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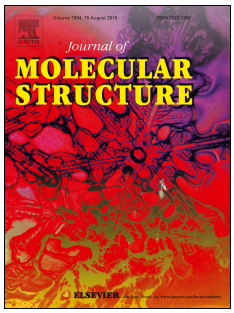

Quantum chemical studies on 4-(2, 6-diphenylpyridin-4-yl) phenol: An electron transport and nonlinear optical molecule

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Quantum chemical studies on 4-(2, 6-diphenylpyridin-4-yl) phenol: An electron transport and nonlinear optical molecule

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Abstract

The present article describes a combined experimental and computational study of 4-(2, 6-diphenylpyridin-4-yl) phenol, denoted as TAP. The TAP has been synthesized and characterized using IR, ^{1}H NMR, and single crystal XRD analysis. Single crystal analysis showed that the crystal belongs to monoclinic system and P21/c space group. The existence of three phenyl rings in a plane is expected to show good NLO activity. Ab initio quantum chemical calculations on the title compound have been performed by density functional theory (DFT) using B3LYP method with 6-31G basis set. First order hyperpolarizability has been predicted, the molecule showed good SHG activity, suggesting that the title compound is a suitable organic NLO active material. Molecular Electrostatic Potential (MEP) analysis showed both electronegative and electropositive potential sites in the molecule. Topology of HOMO-LUMO showed a marked energy gap (3.07eV) indicating the possibility of the molecule to be used as electron transport material.

Keywords: Aryl Pyridine, NLO studies, X-ray structure, DFT Calculations

1. Introduction

Multiaryl-substituted pyridine derivatives are widely used as Electron Transport Molecules (ETMs). They possess good hole blocking properties with suitable LUMO values (>3.5eV) to allow electron injection and HOMO values as large as 6.87 eV which are among the highest reported for molecular semiconductor materials [1-2]. They are used as electron transport materials in non-doped deep blue OLEDs [3]. Due to the presence of π-stacking ability, these compounds are used in supramolecular chemistry [4]. Pyridine derivatives have good electron affinity and are important electron-acceptor species. Many of the derivatives are promising candidates for application in OLEDs [5, 6]. Multiaryl pyridines have remarkable pharmacological activities, such as antitumor [7], cytoprotective [8], anxiolytic [9] and antiviral