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ORIGINAL ARTICLE

Synthesis, Spectroscopic Characterization and DFT/TD-DFT Calculations of new Fluorescent Derivatives of Imidazo[4′,5′:3,4] Benzo[*c*]Isoxazole

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Abstract An increasingly wide variety of fluorescent compounds is used in biotechnology, genomics, immunoassays, array technologies, imaging, and drug discovery. Therefore, synthesis of fluorophores with novel structural features can be interesting and useful in various fields. In this paper, four new fluorescent heterocyclic compounds with high quantum yields are introduced. These new fluorophores are synthesized in moderate to high yields *via* regioselective nitration of 3-alkyl-8-(4-chlorophenyl)-3 *H*-imidazo[4′,5′:3,4]benzo[*c*]-isoxazoles. The latter compounds are obtained from the reaction of 1-alkyl-5-nitro-1 *H*-benzoimidazoles with (4-chlorophenyl)acetonitrile in basic MeOH solution. Physical spectral (UV-vis, IR, ^{1}HNMR, ^{13}C NMR, NOESY and fluorescence) and analytical data have established the structures of synthesized compounds. The fluorescence properties of new fluorescent heterocyclic compounds are studied. The fluorescence of all compounds is very intense and fluorescence quantum yields are high (> 0.52). Density functional theory (DFT) calculations are performed to provide the optimized geometries, relevant frontier orbitals and the prediction of ^{1}H NMR chemical shifts for confirming the exact structure of fluorescent compounds. Calculated electronic absorption spectra were also obtained by time-dependent density functional theory (TD-DFT) method.

Keywords 3 *H*-Imidazo[4′,5′:3,4]benzo[*c*]isoxazole · Density functional theory · NOESY · Fluorescence · Emission and absorption spectra

Introduction

The recent explosion in new fluorescence applications is accelerating the pace of research and development in basic and applied life sciences, including genomics, proteomics, bioengineering, medical diagnosis and industrial microbiology. Fluorescent heterocyclic compounds are of vast interest as useful materials in the emitters of electroluminescence devices and in the molecular probes used for biochemical research, as well as in the traditional textile and polymer fields [1–7]. They are useful materials in the search for new biologically active compounds and diagnostic methods [8]. Fluorescent chromophores are usually known to have planar and rigid pi-conjugated systems, and many fluorescent chromophores are based on rigid ring systems. Naturally occurring substituted imidazoles, as well as synthetic derivatives thereof, exhibit wide ranges of biological activities and optical applications such as fluorescence compounds, dyes, and TPA (Two-photon absorption) materials [9–12] making them attractive compounds for organic chemists. Also, many commercial fluorescent brighteners for application to synthetic fibers contain an imidazole moiety [13]. On the other hand, isoxazoles and fused isoxazoles have found continuing application in medicinal chemistry, several examples of which have advanced to general medical practice. For example, benzo[*c*]isoxazole derivatives are prescribed as antipsychotic risperidone drugs [14] and play a key role in many organic reactions [15]. A literature survey disclosed that there are only a few

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examples of isoxazoles or benzo[*c*]isoxazoles with fluorescence properties. A combination of the benzo[*c*]-isoxazole moiety with the imidazole nucleus may enhance optical and biological properties. Based on these aspects, in current work, we synthesized some imidazo[4′,5′:3,4]benzo[*c*]isoxazoles with high fluorescence properties as new fluorophores. Spectroscopic characterization of these compounds were studied and the structure of the major products was established by NOESY (Nuclear Overhauser Effect Spectroscopy) experiment and explained with DFT and TD-DFT calculations by using the B3LYP hybrid functional and the 6–311++G(d,p) basis set.

