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Synthesis and characterization of functionalized triarylamine bisimidazole derivatives

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Novel triarylamine–bisimidazole derivatives configured with donor–acceptor (D–A) architecture have been synthesized and thoroughly characterized. The parent bisimidazole scaffolds have been obtained in high yields through a simple one-pot condensation, followed by selective functionalization through Buchwald–Hartwig amination using diphenylamine and carbazole donor groups. The structure of the synthesized compound have been confirmed by FT-IR, mass spectrometry, ^{1}H and ^{13}C NMR, and elemental analysis. The synthesized compound display distinctive intramolecular charge-transfer (ICT) absorption bands between 535 to 560 nm with blue fluorescence in the range of 445–452 nm. The estimated optical band gaps fall within 2.59–2.65 eV.

Keywords: Bisimidazole, Triarylamines, Donor-acceptor, Heterocycles, Characterization

Five-membered imidazoles are an important heterocyclic compound broadly present in variety of naturally occurring and synthetic compounds with a broad range of medicinal applications which includes anti-inflammatory[1], anti-allergic[2], antibacterial, antiviral[3] and anticancer[4]. Moreover, other than medicinal chemistry applications, imidazole based compounds have gained a lot of importance in the synthesis of functionalized materials such as organic solar cells (OSC) and organic light emitting diodes (OLED) due to good functional group tolerance and substrate flexibility[5]. π-Conjugated imidazole system with D–A architecture have received great recognition in the last three decades due to their unique optical and bipolar charge transport properties which are useful for organic electronics[5]. In D–A compounds, the donor component donates electrons to the acceptor unit, leading to distinct optoelectronics properties and they are often used in organic electronic gadgets and devices[6]. In these D–A systems, the excited states of the D or A moiety and intramolecular charge transfer (ICT) excited states are the primary sources of photoluminescence[7]. Triarylamines based organic compounds are the most explored compounds by the material chemists for applications in organo electronics due to their rigid, stable molecular structure and efficient electro-photophysical properties[8-11]. Imidazole on coupling with triphenylamine serves as an efficient ambipolar material[12]. Hence inspired with above ambipolar nature of imidazoles coupled with triarylamines, we have designed, synthesized and characterized triarylamines imidazole derivative with D–A architecture. Here triarylamines will act as donor and imidazole central moiety as acceptor unit. In literature, very few reports are available regarding synthesis of triaryl imidazole derivatives[13,14] and certain phenanthroimidazole and diphenylimidazole derivatives are used for generating light emitting devices in the blue region of the electromagnetic spectrum[15-22]. Further radical chemistry and fluorescent sensing of heavy metal ions of compound **1** (1,3-bis(4,5-diphenyl-1*H*-imidazol-2-yl)benzene) under oxidative/reductive condition is reported in the literature (Fig. 1)[23-25].

However, no reports are available for the synthesis and applications of 1,3 disubstituted triarylamine bisimidazole derivatives. Thus, herein we present a straight forward method for synthesis of novel triarylamine bisimidazole based derivatives (compound **3** and **4**) and their detailed characterization using FT-IR, Mass spectrometry, ^{1}H and ^{13}C NMR spectroscopy, and elemental analysis. In addition to characterization, photophysical properties are also discussed briefly.

