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Introduction

Over the past decade, there has been growing interest in the development of organic electronics for applications in organic field effect transistors, nonlinear optic materials and organic light emitting diodes (OLEDs).^{1–6} Although organic materials have noteworthy advantages over inorganic materials, such as cost effectiveness, a wide array of processing options and the ability to tune the photophysical properties using different synthetic approaches, they lack long-term stability and performance. Intensive work has been carried out in both academia and industry with a view to preparing conjugated frameworks of enhanced stability and performance. Incorporation of hetero atoms into the backbone of π -conjugated systems has turned out to be one of the widely used methods to tune the electronic structures thus producing desirable photophysical and electronic properties.^{7,8} In this regard, incorporation of

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Design, synthesis, photophysical and electrochemical properties of 2-(4,5-diphenyl-1-p-aryl-1H-imidazol-2-yl)phenol-based boron complexes†

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New hybrid organic–inorganic boron compounds using an imidazole core have been readily synthesized by a two-step procedure from commercially available simple starting materials. All boron compounds were fully characterized by multinuclear NMR spectroscopy, LC-MS, thermogravimetric analysis, cyclic voltammetry and single crystal X-ray diffraction analysis (for **2a** & **2c**). The photoluminescence measurements of **2a–2c** revealed distinct emission peak maxima located at 378, 379 and 387 nm, respectively. Electroluminescent devices fabricated using these boron compounds (**2a–2c**) suggest that the boron compounds are capable of transporting electrons. A maximum brightness of 6450 cd m⁻² at 12.5 V was realized when compound **2a** was used as an electron-transporting material.

main group elements into organic frameworks with extended conjugation has attracted much attention owing to their unusual optical and electronic properties.

Among various types of main group element-containing π -electron systems, tri-⁹⁻¹⁸ and tetra-¹⁹⁻²¹ coordinated boron compounds have received particular interest because of their applications in nonlinear optics, fluorescent sensors, organic light emitting diodes and biomolecular probes. Much effort has been devoted to the development of different types of tetra-coordinated boron compounds owing to their high stability towards air and moisture over tri-coordinated boron compounds. In particular, boron dipyrromethene²²⁻²⁶ (BODIPYs) dyes synthesized by the condensation of pyrrole, carbaldehyde and boron reagents have been used extensively as organic light-emitting diodes, fluorescent imaging agents and sensors. Although BODIPYs exhibit strong fluorescence and high molar extinction coefficients, they suffer from small Stokes' shift²⁶ and weak solid-state emissions. Efforts have been made to synthesise modified BODIPY fluorophores with pronounced Stokes' shifts²⁷⁻²⁹ and better electroluminescent properties; however, a distinct disadvantage of this approach is that the assemblies made using this method are structurally complex and require multi-step organic synthesis.

Another strategy employed for the development of boron fluorophores^{30–51} with improved properties relies on principles of ligand design. Several examples of boron fluorophores with different architectures have been reported to intrinsically exhibit better photophysical properties, not only in solution



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but also in the solid state. For example, Massue et al.^{52,53} reported a series of boron complexes based on 2-(2'-hydoxyphenyl)benzoxazole. Ahn and co-workers⁵¹ reported the dramatic substituent effect of boron complexes based on 2-(benzothiazol-2-yl)phenols. More recently, Wagner and coworkers⁵⁴ reported aryl(hydro)boranes as versatile boron-containing π -electron materials. In pursuit of a new ligand system, we noticed that imidazoles are highly attractive synthons, especially tetraphenylimidazole based excited-state intramolecular proton-transfer (ESIPT) molecules that showed good electroluminescence, high thermal and morphological stability.55-60 Different synthetic approaches have been employed to modify the optical and charge transport properties of arylimidazoles.^{60–62} In an effort to tune the optical properties of imidazoles, Ziessel and co-workers⁶² introduced boron into the frame work of imidazoles through N,O-chelation. Herein, we report the synthesis and characterization of tetraarylimidazoles based boron complexes from simple starting materials using simple synthetic methodology and also present their photophysical and electroluminescent properties. We chose 2-(4,5-diphenyl-1-p-aryl-1H-imidazol-2-yl)phenol as the building unit due to its ease of synthesis from simple starting materials and its versatility to construct four coordinated boron difluoride complexes.63,64

Results and discussion

Synthesis & characterization

The tetraarylimidazoles (**1a–1c**) were readily synthesized according to a literature procedure^{55,65} using commercially available reagents. The corresponding boron complexes **2a–2c** were prepared by the reaction of **1a–1c** with boron trifluoride etherate in the presence of diisoprolylethylamine, as shown in Scheme 1. All three boron complexes were fully characterized using ¹H, ¹³C, ¹¹B and ¹⁹F NMR spectroscopy and high-resolu-



Scheme 1 Synthetic route to compounds 2a-2c.

tion mass spectrometry. The ¹¹B NMR spectra of complexes **2a–2c** show resonance at around 1 ppm, which is characteristic of tetracoordinated boron and the ¹⁹F chemical shifts appear at around –139 ppm for the fluorine atoms attached to boron.⁶⁶ Compounds **2a** and **2c** were further characterized by X-ray crystallography (Table S5†). Complexes **2a** and **2c** crystallizes in the triclinic $P\bar{1}$ space group and monoclinic C2/c space group, respectively.

