

ORIGINAL PAPER

X-ray molecular structure and theoretical study of 1,4-bis[2-cyano-2-(*o*-pyridyl)ethenyl]benzene

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Received 21 December 2012; Revised 22 April 2013; Accepted 27 April 2013

The structural characterisation of the molecule 1,4-bis[2-cyano-2-(*o*-pyridyl)ethenyl] benzene obtained through Knoevenagel condensation is reported. The single crystals, as light brown rods, were cultured from a chloroform solution using a slow evaporation method at ambient temperature. The compound crystallised in the monoclinic system belonging to the *C2/c* space group with $a = 26.4556(9)$ Å, $b = 3.73562(10)$ Å, $c = 18.4230(6)$ Å, $\beta = 109.841(4)^\circ$ and the asymmetric unit comprising $Z = 4$. The structure is ordered and the molecules of the title compound exhibited a lattice with water molecules located at sites of inversion and two-fold axial symmetries. Thus, only halves of the molecules are symmetrically independent. The lattice is reported and contrasted with X-ray single-crystal diffraction and theoretical calculations of 1,4-bis(1-cyano-2-phenylethenyl)benzene. By using density functional theory (DFT) and second order Moller–Plesset (MP2) theoretical calculations, the ground state geometry in the whole molecule at the B3LYP/6-31+G(d,p), and MP2/6-31+G(d,p) theory levels, respectively, were optimised. The DFT calculations showed a quasi-planar structure of the molecule, whereas the wave function-based MP2 method afforded a non-planar optimised structure with significant torsion angles between the pyridine and phenyl rings.

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Keywords: cyano-substituted acrylonitrile compound, X-ray structure, molecular structure, DFT and MP2 calculations

Introduction

The synthesis and the study of novel series of conjugated cyano-substituted acrylonitrile compounds are topics currently attracting great interest with regard to applications in electroluminescent devices (Friend et al., 1999). The structural analysis and characterisation of these compounds are essential processes for correlating the structural features with possible optical properties. Compounds such as 1,4-distyrylbenzene derivatives have been synthesised using standard Schlenk techniques, while distyrylben-

zene derivatives have been prepared (Wadsworth et al., 1965) via Knoevenagel condensation (Greenham et al., 1993) or by Heck coupling (Renak et al., 1999). The distance and relative orientation between the conjugated polymer chains and the corresponding molecular chromophores play important roles in determining the characteristics of the bulk materials, such as emission quantum yield and transport ability.

To determine the interchange arrangement in polymers (Enkeimann, 1998), the lattice properties of conjugated oligomers, particularly crystalline molecules, have been investigated by simulating model com-

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