



Vibrational spectroscopic and molecular docking study of 4-Methylphenylquinoline-2-carboxylate



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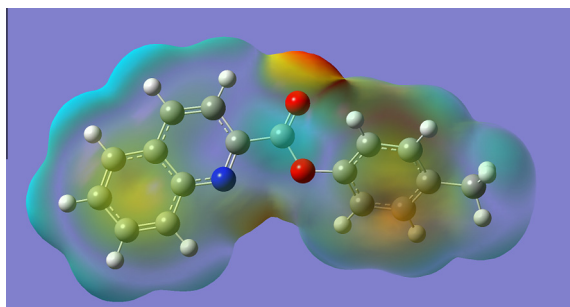
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HIGHLIGHTS

- IR, Raman spectra and NBO analysis were reported.
- The wavenumbers are calculated theoretically using Gaussian09 software.
- The wavenumbers are assigned using PED analysis.
- The geometrical parameters are in agreement with XRD data.
- Molecular docking is reported.

GRAPHICAL ABSTRACT



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ABSTRACT

FT-IR and FT-Raman spectra of 4-Methylphenylquinoline-2-carboxylate were recorded and analyzed. The structure of the molecule has been optimized and structural characteristics have been determined by density functional theory. The geometrical parameters (DFT) are in agreement with the XRD results. HOMO and LUMO and other chemical properties are reported. Nonlinear optical properties are also reported. A detailed molecular picture of the title compound and its interactions were obtained from NBO analysis. The negative (red and yellow) regions of the MEP are related to electrophilic reactivity and the positive (blue) regions to nucleophilic reactivity, as shown in the MEP plot and the carbonyl group and the phenyl rings are observed as electrophilic. PASS analysis predicts that the 4-Methylphenylquinoline-2-carboxylate might exhibit anti-diabetic activity. Molecular docking results suggest that the compound might exhibit inhibitory activity against GPb.

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Introduction

Quinoline-2 carboxylic acid derivatives are a class of important materials used as anti-tuberculosis agents, fluorescent reagents,

hydrophobic field-detection reagents, visualization reagents, fluorescent labeled peptide probes and anti-hyper glycemics. Quinoline derivatives could be used as dopants in the polymer-light emitting diode materials [1]. Certain quinoline derivatives could generate a sharp green electroluminescence and have high quantum efficiency of emission in the blue and the green region [2,3]. Quinoline derivatives represent a major class of hetero-cycles

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and are found in natural products [4], numerous commercial products, including fragrances, dyes and biologically active compounds [5–7]. Quinoline alkaloids such as quinine, chloroquine, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria [8]. Quinoline as a privileged scaffold in cancer drug discovery is reported by Solomon and Lee [9] and the derivatives shows potent-activity as anti-proliferative, anti-asthmatic and anti-inflammatory [10–12]. Quinoline derivatives are well known for its anti-malarial, antifungal and anti-amoebic activities [13]. Quinolines have been detected in meteorite extracts, and in general quinolines are of astro-biological interest, since this class of molecules includes nucleo-bases and basic components of nucleic acids [14,15]. Quinolines have good electron mobility, thermal and oxidative stabilities, high photoluminescence efficiencies and good film forming properties which are important for their use in Organic Light Emitting Diodes (OLEDs) [16,17]. Quinoline derivatives have been extensively studied due to their great potential application in the field of OLEDs [18–28]. Quinoline based dyes have developed with the advent of technology and are applied to electroluminescence and photo-chromism as well as the field of medication [29–31]. Quinoline derivatives possess non-centrosymmetry and hence they are used in the synthesis of molecules having non-linear responses [32–35]. Quinoline derivatives have been widely used as an emissive and electron transporting material in organic light emitting devices [36,37]. The title compound was synthesized by treatment of quinolone-2-carboxylic acid with *p*-cresol. The single crystal XRD study of the title compound was reported by Fazal et al. [38]. In the present study, the vibrational infrared and Raman spectra of the title compound are presented. Also the NBO, Frontier molecular orbital analysis, Molecular electrostatic potential and first hyperpolarizability are also reported. Due to the different potential biological activity of the title compound, molecular docking studies are also reported.

Experimental details

The title compound was synthesized as reported [38] and was recrystallized in absolute ethanol. Infrared spectrum (Fig. 1) was recorded on a Shimadzu IR prestige-21 FT spectrophotometer with KBr pellets (4000–400 cm^{-1}). The FT-Raman spectrum (Fig. 2) was obtained on a Bruker RFS 100/s, Germany. For excitation of the spectrum, the emission of Nd: YAG laser was used with an excitation wavelength of 1064 nm, maximal power 150 mW; measurement on solid sample. One thousand scans were accumulated with a total registration time of about 30 min. The spectral resolution after apodization was 2 cm^{-1} . In the title compound, $\text{C}_{17}\text{H}_{13}\text{NO}_2$, two molecules crystallize in the asymmetric unit. In the crystal weak C–H...O intermolecular interactions are observed.