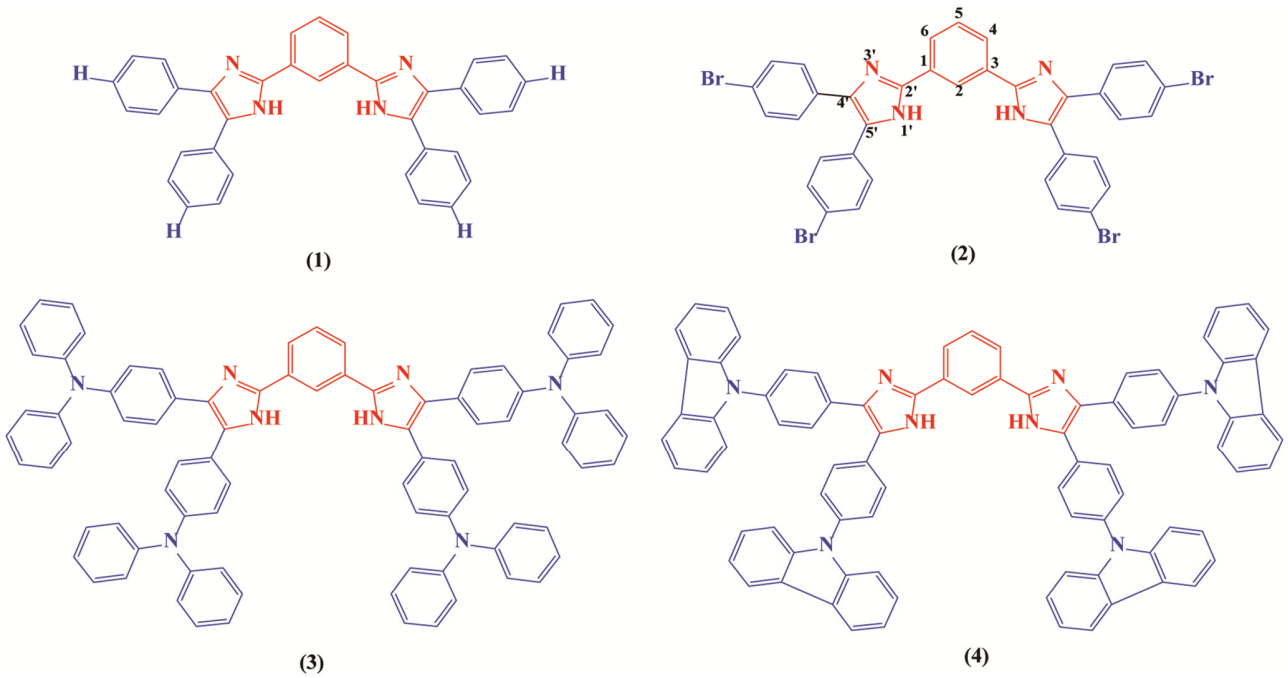


Fig. 1 — Molecular structure of compounds **1–4**

Experimental Section

Without any purification, all of the solvents (HPLC grade) and starting chemicals (AR grade) were procured directly from SD Fine-Chem, Sigma Aldrich and Spectrochem companies. 60–120 mesh silica gels with mixture of *n*-hexane and ethyl acetate as eluting solvent system was used for column chromatography. Aluminum thin layer chromatography (TLC) plates from Merck were used to track the reaction's progress and the purity of the produced compounds. Bruker 300 Ultrashield spectrometer at operative frequencies of 300 MHz and 75 MHz was used to record ^{1}H and ^{13}C NMR spectra respectively, using DMSO-d_6 as solvent and tetramethylsilane as standard internal reference. Perkin-Elmer Frontier 91579 and Thermo Scientific GCMS ITQ 1100 instruments were used to record Fourier transform infrared (FT-IR) and mass spectra respectively, while the EA Euro-elemental analysis instrument was used for elemental analysis. On Shimadzu UV-2401PC, UV-Visible spectra were captured in a dichloromethane solvent. The Perkin-Elmer LS 55 Fluorescence spectrophotometer was used to procure the emission and excitation spectras of compound **1–4**. The intersection of normalized excitation and emission spectra was used to calculate the optical band gap energy. Melting points are determined using open capillaries and are not corrected on a Thomas Hoover melting point apparatus.

