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# New luminescent 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile: Synthesis, crystal structure, DFT and photophysical studies

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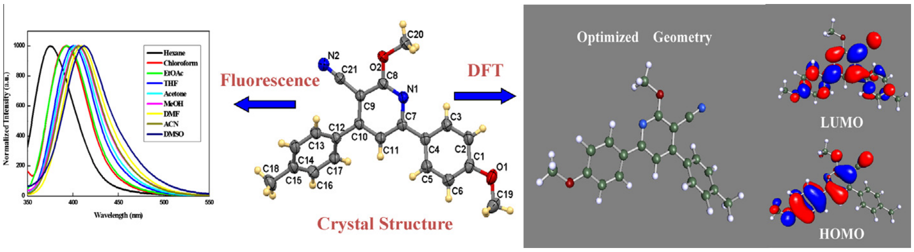
## HIGHLIGHTS

- A new D–A type 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**) compounds was designed and synthesized.
- Its crystal structure analysis confirms the presence of non-conventional intermolecular H-bonds.
- It exhibits positive solvatochromic behaviour with the variation of solvent systems.
- The photophysical studies reveal that the compound is good blue emissive material.
- DFT calculations were performed to obtain optimized geometry and theoretical IR stretching vibrations.

## GRAPHICAL ABSTRACT



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## ABSTRACT

In the current communication, we report the synthesis, spectroscopic, crystal structure, DFT and photophysical studies of a new nicotinonitrile derivative, viz. 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**) as a potential blue light emitting material. The compound **2** was synthesized in good yield via a simple route. The acquired spectral and elemental analysis data were in consistent with the chemical structure of **2**. The single crystal study further confirms its three dimensional structure, molecular shape, and nature of short contacts. Its DFT calculations reveal that compound **2** possesses a non-planar structure and its theoretical IR spectral data are found to be in accordance with experimental values. In addition, its UV–visible and fluorescence spectral measurements prove that the compound exhibits good absorption and fluorescence properties. Also, it shows positive solvatochromic effect when the solvent polarity was varied from non-polar to polar.

## Introduction

In the recent years, there has been a considerable attention among the researchers to synthesize and develop new π-conjugated materials displaying promising luminescent properties. Thus, search for novel luminescent compounds is important for their applications in organic light emitting diodes (OLEDs), fluorescent probes and fluorescent sensors [1,2]. For such applications, the luminescent properties of the materials can be readily tuned by structural modifications to attain required electronic properties. Obviously, on the basis of donor–acceptor (DA) concept, one can develop materials with unusual electrochromic, photochromic, luminescent or nonlinear optical properties by the incorporation of aromatic or heteroaromatic ring containing required electronic properties [3–6].

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**Table 1**
Crystal and structure refinement data for compound (**2**).

| Compound | **2** |
|---|---|
| Formula | $C_{21}H_{18}N_2O_2$ |
| Formula weight | 330.38 |
| CCDC number | 933190 |
| Temperature (K) | 296 (2) |
| Crystal form | Block |
| Colour | Yellow |
| Crystal system | Monoclinic |
| Space group | $P2_1/c$ |
| $a$ (Å) | 7.9324(2) |
| $b$ (Å) | 14.7056(5) |
| $c$ (Å) | 14.7951(5) |
| $\alpha$ (°) | 90 |
| $\beta$ (°) | 97.340(2) |
| $\gamma$ (°) | 90 |
| Volume (Å$^3$) | 97.340(2) |
| $Z$ | 4 |
| Density (g cm$^{-3}$) | 1.282 |
| $\mu$ (mm$^{-1}$) | 0.083 |
| F (000) | 696 |
| $h_{\text{min, max}}$ | −9,9 |
| $k_{\text{min, max}}$ | −18,17 |
| $l_{\text{min, max}}$ | −18,18 |
| Reflections collected | 3370 |
| Independent reflections | 2572 |
| $R_{\text{\_all}}$, $R_{\text{\_obs}}$ | 0.0579, 0.046 |
| $wR_{2\text{\_all}}$, $wR_{2\text{\_obs}}$ | 0.1291, 0.1182 |
| $\Delta\rho_{\text{min, max}}$ (e Å$^{-3}$) | −0.175, 0.222 |
| GOOF | 1.073 |