Experimental

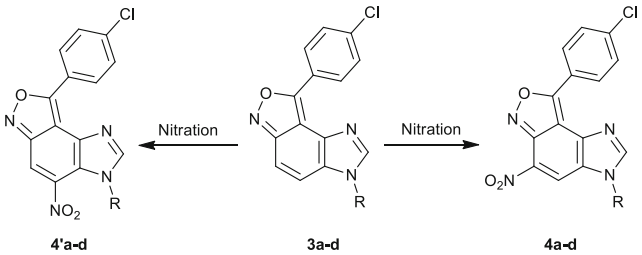
Equipment and Materials

Melting points were measured on an Electrothermaltype-9100 melting-point apparatus. The FT-IR (as KBr discs) spectra were obtained on a Tensor 27 spectrometer and only noteworthy absorptions are listed. The ^{13}C NMR (100 MHz), ^{1} H NMR (400 MHz) and NOESY spectra were recorded on a Bruker Avance DRX-400 spectrometer. Chemical shifts are reported in ppm downfield from TMS as internal standard; coupling constant *J* is given in Hz. The mass spectra were recorded on a Varian Mat, CH-7 at 70 eV. Elemental analysis was performed on a Thermo Finnigan Flash EA microanalyzer. Absorption and fluorescence spectra were recorded on Varian 50-bio UV-Visible spectrophotometer and Varian Cary Eclipse spectrofluorophotometer. UV–vis and fluorescence scans were recorded from 200 to 1000 nm. All measurements were carried out at room temperature. Compounds **1a–d** [16] and **3a–d** [17] were obtained according to the published methods. Other reagents were commercially available.

Computational Methods

DFT calculations were performed with the Gaussian 98 software package [18] by using the B3LYP hybrid functional [19] and the 6–311 + G(d,p) basis set. Firstly, geometry of the compounds 4a and 4a' were fully optimized in the chloroform solution. The optimized geometries were confirmed to have no imaginary frequency. Then, their optimized geometries were used for frequency calculations.

Here, one of self-consistent reaction field methods, the sophisticated Polarized Continuum Model (PCM) [20] has been used for investigation of the solvent effects. The PCM calculations have been performed in the chloroform solution and the zero-point corrections were considered to obtain energies. Based on the optimized geometries and using time-dependent density functional theory (TD-DFT) [21–23] methods, the electronic spectra of the compounds **4a** and **4a'** were predicted.

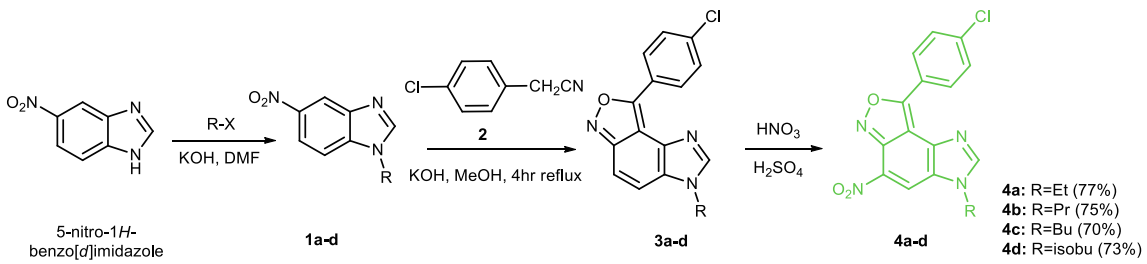


Scheme 2 Two possible structures for the nitration of **3a–d**

General Procedure for the Synthesis of 4a–d from 3a–d

Nitric acid (1 ml) was added with stirring over half an hour period to a solution of **3a–d** (20 mmol) in concentrated sulfuric acid (4 ml) maintained at 0–5 °C. After the addition was completed, the mixture was allowed to warm to room temperature with stirring for 30 min. After pouring this mixture into crushed ice and water (200 ml), the solid that precipitated was removed by filtration, was washed with water, and dried to give crude **4a–d**.

8-(4-Chlorophenyl)-3-ethyl-5-nitro-3 H-imidazo[4′,5′:3,4] benzo[*c*]isoxazoles (**4a**). Compound **4a** was passed through silica-gel column (*n*-hexane-EtOAc 2:1) to give **4a** as a shiny yellow powder. Yield (77 %); mp 277–279 °C. ^{1} H NMR ($CDCl_3$): δ 1.69 (t, J = 7.2 Hz, 3 H), 4.43 (q, J = 7.2 Hz, 2 H), 7.62 (d, J = 8.4 Hz, 2 H), 8.20 (s, 1 H), 8.74 (s, 1 H), 8.90 (d, J = 8.4 Hz, 2 H) ppm; ^{13}C NMR ($CDCl_3$): δ 16.0, 41.2, 109.8, 118.2, 125.6, 126.5, 129.4, 129.5, 132.2, 137.4,