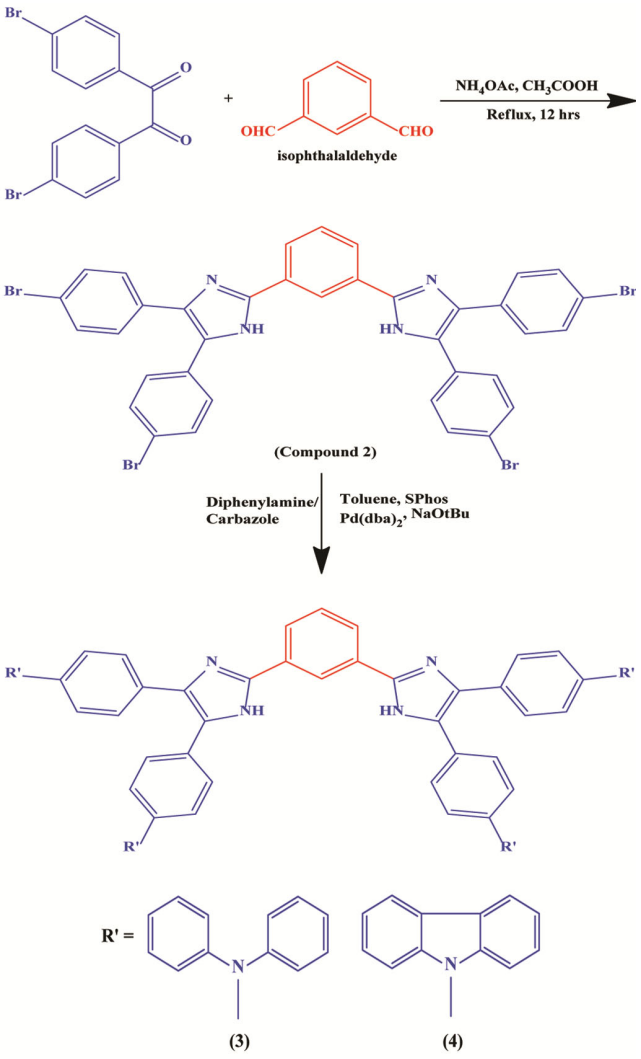
Scheme 1 illustrates the synthetic process employed to synthesize compounds **2–4**. The starting material 4,4'-dibromobenzil was synthesized as per the reported method and confirmed by its physical constant[26]. Compound **1** and **2** were synthesized *via* condensation reactions using benzil/4,4'– dibromobenzil and isophthalaldehyde with ammonium acetate, affording crystalline white and light yellow green solid with excellent yield, respectively[23-25]. Compound **3** and **4** were produced by means of Buchwald Hartwig amination reaction[27,28] by reacting starting material (compound **2**) with diphenylamine and carbazole respectively in the presence of tris(dibenzylideneacetone)dipalladium ($Pd_2(dba)_3$) as catalyst, 2–dicyclohexyl phoshpino–2,6–dimethoxybiphenyl (SPhos) as ligand and base sodium tertiarybutoxide (NaOtBu) in dry toluene.

Further, compound **1–4** were found to be soluble in a variety of solvents which includes both nonpolar and polar solvents such as toluene, *n*-hexane, dichloromethane, dimethyl sulfoxide, acetonitrile, ethyl acetate, and chloroform. Below are the complete synthetic process and characterization information of compound **1–4**.

Synthetic procedure of compound 1–4

1,3-bis(4,5-Diphenyl-1*H*-imidazol-2-yl)benzene, 1

1,2-Diphenylethane-1,2-dione (6.0 g, 30.0 mmol) and isophthaldehyde (1.345 g, 10.0 mmol) with ammonium acetate (5.0 g, 60.0 m mol) was refluxed



Scheme 1 — Synthesis of compounds **2–4**

for 12 hours in 50 cm^3 acetic acid at 100°C. Obtained crude solid was purified subsequently through column chromatography with eluting solvent system of *n*-hexane (70%) and ethyl acetate (30%) to yield purified white solid. Yield 90%. m.p 218–222°C. Mol Wt. 514.22. Anal. for $C_{36}H_{26}N_4$ Found: C, 83.72; H, 5.49; N, 10.79. Requires: C, 84.02; H, 5.09; N, 10.89%. FT-IR (KBr): 3044, 1661, 1587, 1491, 1262, 1137, 997, 696, 548 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d_6): δ H 7.30–7.35 (multiplet, 12H, aromatic), 7.58–7.60 (multiplet, 9H, aromatic), 7.71 (double doublet, J = 7.5 Hz, 2H, aromatic), 7.94 (singlet, 1H, aromatic), 8.76 (singlet, 2H, NH); ^{13}C NMR (75 MHz, DMSO-d_6): δ C 121.4, 127.4, 127.7, 127.9, 128.5, 129.1, 129.1, 130.8, 131.3, 131.7, 132.6, 133.5, 137.5, 143.3, 145.6; MS: *m/z* 514.60.