Pyridine is an interesting stable n-type heterocyclic system, which has attracted attention of many researchers for the design of new conjugated materials [7–16]. In addition, since pyridine is a highly electron-deficient heterocycle, it imparts good electron-transporting ability and brings an excellent optical properties, when it is present in donor and acceptor (DA) type conjugated systems. Further, field of pyridine has been of much interest owing to its high thermal as well as chemical stability. In effect, the presence of highly electron withdrawing nitrile (CN) substituent on the pyridine ring can further promote its electron-transporting nature [17]. In view of the observed fact that cyanopyridine is an attractive molecule with good electron transporting and photophysical properties, many of its derivatives were shown to possess good thermal and photochemical stability [18], high luminescence efficiency and novel optoelectronic properties [18]. Also, it was reported that insertion of an electron withdrawing cyanopyridine ring in a DA type molecular network lowers its band gap [17]. Against this background, Bagley et al. synthesized various cyanopyridine derivatives bearing easily-interchangeable electron-donating and electron-accepting groups, based on DA concept and investigated their photoemissive properties [19]. Interestingly, many cyanopyridine derivatives were found to possess good tuneable photophysical behaviour and excellent quantum yields.

Motivated by the above findings, and keeping in view of developing new cyanopyridine based luminescent materials, we have designed a new DA type compound, viz. 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**). In the new design, 2-methoxy-3-cyanopyridine acts as an electron deficient luminescent core (acceptor) and two substituents, viz. 4-methylphenyl and 4-methoxyphenyl groups attached to 2-methoxy-3-cyanopyridine core, act as electron donor moieties, leading to a good donor–acceptor networking. The newly designed compound **2** was synthesized from 1-(4-methoxy-phenyl)-3-*p*-tolyl-propenone (**1**) by reacting it with malononitrile in basic medium. Its structure was established using $^1$H NMR, FTIR, mass spectral as well as elemental analyses and its photophysical properties were investigated by UV–visible, and fluorescence spectroscopy. Also, the solvatochromic behaviour of the compound was studied in various solvent systems. Further, its 3-D structure, shape and nature of short contacts were investigated by single crystal X-ray study. Finally, its DFT calculations were carried out to obtain optimized geometry and theoretical IR stretching vibrations.

## Experimental details

### *Materials and measurements*

The infrared spectrum of compound **2** was recorded on a Nicolet Avatar 5700 FTIR (Thermo Electron Corporation). UV–visible and fluorescence spectra were taken in GBC Cintra 101 and Perkin Elmer LS55 fluorescence spectrophotometers in different non-polar and polar organic solvents. $^1$H NMR spectrum was recorded on a Bruker Avance DPX spectrometer at 300 MHz using DMSO-$d_6$ as the solvent with Tetramethylsilane (TMS) as internal standard, and data are reported in the order: chemical shift (ppm), number of protons, multiplicity (s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet; br, broad), approximate coupling constant ($J$) in hertz, and assignment of a signal. Mass spectrum was recorded on Agilent technologies LC/MSD Trap XCD mass spectrometry. An elemental analysis was performed on a Flash EA1112 CHNS analyser (Thermo Electron Corporation). Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel plates (Merck 60 Kieselgel F 254) and visualised with UV light. DFT calculations were carried out by using Turbomole software package.

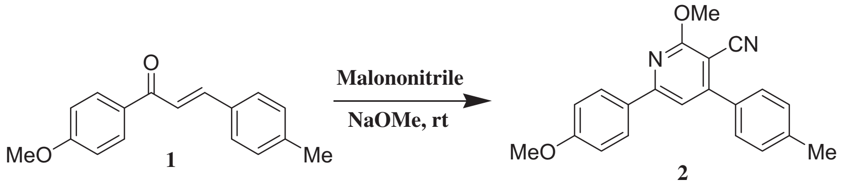
### *Synthesis*

#### *1-(4-Methoxy-phenyl)-3-p-tolyl-propenone (**1**)*

The 4-methoxyacetophenone (1 equivalent) and 4-methylbenzaldehyde (1 equivalent) were taken in 5 mL of ethanol. To this 1 mL of aqueous potassium hydroxide (1.2 equivalents) solution was added slowly. Reaction mixture was then stirred at room temperature for 4 h. The precipitated product was filtered, washed with water and recrystallized from methanol. White solid, yield 92%, m.p. 197–198 °C. IR (ATR, cm$^{-1}$): 2917, 2841, 1651, 1253, 1019, 804. Anal. Calcd. For. $C_{17}H_{16}O_2$: C, 80.93; H, 6.39; Found: C. 81.09; H. 6.44.