Scheme 1 Synthesis of the new fluorophores **4a–d**

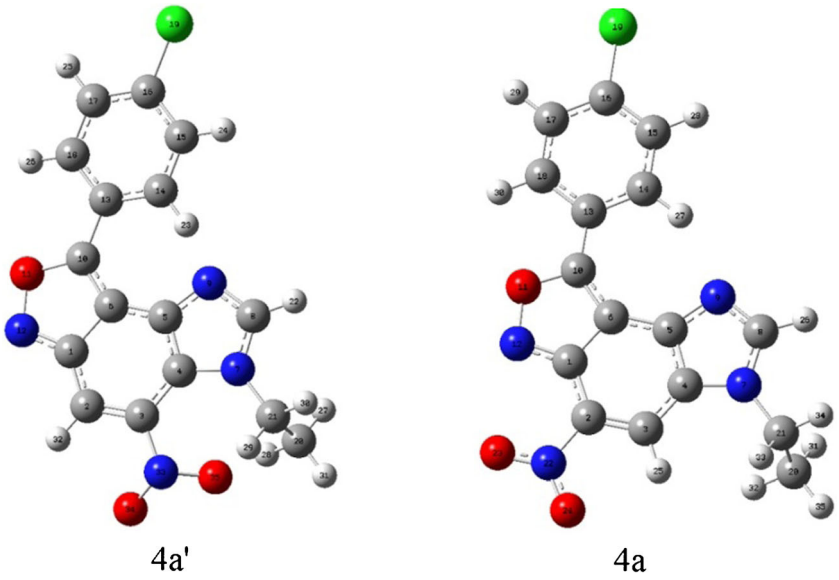


Fig. 1 Optimized geometries of the **4a** and **4a'**

140.4, 144.2, 151.0, 165.6 ppm. IR (KBr): 1358, 1542 cm^{-1} (NO_2), MS (m/z) 344 (M^++2). Anal. Calcd for $C_{16}H_{11}ClN_4O_3$ (342.7): C, 56.07; H, 3.23; N, 16.35. Found: C, 55.97; H, 3.20; N, 16.27.

8-(4-Chlorophenyl)-3-propyl-5-nitro-3 H-imidazo[4′,5′:3, 4] benzo[*c*]isoxazoles (**4b**). Compound **4b** was passed through silica-gel column (*n*-hexane-EtOAc 2:1) to give **4b** as a shiny yellow powder. Yield (75 %); mp 275–277 °C. ^{1} H NMR ($CDCl_3$): δ 1.07 (t, J = 7.3 Hz, 3 H), 1.90–2.02 (m, 2 H), 4.33 (t, J = 7.2 Hz, 2 H), 7.62 (d, J = 8.4 Hz, 2 H), 8.17 (s, 1 H), 8.71 (s, 1 H), 8.90 (d, J = 8.4 Hz, 2 H) ppm; ^{13}C NMR ($CDCl_3$): δ 12.2, 23.5, 53.8, 109.7, 117.8, 125.9, 126.3, 129.0, 129.9, 132.1, 137.9, 140.3, 144.5, 150.6, 165.4 ppm. IR (KBr): 1357, 1543 cm^{-1} (NO_2), MS (m/z) 358 (M^++2). Anal. Calcd for $C_{17}H_{13}ClN_4O_3$ (356.8): C, 57.23; H, 3.67; N, 15.70. Found: C, 57.11; H, 3.65; N, 15.83.

3-Butyl-8-(4-chlorophenyl)-5-nitro-3 H-imidazo[4′,5′:3,4] benzo[*c*]isoxazoles (**4c**). Compound **4c** was passed through silica-gel column (*n*-hexane-EtOAc 2:1) to give **4c** as a shiny yellow powder. Yield (70 %); mp 272–275 °C. ^{1} H NMR ($CDCl_3$): δ 0.93 (t, J = 7.2 Hz, 3 H), 1.40–1.48 (m, 2 H), 1.95–2.02 (m, 2 H), 4.37 (t, J = 7.2 Hz, 2 H), 7.62 (d, J = 8.4 Hz, 2 H), 8.17 (s, 1 H), 8.73 (s, 1 H), 8.90 (d, J = 8.4 Hz, 2 H) ppm; ^{13}C NMR ($CDCl_3$): δ 13.7, 21.3, 33.6, 54.2, 109.8, 117.9, 125.9, 126.4, 129.2, 130.4, 132.3, 138.3, 140.0, 144.7, 150.5, 165.3 ppm. IR (KBr): 1352, 1541 cm^{-1} (NO_2), MS (m/z) 372 (M^++2). Anal. Calcd for $C_{18}H_{15}ClN_4O_3$ (370.8): C, 58.31; H, 4.08; N, 15.11. Found: C, 58.21; H, 4.06; N, 14.97.