1,3-bis(4,5-bis(4-Bromophenyl)-1*H*-imidazol-2-yl)benzene, 2

1,2-bis(4-Bromophenyl)ethane-1,2-dione (10.0 g, 20.0 mmol) and isophthaldehyde (1.345 g, 10.0 mmol.) with ammonium acetate (5.0 g 60 mmol) was refluxed for 12 hour in 50 cm^3 acetic acid at 100°C. Obtained crude solid was purified subsequently through column chromatography with eluting solvent system of *n*-hexane (50%) and ethyl acetate (50%) to yield pale yellow green solid. Yield 95%. m.p 258–262°C. Mol Wt. 830.20. Anal. Calcd for $C_{36}H_{22}Br_4N_4$ Found: C, 52.54; H, 2.47; N, 6.85; Br, 38.15. Requires: C, 52.08; H, 2.67; N, 6.75; Br, 38.50%. FT-IR (KBr): 2926, 1661, 1593, 1483, 1256, 989, 686, 505 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d_6): δ H 7.46–7.48 (multiplet, 8H, aromatic), 7.56–7.59 (multiplet, 9H, aromatic), 7.70 (double doublet, *J* = 7.9 Hz, 2H, aromatic), 7.92 (singlet, 1H, aromatic), 8.68 (singlet, 2H, NH); ^{13}C NMR (75 MHz, DMSO-d_6): δ C 121.4, 122.3, 124.3, 129.1, 129.3, 129.4, 130.3, 131.6, 131.7, 132.4, 132.6, 137.5, 143.3, 145.6; MS: *m/z* 829.87.

Buchwald Hartwig coupling reaction procedure for compounds 3 and 4

To a mixture of 1,3-bis(4,5-bis(4-bromophenyl)-1*H*-imidazol-2-yl)benzene (208 mg, 0.25 mmol) and diphenylamine or carbazole (1.20 mmol) in dry toluene (30 cm^3). To above emulsion, $Pd(dba)_2$ (32 mg, 5.21 × 10^{-5} mol), SPhos (45 mg, 11 × 10^{-5} mol and NaOtBu (300 mg, 3.1 mmol) added under inert condition of nitrogen atmosphere and continuously refluxed at 100°C till completion of the reaction (1−2 hours). Hot reaction mixture was subsequently brought to room temperature and resulting crude product was extracted and purified using column chromatography to obtained light to dark orange purified products.

1,3− bis(4,5-bis(N-Diphenyl amine)-1*H*-imidazol-2-yl)benzene, 3

Compound **2** (208 mg, 0.25 mmol) and diphenylamine (220 mg, 1.2 mmol) were reacted in dry toluene as discusses above. Obtained crude solid was purified subsequently through column chromatography with eluting solvent system of *n*-hexane (80%) and ethyl acetate (20%) to yield light orange solid. Yield 56%. m.p 270–274°C. Mol. Wt 1183.44. Anal. Calcd for $C_{84}H_{62}N_8$ Found: C, 84.56; H, 5.49; N, 9.96. Requires: C, 85.26; H, 5.29; N,

9.48%. FT-IR (KBr): 2934, 1667, 1587, 1498, 1233, 1035, 828 cm^{-1}; ^1H NMR (300 MHz, DMSO-d_6): δ H 6.61 (singlet, 2H, NH), 6.99–6.96 (multiplet, 8H, aromatic), 7.11 (doublet, J = 7.5 Hz, 4H, aromatic), 7.10–7.33 (multiplet, 35H, aromatic), 7.48 (triplet, J = 7.9 Hz, 8H, aromatic), 7.58 (double doublet, J = 7.5 Hz, 4H, aromatic), 7.96 (singlet, 1H, aromatic); ^{13}C NMR (75 MHz, DMSO-d_6): δ C 121.4, 123.7, 124.2, 124.5, 124.6, 124.8, 126.2, 129.4, 129.8, 130.3, 132.5, 132.6, 137.5, 142.3, 143.3, 145.4, 145.6; MS: *m/z* 1182.52.