#### *2-Methoxy-6-(4-methoxy-phenyl)-4-p-tolyl-nicotinonitrile (**2**)*

1-(4-Methoxy-phenyl)-3-*p*-tolyl-propenone (**1**) (1 equivalent) was added slowly to a freshly prepared solution of sodium



**Scheme 1.** Synthesis of 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile.

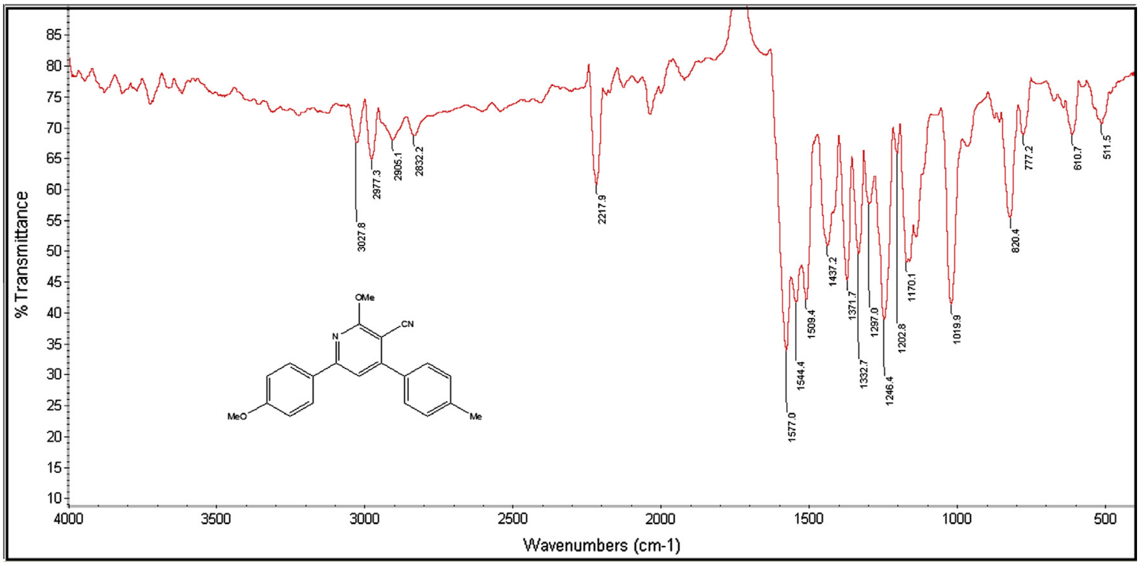


**Fig. 1.** FTIR spectrum of compound **2**.

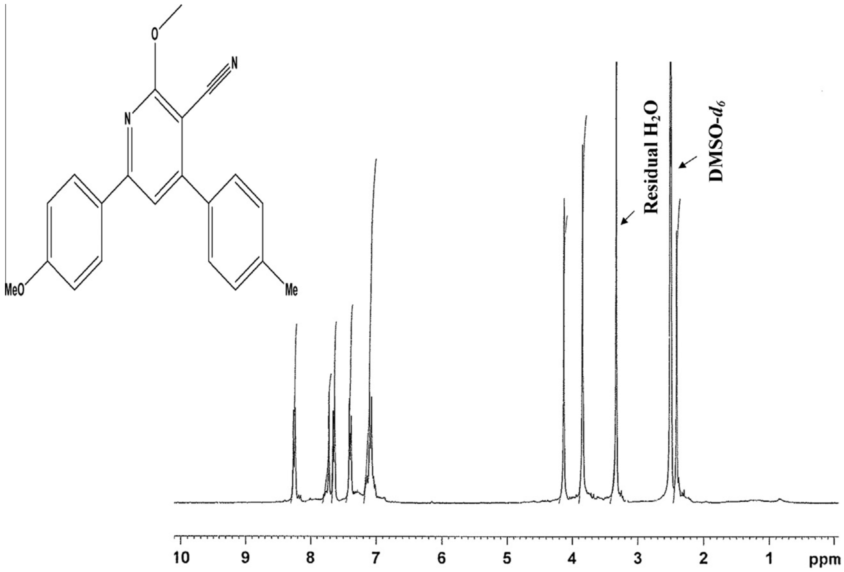


**Fig. 2.** $^1$H NMR spectrum of compound **2** in DMSO-$d_6$ (300 MHz).

methoxide (20 mmol of sodium in 10 mL of methanol) while stirring. Malononitrile (1.1equivalent) was then added with continuous stirring at room temperature until the precipitate separates out. The solid separated was collected by filtration, washed with methanol and recrystallized from chloroform. Yellow solid, yield 76%, m.p. 188–189 °C. $^1$H NMR (300 MHz, DMSO-$d_6$) δ (ppm) 8.24 (*d*, *J* = 9 Hz, 2H, Ar—H), 7.72 (s, 1H, Ar—H (Pyridine)), 7.64 (*d*, *J* = 9 Hz, 2H, Ar—H), 7.39 (*d*, *J* = 9 Hz, 2H, Ar—H), 7.08(*d*, *J* = 9 Hz, 2H, Ar—H), 4.13 (s, 3H, —OCH$_3$, Pyridine), 3.99 (s, 3H, —OCH$_3$, Phenyl), 2.41 (s, 3H, —CH$_3$, Phenyl). LC/MS (*m*/*z*): found, 331.3 ([M + H]$^+$); Calcd. for $C_{21}H_{19}N_2O_2$, 331.3. IR (ATR, cm$^{-1}$): 2948, 2856, 2218, 1543, 1445, 1014, 822. Anal. Calcd. For $C_{21}H_{18}N_2O_2$: C, 76.34; H, 5.49; N, 8.48; Found: C. 76.18; H. 5.8; N.8.43.