8-(4-Chlorophenyl)-3-isobutyl-5-nitro-3 H-imidazo[4′, 5′:3,4] benzo[*c*]isoxazoles (**4d**). Compound **4d** was passed through silica-gel column (*n*-hexane-EtOAc 2:1) to give **4d** as a shiny yellow powder. Yield (73 %); mp 269–271 °C. ^{1} H NMR ($CDCl_3$): δ 0.90 (d, J = 6.4 Hz, 6 H), 2.15–2.19 (m, 1 H), 4.32 (d, J = 7.2 Hz, 2 H), 7.62 (d, J = 8.4 Hz, 2 H), 8.16 (s, 1 H), 8.72 (s, 1 H), 8.90 (d, J = 8.4 Hz, 2 H) ppm; ^{13}C NMR ($CDCl_3$): δ 20.4, 29.8, 58.9, 109.9, 117.7, 125.5, 126.0, 128.7, 130.7, 132.2, 138.6, 140.3, 144.8, 150.7, 165.0 ppm. IR (KBr): 1355, 1541 cm^{-1} (NO2), MS (m/z) 372 (M^++2). Anal. Calcd for $C_{18}H_{15}ClN_4O3$ (370.8): C, 58.31; H, 4.08; N, 15.11. Found: C, 58.15; H, 4.06; N, 15.0.

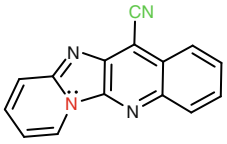
Table 1 Experimental and DFT calculated ^{1}H NMR chemical shifts of **4a** and **4a'**

Atom number (**4a'**)	Chemical shift		Atom number (**4a**)	Chemical shift	
	Calc.	Exp.		Calc.	Exp.
H24, H25	8.66	8.90	H28, H29	9.02	8.90
H32	8.27	8.75	H25	8.80	8.75
H22	8.01	8.21	H26	8.26	8.21
H23, H26	7.70	7.62	H27, H30	7.71	7.62

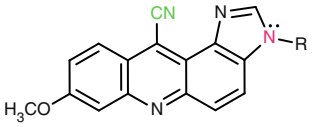
Synthesis of 8-(4-Chlorobenzoyl) -5-Ethyl-5 *H*-Imidazo[4′,5′:4,5]Benzo[1,2-*c*] [1, 2, 5] Oxadiazole 3-Oxide (5)

Compound **4a** (0.5 g) was heated 1 h under reflux in 10 ml of glacial acetic acid. The solution was cooled, and an equal volume of water was added. The precipitated solid was crystallized from EtOH as yellow needles (0.33 g, 65 %) mp > 300 °C (decomp). ^{1}H NMR ($CDCl_3$): δ 1.54 (t, J = 7.2 Hz, 3 H), 4.39 (q, J = 7.2 Hz, 2 H), 6.88 (s, 1 H), 8.12 (d, J = 8.7 Hz, 1 H), 8.32 (d, J = 8.7 Hz, 2 H) 8.41 (s, 1 H), ppm; ^{13}C NMR ($CDCl_3$): δ 15.7, 45.8, 104.6, 116.3, 128.4, 129.6, 130.0, 132.1, 132.8, 136.7, 145.5, 150.4, 159.8, 185.6 ppm. IR (KBr): 1685 cm^{-1} (C = O), MS (m/z)

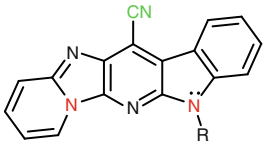
Scheme 3 Some recently synthesized fluorescent heterocyclic compounds containing donor sites (endocyclic N or S) and the CN group as an acceptor moiety



Pyrido[2',1':2,3] imidazo[4,5-b]quinoline-12-ylcyanides[23]



3-alkyl-8-methoxy-3*H*-imidazo[4,5-*a*] acridine-11-carbonitrile[24]



pyrido[1",2":1',2']imidazo[4',5':5,6] pyrido[2,3-b]indole[25]

344 (M^++2). Anal. Calcd for $C_{16}H_{11}ClN_4O_3$ (342.7): C, 56.07; H, 3.23; N, 16.35. Found: C, 55.95; H, 3.21; N, 16.49.