The molecular structures of **2a** and **2c** along with selected bond lengths and bond angles are depicted in Fig. 1 and 2, respectively. The boron atoms in both **2a** and **2c** adopt a slightly distorted tetrahedral geometry. The B–O and B–N bond lengths in **2a** and **2c** are comparable to those of the other literature reported boron complexes.^{62,67} In both structures, the six-membered ring formed by the boron chelation takes a twisted conformation. The boron and oxygen atoms deviate from the imidazole plane by 0.06 Å and 0.66 Å in the case of **2a** and 0.15 Å and 0.83 Å in the case of **2c**. The dihedral angle between the imidazole and the phenolate is 19.46° (for **2a**) and 22.13° (for **2c**), which indicates that the π -system is distorted from the coplanar framework. The phenyl rings at the **1**, **4** and 5-positions are severely twisted, the twist observed



Fig. 1 Molecular structure of 2a. (a) ORTEP view of 2a with thermal ellipsoids at the 30% probability level. (b) Side view of 2a (capped stick model). Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and bond angles (°) are as follows: B1–F1 1.383(2), B1–F2 1.357(2), B1–O1 1.455(3), B1–N1 1.582(2), F1–B1–F2 111.76(16), F1–B1–O1 110.55(16), F2–B1–O1 108.89(17), F1–B1–N1 107.49(15), F2–B1–N1 110.71(15), O1–B1–N1 107.35(14).



Fig. 2 Molecular structure of 2c. (a) ORTEP view of 2c with thermal ellipsoids at the 50% probability level. (b) Side view of 2c (capped stick model). Co-crystallized solvent molecule and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and bond angles (°) are as follows. B1–F1 1.3751(13), B1–F2 1.3894(14), B1–O1 1.4585(14), B1–N1 1.5851(15), F1–B1–F2 111.58(9), F1–B1–O1 108.39(9), F2–B1–O1 111.09(9), F1–B1–N1 110.16(9), F2–B1–N1 108.13(9), O1–B1–N1 107.40(8).

for **2a** is 70.34, 45.06 and 58.83°, and for **2c** is 64.17, 46.50 and 53.03°, respectively (Fig. S2†). This ring twist leads to a propeller type conformation for the chromophore, which helps in preventing the π - π stacking interactions. The π - π stacking interactions are blamed for the quenching of the fluorescence in the solid state.

Photophysical properties

As shown in Fig. 3 & Table 1, all three boron complexes (2a–2c) exhibited similar UV-Visible absorption and emission spectra. The absorption spectra of 2a–2c in dichloromethane (Fig. 3) consist of two bands. The first band is centered at around 284 nm while the second band appeared at 325 nm (ε = 20 500 M⁻¹ cm⁻¹) for 2a, 325 nm (ε = 21 200 M⁻¹ cm⁻¹) for 2b and 328 nm (ε = 19 100 M⁻¹ cm⁻¹) for 2c. The origin of this absorption was studied using theoretical calculations and will be



Fig. 3 Normalized UV-Vis absorption (top) and fluorescence (bottom) spectra of compounds 2a–2c. Insets: fluorescence photograph under UV light (wavelength of light is 365 nm).

described in the following section. Upon excitation of a dichloromethane solution of boron complexes 2a-2c, a broad emission band with $\lambda_{max} = 378$ (2a), 379 (2b) & 387 (2c) nm (Fig. 3) is observed. All three complexes showed moderate emission quantum yields (quantum yields in CH₂Cl₂: 0.44 (2a); 0.45 (2b); 0.50 (2c)) with larger Stokes' shifts in comparison to typical BODIPYs systems. There is a considerable red shift for complex 2c, both in the absorption and fluorescence spectra, which can be attributed to the electron-withdrawing nature of the $-CF_3$ substituent. We tested the solvent effect of all three boron complexes (2a-2c) using different solvents (Table 1), ranging from toluene to dimethylformamide, and found that our boron complexes (2a-2c) are not sensitive towards solvent polarity, which is quite a contrasting result compared to the majority of BODIPY dyes.

