Vibrational spectra and analyses of phenylcyanamide. Badawi, Hassan M.; Forner, Wolfgang.

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.