### *Structure determination and refinement*

A single crystal of dimension 0.25 × 0.23 × 0.20 mm$^3$ was grown by dissolving the 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**) in chloroform at room temperature, followed by slow evaporation of solvent through a parafilm plastic containing pinholes. A crystal of suitable size was mounted using a Mitigen micromount, and single-crystal data collection was done on a Bruker Smart X2S bench-top diffractometer equipped with a micro-focus Mo Kα radiation (λ = 0.71073) at room temperature [20]. The machine was operated at 50 kV and 1 mA. Data reduction was performed using SAINTPLUS. Scaling, absorption correction was done using SADABS, all embedded in the Apex2 software suite [20]. The crystal structure was solved by direct methods using XS and the structure refinement was done using XL in the SHELXTL package [21]. The position and thermal parameters of all the non-hydrogen atoms were refined. The hydrogen's were fixed in geometrically calculated positions and refined isotropically. The ORTEP diagrams and packing diagrams were created using Mercury 3.0 and POV ray. Crystal and experimental data for compound **2** are listed in Table 1. Its molecular structure is shown in Scheme 1.

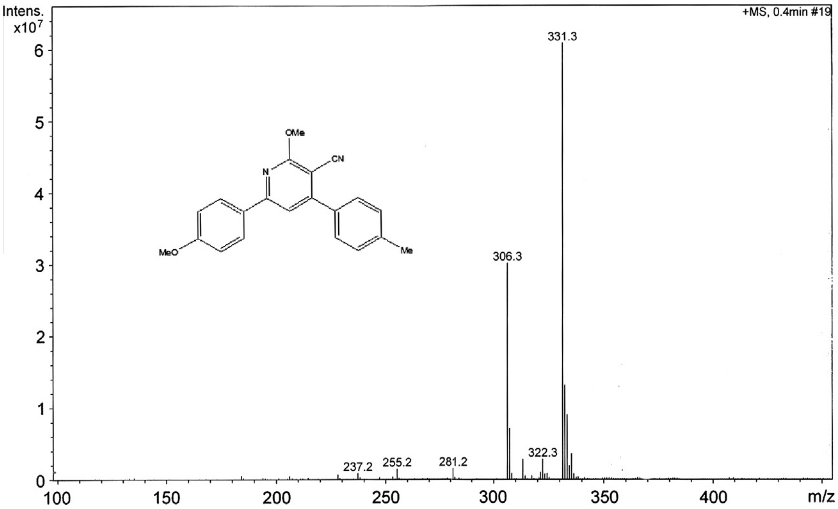


**Fig. 3.** Mass spectrum of compound **2**.

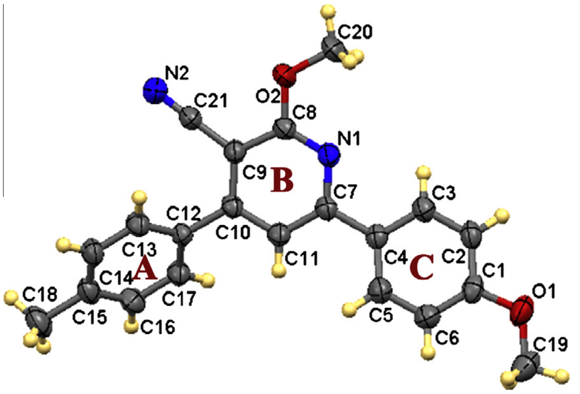


**Fig. 4.** ORTEP diagram of 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**) with numbering scheme (here 'A', 'B', and 'C' indicate 4-methylphenyl-, pyridyl- and 4-methoxyphenyl-rings, respectively).

## Results and discussion

### *Synthesis*

The synthetic rout for the preparation of new compound **2** is depicted in Scheme 1. The compound **2** was obtained in good yield when 1-(4-methoxy-phenyl)-3-*p*-tolyl-propenone (**1**) was treated with malononitrile at room temperature in presence of sodium methoxide as catalyst. Further, its chemical structure was confirmed by using FTIR, $^1$H NMR, mass spectral and elemental analyses. Finally, its three dimensional structure was determined with the help of single crystal X-ray diffractometer.