Thermal and electrochemical properties

The thermal properties of complexes 2a-2c were studied using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) under a nitrogen atmosphere at a heating rate of 20 °C min⁻¹. All three boron complexes exhibit good

Table 1	Computed and	experimental	photophysical	data of	compounds	2a-2c
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	Experimental data				Theoretical calculations		
Compound	Solvent	λ_{\max}^{a} (nm)	$\epsilon_{\rm max} \ ({ m M}^{-1} \ { m cm}^{-1} imes 10^3)$	$\lambda_{\mathrm{em}}^{a,b} (\mathrm{nm})((\Phi)^c)$	MO contributions	$\lambda_{\rm exc} ({\rm nm})$	Oscillator strength
2a	CH ₃ CN	321	17.9	379 (0.44)	HOMO-LUMO	331	0.274
	THF	326	17.6	382 (0.40)			
	CH ₂ Cl ₂	325	20.5	379 (0.44)			
	DMF	323	18.7	382 (0.45)			
	Toluene	328	19.4	385 (0.46)			
2b	CH ₃ CN	321	16.6	379 (0.44)	HOMO-LUMO	329	0.313
	THF	326	16.6	382 (0.58)			
	CH ₂ Cl ₂	325	21.2	379 (0.45)			
	DMF	323	17.7	381 (0.36)			
	Toluene	328	17.9	384 (0.40)			
2c	CH ₂ CN	323	16.5	386 (0.48)	HOMO-LUMO	362	0.065
	THF	327	15.1	390 (0.49)			
	CH ₂ Cl ₂	328	19.1	387 (0.50)			
	DMF	325	18.0	388 (0.39)			
	Toluene	331	16.8	392 (0.51)			

^{*a*} Concentrations were 4.00×10^{-5} M. ^{*b*} Excited at the absorption maximum. ^{*c*} Quantum yields were measured according to literature reported^{69,70} methods using quinine sulphate as the reference.

thermal stability (decomposition starts above 300 °C for 2a & 2b-see ESI†) with high melting points (>270 °C).

The electrochemical properties of complexes 2a-2c were measured in DMF (and CH₃CN) solution using Bu₄NPF₆ as the electrolyte and the data are summarized in Table S1 (ESI[†]). As shown in Fig. 4, all three complexes exhibit one electron reduction; the reduction potential for 2c is less negative than 2a and 2b, attributed to the electron withdrawing nature of the -CF₃ moiety present in 2c. The reduction potentials of our boron complexes (2a-2c) are comparable with those of the anilido-benzoxazole boron complexes reported by Lee and coworkers,⁵⁰ however notably more highly negative than those of BODIPYs.⁶⁸



Fig. 4 Cyclic voltammograms of compounds 2a-2c (vs. ferrocene/ferrocenium) with 0.1 M Bu₄NPF₆ in DMF as the supporting electrolyte (scan rate 100 mV s⁻¹).

Molecular orbital calculations

To obtain a better understanding of the electronic structures of complexes 2a-2c, we carried out density functional theory (DFT) calculations by the Gaussian 03 programmes using the B3LYP/6-31G basis set. The plots and the calculated HOMO and LUMO energy levels for complexes 2a-2c are provided in Fig. 5, Table 1 and Tables S2-S4 (ESI[†]), respectively. As shown in Fig. 5, the HOMO levels for all three complexes are π -orbitals that involve contributions from the central imidazole, 2,4phenyl and the oxygen atom, whereas the LUMO levels for 2a and 2b are π^* orbitals consisting of atomic orbitals from central imidazole, 1, 2 and 5-phenyl moieties. An important observation is that the LUMO for 2c is more effectively stabilized than the HOMO so that the gap gets smaller for 2c (4.000 eV) compared to 2a (4.245 eV) and 2b (4.274 eV). The electronic excitations for complexes 2a-2c were calculated using TD-B3LYP/6-31-G. The calculated excitation values are comparable with the experimental results, especially the calculation nicely reproduced the red shift for the complex 2c.

Electroluminescent properties

To assess the electron transfer properties of the complexes (2a-2c) in polymer LEDs, we fabricated solution-processed electrophosphorescent devices using a green phosphor, Ir-(ppy)₃, as the dopant. Single layer devices with the configuration of ITO/PEDOT:PSS/PVK:Ir(ppy)₃ (8 wt%–16 wt%): 2(40 wt%)/Mg/Ag were fabricated (Fig. 6), where the ITO glass was used as a transparent anode; the conducting polymer poly(3,4-ethyle-nedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) was used as the hole-injection layer; poly(*N*-vinylcarbazole)(PVK) was used as the host material; the electron-transporting material 2 was mixed into the host materials to facilitate electron trans-



Fig. 5 Computed orbitals for compounds 2a-2c.