Results and Discussion

Synthesis and Structures of new Compounds 4a–d

As depicted in Scheme 1, to obtain the desired new fluorescent compounds, in the first place, the commercially available 5-nitro-1 *H*-benzimidazole was alkylated with different alkyl halides in KOH and DMF to give 1-alkyl-5-nitro-1 *H*-benzimidazoles (**1a–d**) at rt. [16]. Reaction of **1a–d** with (4-chlorophenyl)acetonitrile (**2**) in basic MeOH solution led to the formation of 3-alkyl-8-(4-chlorophenyl)-3 *H*-imidazo [4′, 5′:3,4] benzo[*c*]isoxazoles (**3a–d**) in excellent yields [17]. Finally, new 3-alkyl-8-(4-chlorophenyl)-5-nitro-3 *H*-imidazo [4′,5′:3,4]benzo[*c*]isoxazoles (**4a–d**) were synthesized by nitration of **3a–d** in moderate to high yields.

Structural assignments of new compounds **4a–d** were based upon their spectral and microanalytical (C, H and N) data. For example, in the aromatic region of the ^{1}H NMR spectrum of compound **4a** (Supporting Information), there are two doublet signals at δ 7.62 and 8.90 ppm attributed to four aromatic protons of 4-chlorophenyl ring and two singlet signals at δ 8.21 and 8.75 ppm assignable to two aromatic protons of imidazole and phenyl ring respectively. Also, there are 14 different carbon atoms in the ^{13}C NMR spectrum of compound **4a**. Moreover, the FT-IR spectrum of the 4a in KBr showed two absorption band at 1542 and 1358 cm^{-1} corresponding to the nitro group. All this evidence taken in conjunction with molecular ion peak at m/z 344 (M^++2) strongly support the structure of compound **4a**. However, these spectral characteristics are consistent with another possible structure which is isomeric with **4a** (Scheme 2).

In order to clarify the exact structure for the nitration of **3a–d**, after the compounds were passed through silica-gel column (*n*-hexane-EtOAc), we made a great attempt to obtain an appropriate single crystal of the products for crystallography in different solvents, but the obtained crystals were not suitable for X- ray crystallography. However, there are some convincing reasons that confirm that the **4a–d** are the major products for the nitration of **3a–d**. For example, electron release from the imidazole ring would make the C-5 position more susceptible to electrophilic attack than C-4. Furthermore the latter is also hindered by its proximity to the N-3 alkyl group.

In addition, **4a–d** intermediates have more resonance structures than **4'a–d** intermediates (Supporting Information) and this leads to the stability of **4a–d** intermediates and thus faster formation of **4a–d** compared to **4'a–d** products.

Also, DFT calculations at the level of B3LYP/6–311 + G(d, p) can help identify the structure of the main product. For this purpose, optimized geometries of compounds **4a** and **4a'** were obtained (Fig. 1) and then, DFT calculated chemical shifts (δ) of compounds **4a** and **4a'** were compared with the experimental values (Table 1). It can be induced from Table 1, the calculated chemical shifts (δ) of compound **4a** are more in agreement with the experimental values, confirming validity of the structure of compound **4a**. Selected structural parameters of **4a** and **4'a** can be found in Supporting Information.