### *Spectroscopic properties*

The structure of compound **2** was established by FTIR, $^1$H NMR and mass spectroscopic techniques. Its FTIR spectrum shows two strong IR absorption bands at 2948 and 2856 cm$^{-1}$ that correspond to asymmetric and symmetric C—H stretching vibrations of methoxy group (Fig. 1). Further, a strong IR absorption band at 2218 cm$^{-1}$ indicates the presence of cyano group in its molecular structure. Also, the absorption band at 1543 cm$^{-1}$ accounts for C≡N stretching, confirming the formation of pyridine ring. The compound **2**, in its $^1$H NMR spectrum (Fig. 2) shows unique resonances at 8.24, 7.64, 7.39 and 7.08 ppm for the protons of aromatic moieties. The appearance of a singlet at 7.72 ppm is for one proton of aromatic pyridine ring. Also, three types of singlet were observed; one singlet at 4.13 ppm for three protons -OMe of pyridine, a second singlet resonated at 3.99 ppm for three protons -OMe of phenyl, and a third singlet appeared at 2.41 ppm for three protons of -Me of phenyl, confirm the formation of compound **2**. Finally, its structure was confirmed by mass spectral analysis and the experimentally obtained mass 331.3 (M + H)$^+$ is in agreement with that of the calculated mass (Fig. 3).

**Table 2**
Selected bond lengths (Å) and angles (°) for Compound **2**.

| | | | |
|---|---|---|---|
| *Bond lengths (Å)* | | | |
| O1—C1 | 1.3660(19) | C41—C7 | 1.475(2) |
| O11—C19 | 1.419(2) | C51—C6 | 1.378(2) |
| O21—C8 | 1.3433(18) | C81—C9 | 1.409(2) |
| O21—C20 | 1.4323(19) | C91—C21 | 1.425(2) |
| N11—C7 | 1.3549(18) | C121—C13 | 1.390(2) |
| N11—C8 | 1.3129(19) | C131—C14 | 1.382(2) |
| N21—C21 | 1.141(2) | C151—C18 | 1.508(2) |
| C11—C2 | 1.380(2) | C161—C17 | 1.380(2) |
| C11—C6 | 1.381(2) | C171—H17 | 0.9300 |
| C21—C3 | 1.376(2) | C201—H20C | 0.9600 |
| *Bond angles (°)* | | | |
| C11—O11—C19 | 117.64(13) | C81—C91—C10 | 118.07(13) |
| C81—O21—C20 | 118.13(13) | C81—C91—C21 | 118.76(13) |
| C71—N11—C8 | 117.85(12) | C111—C101—C12 | 120.74(12) |
| O11—C11—C2 | 115.99(13) | C101—C121—C13 | 122.45(12) |
| O11—C11—C6 | 124.72(14) | C131—C121—C17 | 118.19(13) |
| C21—C11—C6 | 119.30(14) | C131—C141—C15 | 121.91(14) |
| C11—C21—C3 | 120.43(14) | N21—C211—C9 | 179.19(17) |
| N11—C71—C4 | 115.93(12) | C141—C151—C16 | 117.47(14) |
| N11—C71—C11 | 121.50(12) | C91—C101—C11 | 117.19(12) |
| O21—C81—N1 | 120.67(13) | C101—C91—C21 | 123.16(12) |
| O21—C81—C9 | 114.96(13) | C71—C111—C10 | 121.02(13) |
| N11—C81—C9 | 124.37(13) | O21—C201—H20A | 109.00 |
| C31—C21—H2 | 120.00 | C91—C101—C12 | 122.06(12) |
| C21—C31—H3 | 119.00 | H20B1—C201—H20C | 109.00 |
| C21—C31—C4 | 121.54(15) | C101—C121—C17 | 119.36(12) |
| C31—C41—C5 | 116.81(14) | C121—C131—C14 | 120.14(14) |
| C31—C41—C7 | 120.81(13) | C141—C151—C18 | 121.14(15) |
| C41—C51—C6 | 122.26(15) | C41—C31—H3 | 119.00 |
| C41—C71—C11 | 122.57(13) | H18A1—C181—H18C | 109.00 |

### *Crystal structure of 2-methoxy-6-(4-methoxy-phenyl)-4-p-tolyl-nicotinonitrile (**2**)*

Single-crystal X-ray study reveals that compound (**2**) crystallizes in monoclinic space group $P2_1/c$ with cell parameters are

