses of phenylcyanamide. Badawi, Hassan M.; Forner, Wolfgang. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2004), 673(1-3), 223-229.

Abstract

The structure of phenylcyanamide *c*-Ph-NHCN was studied by DFT-B3LYP and ab initio MP2 calcns. with 6-311+G basis set. The planar to the perpendicular rotational barrier is of .apprx.4 kcal/mol by both levels of calcn. The stability of the planar structure of phenylcyanamide was explained from conjugation effects between the cyanamide-NHCN moiety and the Ph *c*-Ph ring in agreement with earlier NMR results. The CNC and the HNC bond angles are .apprx.120° esp. by MP2 calcn. that is consistent with sp² (planar -NH-CN group) and not sp³ (pyramidal -NH-CN group) structure. The vibrational frequencies of the d₀-, d₁- and d₅-phenylcyanamide and the potential energy distributions among symmetry coordinates of the normal modes of the parent mol. were computed at the DFT-B3LYP level. The calcd. IR and Raman spectra of the mol. were plotted. Complete vibrational assignments were made from isotopic substitution and normal coordinate calcns.