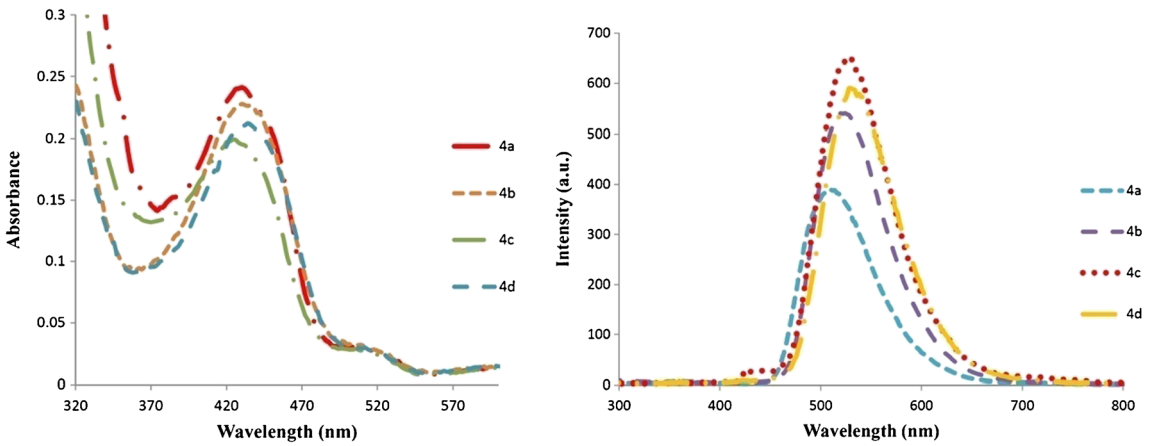


Fig. 2 Visible absorption (*left*) (5×10^{-5} mol L^{-1}) and emission spectra (*right*)) (2×10^{-6} mol L^{-1}) of compounds **4a–d** in chloroform solvent

Investigation on the photophysical properties of the nitrated compounds can also help further to confirm the exact structure. Recently, we have succeeded in synthesizing some new heterocyclic compounds which had fluorescent properties [24–26]. In these compounds, there are efficient intramolecular charge transfer (ICT) states from the donor sites (endocyclic N or S) to the CN group as an acceptor moiety (Scheme 3).

In the present study, there are endocyclic N and O as donor sites in compounds **3a–d** and these compounds are nitrated to obtain new fluorophore with an acceptor site (NO_2 group). Fortunately, new nitrated compounds have fluorescence emission at concentration of 2×10^{-6} mol L^{-1} in chloroform solvent (Fig. 2). The fluorescence excitation (λ_{ex}) wavelength at 425 nm (λ_{ex}/nm) was used for all of them. Their fluorescence quantum yields (Φ_F) were determined via comparison methods, using fluorescein as a standard sample in 0.1 M NaOH and MeOH solution [27]. Visible absorption spectra of nitrated compounds were also obtained in chloroform solvent at concentration of 5×10^{-5} mol L^{-1} (Fig. 2). Photophysical properties of nitrated compounds are presented in Table 2. As is shown in the table, extinction coefficients (ε) calculated as the slope of the plot of absorbance vs concentration are very high, and this is remarkable for optical properties of these compounds. Further, the fluorescence spectral properties (Table 2) of compounds **4a–d** are similar to each other and fluorescence intensity in compound **4c**, with a butyl group, was the highest.

The solvatochromic properties of **4a** in different solvents were also investigated (Table 3). The fluorescence absorption and emission spectra of **4a** in polar solvents undergo a relatively modest red shift. Increasing the solvent polarity stabilizes the ICT excited-state molecule relative to the ground-state molecule with the observed red shift of the absorption maximum as the experimentally observed result (Tables 3). For example, in the absorption and emission spectra of compound **4a**, λ_{abs} and λ_{flu} shift from 415 to 435 nm and 495 to 545 nm respectively, as the solvent changes from *n*-hexane to DMF (Table 3).

Table 2 Photophysical data for absorption (abs) and fluorescence (flu) of **4a–d** (Chloroform)

Dye	4a	4b	4c	4d
λ_{abs} (nm)[a]	427	427	423	427
$\varepsilon \times 10^{-3}$ [(mol L^{-1})$^{-1}$ cm^{-1}][b]	5.6	5.2	4.8	4.6
λ_{ex} (nm)[c]	425	425	425	425
λ_{flu} (nm)[d]	525	533	535	535
Stokes shift (cm^{-1})	102,040	94,339	89,285	92,592
Φ_F[e]	0.52	0.55	0.57	0.55

[a] Wavelengths of maximum absorbance; [b] Extinction coefficient; [c] Wavelengths of fluorescence excitation; [d] Wavelengths of fluorescence emission; [e] Fluorescence quantum yield