**Table 3**
Intra and intermolecular C1—H···N interactions in the crystal structure of compound **2**.

| Compound | D1—H···A | D—H/Å | H···A/Å | D···A/Å | ∠ D—H···A/° | Symmetry |
|---|---|---|---|---|---|---|
| 2 | C3—H3···N1 | 0.930 | 2.480 | 2.798(2) | 100.00 | $x, y, z$ |
| | C17—H17···N2 | 0.930 | 2.520 | 3.383(2) | 154.00 | $-x+1, y+1/2, -z+1/2$ |
| | C20—H20A···N2 | 0.960 | 2.591 | 3.116(2) | 115.00 | $x, -y+1/2, z+1/2$ |

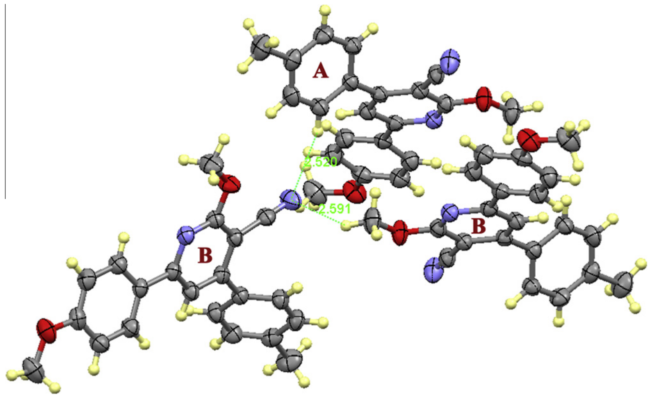


**Fig. 5.** Crystal structure of compound **2** depicting C—H···N intermolecular interactions.

$a = 7.9324(2)$ (Å), $b = 14.7056(5)$ Å, $c = 14.7951(5)$ Å, $V = 97.340(2)$ Å, $Z = 4$ (Table 1). Fig. 4 shows the labelled ORTEP diagram of the compound. In the figure, the three rings are distinguished by labelling with alphabets 'A', 'B', and 'C'. This labelling is useful for explaining the intermolecular interactions in the later stages. However, from the X-ray analysis data, it is evident that the molecule is not planar and but distorted. Interestingly, the 4-methylphenyl ring substituted at the position-4 of the central pyridine ring makes a torsion angle χ[C(9), C(10), C(12), C(13)] of −47.65° with the central pyridine ring, while the other 4-methoxyphenyl ring, substituted at the position-6, forms a torsion angle χ[N(1), C(7), C(4), C(3)] of −14.97°, which is less than the previous one. Further, bond length and bond angle values are all within the expected range, as shown in Table 2. From the data of Table 2, it is observed that C—C, C—N and C—O bond length values in the three ring system are possessing partial double bond character, which clearly indicates that the π-electrons in the three ring system are involved in delocalization.

Further, it is interesting to note that the structure is stabilized by intra-molecular C3—H3···N1 hydrogen bond (Table 3), besides two kinds of intermolecular, *i.e.* C17—H17···N2 (formed by the nitrogen atom of cyano group at position-3 on 'B' ring of one molecule and the nearby aromatic proton of 'A' ring of other molecule) and C20—H20A···N2 (formed by the nitrogen atom of cyano group at position-3 on 'B' ring of one molecule and the nearby methoxy protons at position-2 of 'B' ring of other molecule) hydrogen bonds and their values are tabulated in Table 3. Packing diagram, depicting C—H···N intermolecular interactions and their values is shown in Fig. 5. Also, the crystal assembly of **2**, as shown in Fig. 6(a) contains C—H···π and π···π short contacts, which is responsible for the formation of dimers in its structure. In the dimer, the methoxy group of 'B' ring is interacting with the π cloud of the other 'B' ring and vice versa (C(20)—H···CgB = 3.159 Å, where CgB is the centroid of 'B' ring). In fact, the contribution of π···π interactions in crystal assembly is noteworthy. In the crystal assembly of **2**, π-electron cloud of 'B' ring is involving face–face to interactions with the π-electron cloud of 'C' ring of the nearby molecule with a separation of 3.753 Å (Fig. 6(b)).