1,3-bis(4,5-bis(4-(9*H*-Carbazol-9-yl)phenyl)-1*H*-imidazol-2-yl)benzene, 4

Compound **2** (208 mg, 0.25 mmol) and carbazole (202 mg, 1.2 mmol) were reacted in dry toluene as discussed above. Obtained crude solid was purified subsequently through column chromatography with eluting solvent system of *n*-hexane (70%) and ethyl acetate (30%) to yield dark orange solid. Yield 61%. m.p 298–302°C. Mol. Wt 1175.38. Anal. Calcd for $C_{84}H_{54}N_8$ Found: C, 85.45; H, 4.79; N, 9.76. Requires: C, 85.85; H, 4.60; N, 9.55%. FT-IR (KBr): 3390, 2911, 1661, 1506, 1300, 1175, 711, 505 cm^{-1}; ^1H NMR (300 MHz, DMSO-d_6): δ H 7.19–7.35 (multiplet, 8H, aromatic), 7.34–7.39 (multiplet, 13H, aromatic), 7.72–7.78 (multiplet, 21H, aromatic), 8.06 (doublet, J = 7.5 Hz, 4H, aromatic), 9.42 (double doublet, J = 7.9 Hz, 8H, aromatic); ^{13}C NMR (75 MHz, DMSO-d_6): δ C 114.2, 120.6, 121.4, 122.0, 123.2, 123.7, 123.8, 124.8, 127.0, 129.1, 130.3, 132.6, 133.0, 137.5, 139.0, 139.1, 142.8, 143.3, 145.6; MS: *m/z* 1174.44.

Results and Discussion

The material design of compound **3** and **4** was guided by the concept of enhancing the donor–acceptor (D–A) interactions within the triarylamine–imidazole framework. Diphenylamine and carbazole substituents were selected as donor fragments because of their strong electron-donating ability and well-established roles in charge-transporting materials. Their incorporation at the 4,5-positions of the bisimidazole scaffold was expected to increase conjugation, facilitate intramolecular charge transfer (ICT), and modulate emission properties, particularly in the blue region, making them suitable candidate for optoelectronics.

Compound **1** and **2** serve as the parent scaffolds for further functionalization. Although compound **1** has reported in the literature,[23-25] we have carried out its complete characterization, along with compounds **2**–**4** by FT-IR, ^1H and ^{13}C NMR, mass spectrometry and elemental analysis (complete detailed information given in the experimental section). The identity and purity of synthesized compound were established by multiple spectroscopic and analytical techniques. FT-IR spectra showed strong absorptions at 1661–1667 cm^{-1} corresponding to the imidazole C=N stretch. The ^1H NMR spectra confirmed the presence of imidazole N–H protons, alongside characteristic aromatic resonances. ^{13}C NMR spectra displayed signals consistent with aromatic carbons and imidazole carbons. In addition to precise elemental composition, prominent molecular ion peak was seen in the mass spectra of all the produced compounds.

The UV–Vis absorption spectra of compounds **1**–**4** exhibited strong bands between 269 and 308 nm, assignable to n–π* and π–π* transitions of the conjugated aromatic backbone (Fig. 2a) [29,30].

Weaker, lower-energy absorptions appeared in the 418–560 nm region, attributed to ICT transitions from the electron-rich donor units (triarylamine, diphenylamine, or carbazole) to the imidazole