Table 3 Spectroscopic data for compound **4a** at 298 K in different solvents

Solvent	λ_{abs} (nm)	λ_{flu} (nm)
n-hexane	415	495
DCM	425	525
Acetone	430	540
Acetonitrile	435	540
DMF	435	545

Furthermore, TD-DFT electronic spectra calculations of **4a** and **4a'** show electronic transition bands at 420 nm (oscillator strength: 0.3594) and 338 nm (oscillator strength: 0.4001) respectively. When these electronic transition bands are compared with the experimental value of 427 nm, structures of **4a** gets more confirmation than structures of **4a'**. Electronic transition band of **4a** can be corresponded to π- π* transitions from donor endocyclic nitrogen to the acceptor nitro group. The calculated electronic absorption spectra of **4a** and **4a'** can be found in Supporting Information.

Study on the HOMO and LUMO frontier orbitals and the energy difference between them can provide a deeper insight

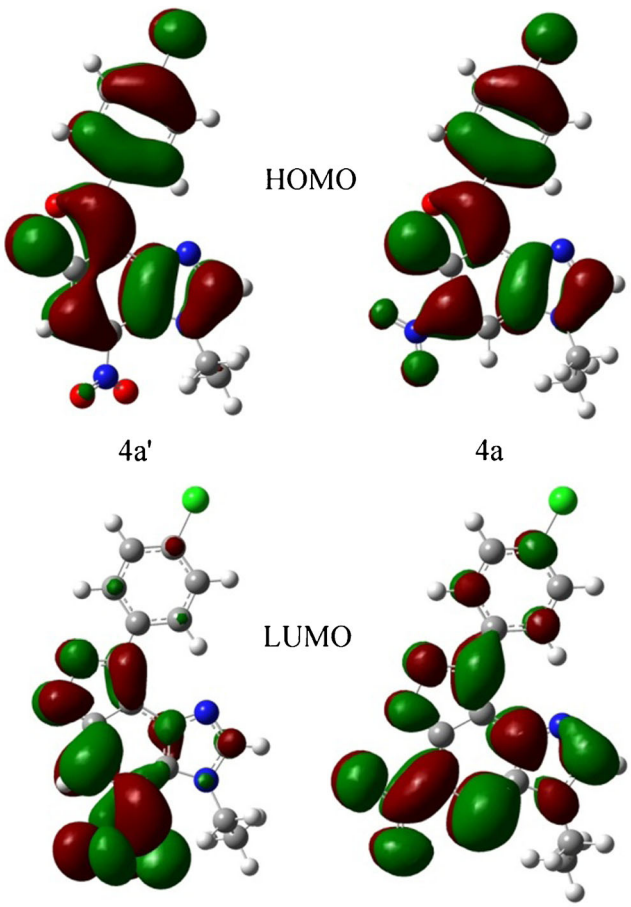
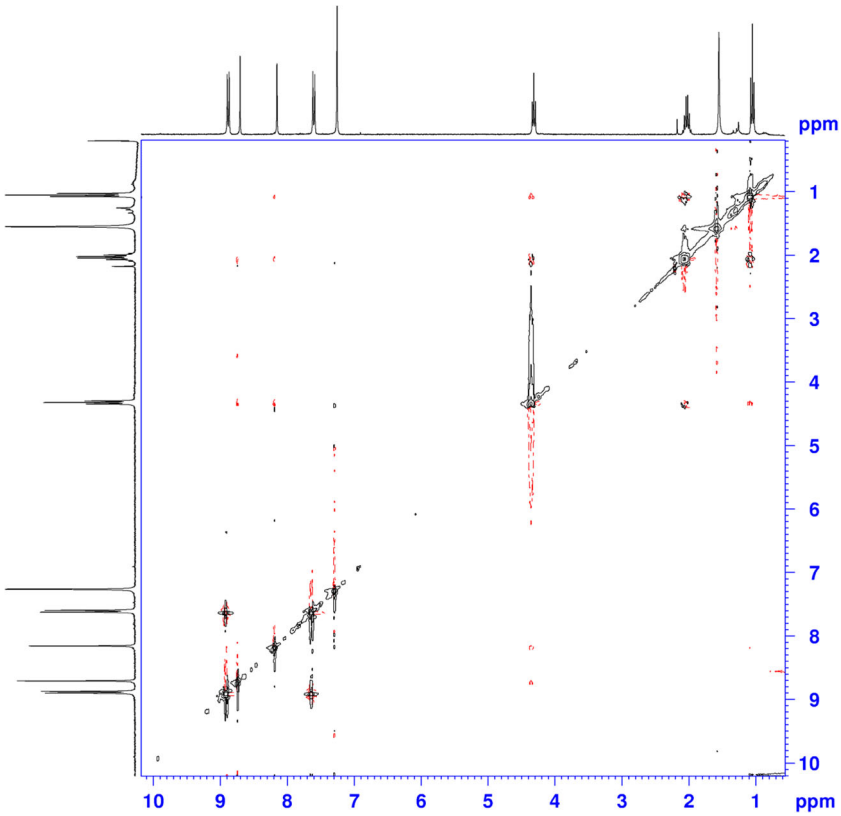


