Normal coordinate analyses of 3,5-dichlorophenylcyanamide. Badawi, Hassan M.; Foerner, Wolfgang. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of Molecular Modeling (2004), 10(3), 178-184.

Abstract

The structure of 3,5-dichlorophenylcyanamide c-C6H3Cl2-NHCN was investigated by DFT-B3LYP and ab initio MP2 calcns. with the 6-311+G++ basis set. The planar to perpendicular rotational barrier was calcd. to be of about 5 kcal mol-1 at both levels of calcn. The stability of the planar structure of the mol. was explained on the basis of conjugation effects between the cyanamide-NHCN moiety and the Ph c-C6H5 ring in agreement with earlier NMR results. The CNC and the HNC bond angles were calcd. to be about 120° esp. by MP2 calcn., which is consistent with sp2 (planar-NH-CN group) and not sp3 (pyramidal -NH-CN group) structure. The vibrational frequencies of the d0, d1 and d3 species of 3,5-dichlorophenylcyanamide 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 on the basis of isotopic substitution and normal coordinate calcns.