Computational details

In this work the DFT using Becke's three parameter exchange functional in combination with the Lee–Yang–Parr correlation functional (B3LYP) and standard 6-31G(d) (6D, 7F) and 6-311G(d) (5D, 7F) basis sets calculations were performed with Gaussian09 program [39]. As the hybrid B3LYP functional tends to overestimate the fundamental normal modes of vibration, the computed frequencies in the harmonic approximation were scaled to closer reproducible experimental values and a scaling factor of 0.9613 is used [40]. The optimum geometry was determined by minimizing the energy, with respect to all geometrical parameters without imposing molecular symmetry constraints. The second one was to perform the frequency analysis which was completed again with DFT method. Thereafter, the vibrational frequencies, infrared intensities and Raman activities have been calculated. The graphi-

cal presentation of the calculated IR and Raman spectra were made using Gaussview program [41]. The assignments of the normal modes were also made on the basis of the PED analysis using GAR2PED software [42]. The optimized geometrical parameters (Fig. 3) (B3LYP/6-311G(d) (5D, 7F)) with XRD data is given in Table S1 as supporting material.

Results and discussion

IR and Raman spectra

The calculated (scaled) frequencies, observed IR and Raman bands with assignments are given in Table 1. In the following discussion, the 1,4-, 1,2-phenyl and quinoline rings are designated as PhI, PhII and RingIII, respectively. The experimentally observed values are in agreement with that given by B3LYP/6-311G(d) (5D, 7F) and hence the theoretical values of frequencies given by B3LYP/6-311G(d) (5D, 7F) is discussed in the following section. The vibrations of the CH_3 group are expected in the range 2900–3000 cm^{-1} [43,44]. The first of these result from asymmetric stretching $\nu_{\text{as}}\text{CH}_3$ modes in which two C–H bonds of the methyl group are extending while the third one is contracting and the other results from the symmetric stretching $\nu_{\text{s}}\text{CH}_3$ in which all three of the C–H bonds extend and contract in phase. The asymmetric stretching modes of methyl group are calculated to be at 2983, 2959 cm^{-1} and the symmetric mode at 2909 cm^{-1} . The bands at 3000, 2957, 2915 cm^{-1} in the IR and 3004, 2920 cm^{-1} in the Raman spectrum of the title compound are assigned as CH_3 stretching vibrations. Two bending modes can occur within a methyl group. The asymmetric deformations are expected in the range 1400–1485 cm^{-1} [43]. The calculated values of $\nu_{\text{as}}\text{CH}_3$ modes are 1455, 1450 cm^{-1} . Experimentally bands are observed at 1457 cm^{-1} in IR and 1458 cm^{-1} in Raman spectrum. In many molecules the symmetric deformation $\delta_{\text{s}}\text{CH}_3$ appears with an intensity varying from medium to strong and expected in the range $1380 \pm 25 \text{ cm}^{-1}$ [43]. Bands at 1375 cm^{-1} in the IR spectrum, 1380 cm^{-1} in the Raman spectrum and at 1376 cm^{-1} (DFT) are assigned as the $\delta_{\text{s}}\text{CH}_3$ modes for the title compound. The methyl rocking modes are expected in the regions 900–1100 cm^{-1} [43]. For the title compound these modes are calculated at 1069, 975 cm^{-1} . The band at 978 (IR) is assigned as rocking modes of the CH_3 group.

According to literature [45] the stretching mode of C=O is expected in the range 1850–1550 cm^{-1} . The in-plane bending mode of C=O is reported in the range $725 \pm 95 \text{ cm}^{-1}$ [43]. The C=O out of plane vibration is reported in the region $595 \pm 120 \text{ cm}^{-1}$ [43]. Kumar et al. reported the C=O stretching modes at 1728, 1703 cm^{-1} in the IR spectrum and the theoretical values are 1739, 1720 cm^{-1} [46]. For the title compound, the band at 1720 cm^{-1} in IR, 1730 cm^{-1} in Raman spectrum and at 1715 cm^{-1} (DFT) is assigned as the C=O stretching mode. The deformation modes of C=O are assigned at 765 cm^{-1} in the IR spectrum, 767 cm^{-1} in the Raman spectrum and at 761, 717 cm^{-1} theoretically. The C–O–C stretching vibrations are expected in the regions 1200–1100 cm^{-1} (asymmetric) and 1050–950 cm^{-1} (symmetric) [43,47]. The skeletal deformation modes of C–O–C can be found in the region $320 \pm 50 \text{ cm}^{-1}$ [43]. As expected the asymmetric C–O–C vibration is assigned at 1103 cm^{-1} in the IR spectrum with DFT value at 1105 cm^{-1} . The symmetric C–O–C stretching vibration is assigned at 1069 cm^{-1} theoretically for the title compound [48]. The deformation modes of C–O–C are reported at 604, 606 and 287 cm^{-1} experimentally [49]. Mary et al. reported the C–O–C stretching modes at 1101, 1099 (experimentally) and at 1102, 942, 940 cm^{-1} theoretically [50,51].

Louren et al. [52] reported a value at 1220 cm^{-1} for $\nu_{\text{C}}\text{–N}$ for poly aniline. In the case of aromatic amines a strong C–N stretching

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