Fig. 3 The HOMO and LUMO frontier orbitals of **4a** and **4a'**

Scheme 4 NOESY spectrum of compound **4b**



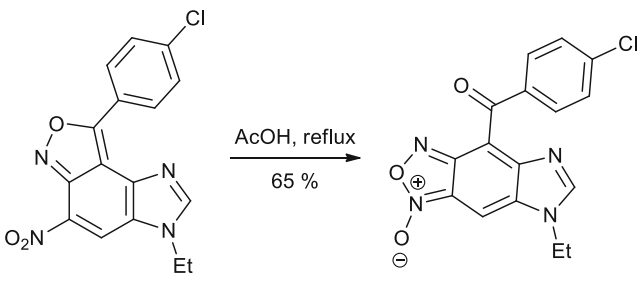
into the charge transfer properties and electronic transition bands. The HOMO and LUMO maps of the **4a** and **4a'** are shown in Fig. 3. Separation energies between the HOMO and LUMO ($\Delta\varepsilon = \varepsilon_{LUMO} - \varepsilon_{HOMO}$) in **4a** and **4a'** are 2.97 and 3.11 eV (417 and 399 nm) respectively. As seen in Fig. 3, the HOMO and LUMO of **4a** are also delocalized on NO_2 group which led to the lower separation energies between the HOMO and LUMO in **4a** compared to the $\Delta\varepsilon$ in **4a'**. It could also be considered as another reason for the confirmation of visible absorption in 427 nm in the nitrated compounds and therefore the position of the nitro group in these compounds.

The data from NOESY experiment of compound **4b** showed a massive cross-peak between the H-4 proton (δ_H 8.71, *s*, CH-benzene) and the N-3 alkyl group (δ_H 4.33 (*t*, $J = 7.2$ Hz, NCH_2), confirming the product structure (**4b**) for the nitration of **3a–d** (Scheme 4). As can be seen in Scheme 4, there are also interactions between proton of imidazole ring (δ_H 8.17, *s*, CH-imidazole) and CH_2 protons of propyl group (δ_H 4.33 (*t*, $J = 7.2$ Hz, NCH_2).

Indeed, compound **4a** underwent thermal rearrangement in high yield to its new corresponding 8-(4-chlorobenzoyl)-5-ethyl-5 *H*-imidazo[4′,5′:4,5]benzo[1,2-*c*] [1, 2, 5]oxadiazole-3-oxide **5** in AcOH [28] (Scheme 5). Structural assignments of compound **5** were based on its spectral and microanalytical data.

In conclusion, we have synthesized some new donor–acceptor fluorescent heterocyclic compounds in good yields with interesting optical properties such as high extinction coefficients and high quantum yields. These compounds were obtained from regioselective nitration of 3-alkyl-8-(4-chlorophenyl)-3 H-imidazo [4′,5′:3,4] benzo[*c*]isoxazoles in rt. Confirmation of the correct structure has been examined by investigation on the resonance structures of intermediates for the nitration reaction, DFT calculated chemical shifts (δ), photophysical properties, TD-DFT electronic spectra calculations, HOMO and LUMO frontier orbitals and finally NOESY experiment of nitrated compounds. Furthermore, the transformation of **4a** to **5** would support the site of nitration.

This research can help to the synthesis of new fluorophores and stereochemical determining in similar reactions. In addition, the new synthesized compounds can play a key role in



4a **5**

Scheme 5 Synthesis of the new compound **5**

many organic reactions, leading to the formation of the other significant compounds.

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