**Table 4**
Dielectric constant, photophysical properties, and Stoke shift values of compound **2** in different solvents.

| Solvent | Dielectric constant (25 °C) | $\lambda_{abs}$ (nm) | $\lambda_{em}$ (nm) | Stoke shift (nm) |
|---|---|---|---|---|
| Hexane | 1.87 | 334 | 375 | 41 |
| Chloroform | 4.80 | 341 | 392 | 51 |
| Ethyl acetate | 6.02 | 335 | 394 | 59 |
| Tetrahydrofuran | 7.58 | 339 | 400 | 61 |
| Acetone | 20.70 | 340 | 403 | 63 |
| Methanol | 32.70 | 338 | 405 | 67 |
| Dimethylformamide | 36.71 | 343 | 409 | 66 |
| Acetonitrile | 37.5 | 338 | 406 | 68 |
| Dimethyl sulphoxide | 46.68 | 344 | 412 | 70 |

## *Photophysical properties*

UV–visible absorption ($10^{-5}$ M) and fluorescence emission ($10^{-6}$ M) spectra were recorded for compound **2** in hexane, chloroform, tetrahydrofuran (THF), acetone, methanol (MeOH), dimethylformamide (DMF) and dimethyl sulfoxide (DMSO), in order to explore its photophysical properties and its molecular interactions with different non-polar and polar organic solvents. These solvents were selected on the basis of increasing order of their dielectric constant values. The absorption and fluorescence spectral data along with the dielectric constants of solvents are tabulated in Table 4. Figs. 7 and 8 show the UV–visible absorption and