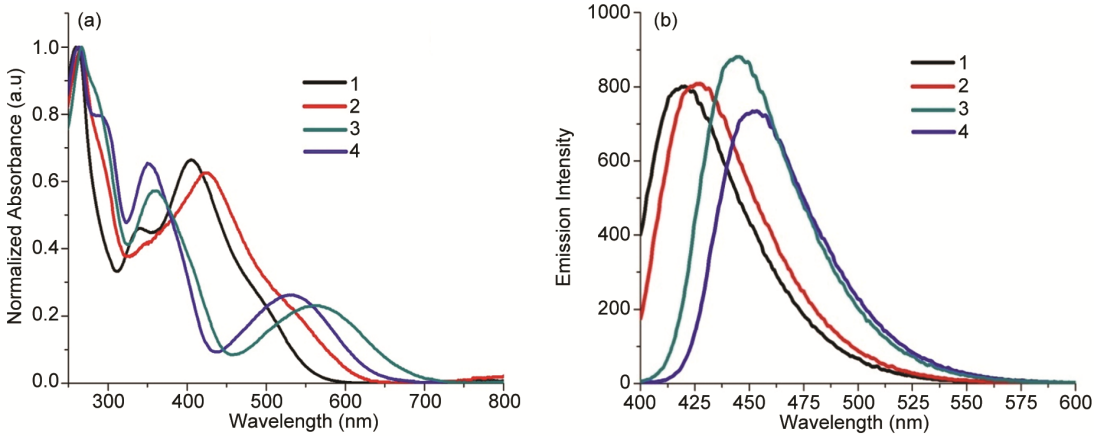


Fig. 2 — Absorption (a) and emission spectra (b) of compounds **1–4** in dichloromethane (10^{-5} mol L^{-1}).

Table 1 — Photophysical characteristics of compounds **1–4**

Compd	λ_{abs} (nm)[a]	λ_{emi} (nm)[a]	logε[b]	E_g^{opt} (eV)[c]	Stoke shift (cm^{-1})[d]
1	297, 418	420	4.788	2.83	9860
2	269, 447	425	4.886	2.89	13645
3	308, 535	445	4.976	2.59	9995
4	270, 302, 560	452	4.986	2.65	14913

[a] measured in 10^{-5} mol L^{-1} of dichloromethane.
[b] ε, molar extinction coefficient in dichloromethane.
[c] Optical band gap E_g^{opt} = 1240.8 /$\lambda_{optedge}$ (eV) [Ref. 21]
[d]Stokes shift calculated from following equation $\left(\nu_{Abs} - \nu_{Em}\right) = \left(\frac{1}{\lambda_{Abs}} - \frac{1}{\lambda_{Em}}\right) X\ 10^7$

acceptor core. Bathochromic shift of around 88 and 113 nm was observed in ICT transition compound **3** and **4** respectively with respect to parent core structure, showing the significant influence of electron donor nature of diphenylamine/carbazole moiety[29,30].

The fluorescence spectra revealed blue emission in the 445–452 nm range for compound **3** and **4** (Fig. 2b). A red shift of around 25–30 nm was observed for compounds **3** and **4** relative to **1** and **2**, consistent with extended conjugation and stronger donor substitution. Photophysical parameters are summarized in Table 1.

Compounds **3** and **4** show high value of stokes shifts of 9995 and 14913 cm^{-1} respectively, in dichloromethane, ensuring that the emitted radiation is not re-absorbed and allowing favourable excited state relaxation[29,30]. The optical band gaps of compound **3** and **4**, calculated from the intersection of normalized excitation and emission spectra, found to be 2.59 and 2.89 eV respectively.

Conclusions

In conclusion, novel triphenyl bisimidazole derivatives (compounds **3** and **4**) were synthesized with good yield using buchwald hartwig coupling. Characterization of the produced compound was done by using ^{1}H and ^{13}C NMR, FT-IR, elemental analysis and mass spectrometry. Optical studies revealed distinct ICT transitions and efficient blue emission. The incorporation of diphenylamine and carbazole donors resulted in red-shifted absorption and emission compared to the parent systems, consistent with enhanced conjugation and donor strength. These findings establish triarylamine bisimidazole hybrids as promising candidates for future studies in organic electronics and fluorescent sensors. Additional efforts are underway to functionalize the 4th and 5th position of compound **2** with other novel electron donating amines. The electrochemical, thermal and biological studies of the compound **3 and 4**, would be investigated and published later.

Supplementary Information

Supplementary information is available in the website https://nopr.niscpr.res.in/handle/123456789/58776.

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