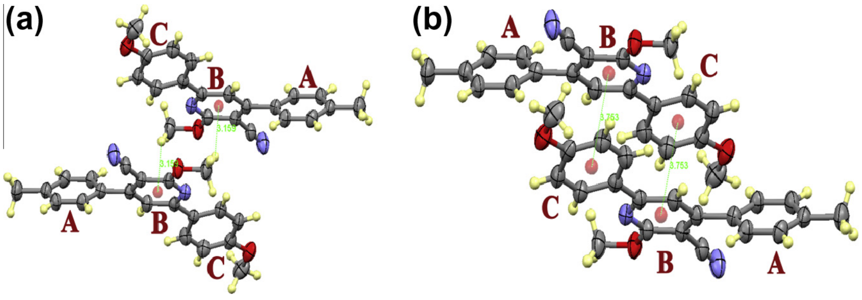


**Fig. 6.** Crystal structure of compound **2** representing (a) C—H···π, and (b) π···π short contacts.

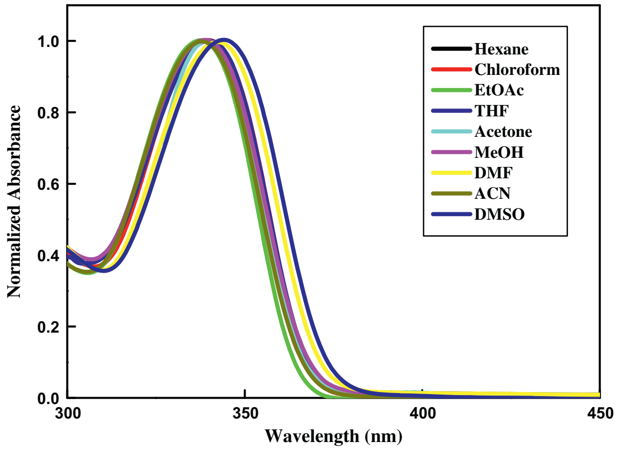


**Fig. 7.** UV–visible spectra of compound **2** in different solvents ($10^{-5}$ M).

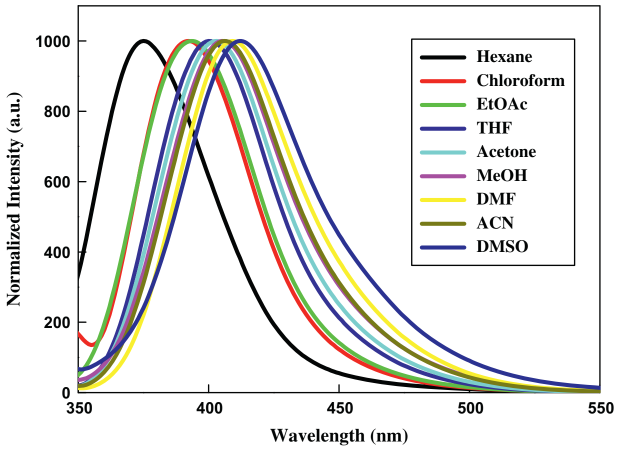


**Fig. 8.** Fluorescence spectra of compound **2** in different solvents ($10^{-6}$ M).

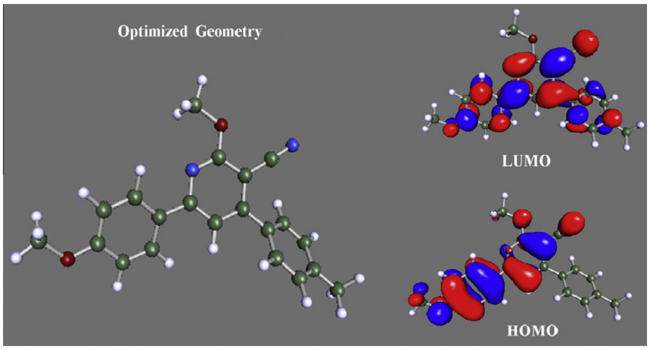


**Fig. 9.** Optimized geometric structure and frontier molecular orbital diagram of **2**.

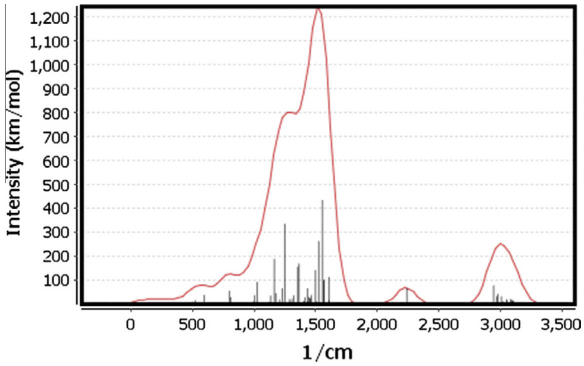


**Fig. 10.** Theoretically obtained FTIR spectrum of compound **2**.

fluorescence spectra in different solvents, respectively. In its absorption spectra, the compound showed one intense absorption band in UV region both in non-polar and polar solvents and the position of the absorption band lies in between 301 and 344 nm. These absorption bands were attributed to a $\pi \rightarrow \pi^*$ electronic transition occurring in it. Table 3 shows that the absorption band ($\lambda_{abs}$) has shifted to a longer wavelength *i.e.* from 301 nm to 343 nm, with the increase in solvent polarity.

In its fluorescence spectra, an intense blue emission band appearing between 375 nm (hexane) and 412 nm (DMSO) has been observed under their excitation wavelengths. Similar to absorption spectra, the fluorescence spectra of compound **2** showed significantly larger solvatochromic effect. There was an appreciable change in emission maxima with the variation of solvent systems from non-polar (hexane) to highly polar (DMSO) solvent with Stokes shift of 50–75 nm. Also, there was a considerable red shifting of emission bands in the fluorescence spectrum, which is attributed to the enhanced interaction between fluorescent molecule and polar solvent. However, in case of acetonitrile no such observation was made due to its weak interactions with the chromophore. Also, the material was found to be blue fluorescent under UV lamp ($\lambda$ = 365 nm). From the results of photophysical studies it can be concluded that compound **2** is a promising material for its applications in organo-electronic devices.

### *Theoretical study*

The geometry optimization and theoretical IR stretching vibrations of molecule **2** were evaluated by density functional theory (DFT) calculations at the def-TZVP level [22–30]. The optimized structure and the frontier molecular orbital profile of **2** are shown in Fig. 9. The study suggests that the compound **2** possesses distorted molecular structure, wherein 4-methylphenyl ring substituted at the position-4 of the central pyridine ring possesses a non-planar arrangement, while 4-methoxyphenyl ring substituted at position-6 of central pyridine ring is having nearly planar arrangement. This observation may be attributed to the interaction exerted by the —CN functional group at position-3 of pyridine ring. Therefore, the HOMO is mainly localized on the 4-methoxyphenyl and central pyridine ring, while the LUMO is delocalized along the whole molecule, indicating that the molecule possesses better intra-molecular charge transfer ability. Fig. 10 shows the calculated IR-spectrum of **2**. Here, the peaks within the range of 1600–650 $cm^{-1}$ are attributed to the aromatic C—C and C—N bond vibrations. Further, the peaks centred at 2220 $cm^{-1}$ and 3000 $cm^{-1}$ are due to the stretching vibrations of cyano and aromatic C—H groups, respectively. Thus, theoretical calculated IR stretching vibrations for the compound **2** is in accordance with that of the experimentally obtained results (as shown in Fig. 1).

## Conclusion

In the present study, a new luminescent material, viz. 2-methoxy-6-(4-methoxy-phenyl)-4-*p*-tolyl-nicotinonitrile (**2**) was successfully synthesized using a simple route and was well-characterised with spectral techniques. Its single crystal and DFT study revealed the existence of non-planar structure. Theoretically calculated IR stretching vibrations are in well agreement with that of the experimental results. In addition, its photophysical measurements indicate that it is a good absorbent and fluorescent material with positive solvatochromic behaviour in both polar and nonpolar solvents. From the results it can be concluded that compound **2** is a promising candidate for its applications in organo-electronic devices.

## Supplementary material

Crystallographic data for the structure reported in this article have been deposited with the Cambridge Crystallographic Data Centre with the deposition number 933190. A copy of the data can be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336 033; E-mail: deposit@ccdc.cam. ac.uk or www.ccdc.cam.ac.uk).

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