Fig. 6 Schematic illustration of EL device structure.

port in the emitting layer; $Ir(ppy)_3$ with a concentration of 8 and 16 wt% was used as the emitter. Fig. 7(a) shows the brightness-voltage (*B-V*) characteristics of the devices. According to the resulting characteristic curves, the turn-on voltages of **2a**, **2b**, and **2c** were 12.5 V, 23.5 V and 15 V, respectively (corresponding to 1 cd m⁻²). The maximum brightnesses obtained for **2a–2c** were 4760, 1600, and 200 cd m⁻², respectively; and highest current efficiencies of 10.6, 5, and 0.8 cd A⁻¹ respectively (Fig. 7(b) and Table 2). The device characteristics suggest that the electron withdrawing groups (**2c**) are likely to prevent the current inject into the system and the electron donating



Fig. 7 EL characters of the devices using **2a–2c**. (a) Brightness–voltage and (b) current efficiency–current density.

Table 2 EL performances of the device 2a-2c

Device	Turn-on voltage at 1 cd m^{-2} (V)	Max. brightness (cd m^{-2})	Efficiency (cd A ⁻¹)/ voltage (V)
2a	12.5	4760	10.6
2b	23.5	1600	5
2c	15	200	0.8

group (-CH₃) of **2b** not only exhibits poor efficiency but also reduces the brightness, which is attributed to steric-hindrance limiting electron injection.

To balance the hole and electron injection (compound **2a**), the amount of guest molecule $(Ir(ppy)_3)$ was increased from 8 wt% to 16 wt%. The *B*-*V* curves of these two samples are summarized in Fig. S3 and Table S6.† The device with 16 wt% of guest molecule $(Ir(ppy)_3$ exhibits maximum brightness of 6450 cd m⁻² at 12.5 V, with maximum current efficiency $(\eta_{c,max})$ of 11.8 cd A⁻¹. The improved device performance may be attributed to the balanced recombination of holes and electrons.

Experimental section

All reagents and starting materials were purchased from Sigma-Aldrich, Alfa Aesar and Spectrochem chemical companies and used as received unless otherwise noted. Chlorinated solvents and acetonitrile were distilled from CaH₂. THF and toluene were distilled from Na/benzophenone prior to use. Tetraarylimidazoles (**1a–1c**) were prepared according to literature procedures.^{55,65} All 400 MHz ¹H, 100 MHz ¹³C, 128 MHz

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¹¹B, and 376 MHz ¹⁹F NMR spectra were recorded using a Bruker ARX 400 spectrometer operating at 400 MHz. All ¹H and ¹³C NMR spectra were referenced internally to solvent signals. ¹¹B NMR spectra were referenced externally to BF₃·Et₂O in CDCl₃ $(\delta = 0)$, ¹⁹F NMR spectra, to α, α, α -trifluorotoluene (0.05% in CDCl₃; $\delta = -63.73$). All NMR spectra were recorded at ambient temperature. ESI mass spectra were recorded using a Bruker micrOTOF-OII mass spectrometer. The absorbance spectra were recorded using a PerkinElmer Lambda 750 UV-visible spectrometer. The fluorescence spectra were recorded using a PerkinElmer LS-55 fluorescence spectrometer. The fluorescence spectra were corrected for the instrumental response. The quantum yield was calculated by measuring the integrated area under the emission curves and by using the following equation: $\Phi_{\text{sample}} = \Phi_{\text{standard}} \times (I_{\text{sample}}/I_{\text{standard}}) \times (\text{OD}_{\text{standard}}/I_{\text{standard}})$ OD_{sample} × ($\eta_{sample}^2 / \eta_{standard}^2$) where ' Φ ' is the quantum yield, 'T the integrated emission intensity, 'OD' the optical density at the excitation wavelength, and ' η ' the refractive index of the solvent. The subscripts "standard" and "sample" refer to the fluorophore of reference and unknown respectively. In this case, the unknown is 2a-2c and the reference is guinine sulphate (quantum yield of quinine sulphate in 1 N H₂SO₄ is 0.55). Optically matched solutions with very similar optical densities of the "sample" and "standard" at a given absorbing wavelength were used for quantum yield calculations.

Elemental analyses were carried out using a Thermo quest CE instrument model EA/110 CHNS-O elemental analyzer. Single-crystal X-ray diffraction data were collected on a Bruker APEX-II diffractometer equipped with an Oxford Instruments low-temperature attachment. The data were collected at 296 K (2a) and 100 K (2c) using Mo-Kα radiation (0.71073 Å). Crystallographic data for 2a and 2c, and details of X-ray diffraction experiments and crystal structure refinements are given in Table S5.† SADABS absorption corrections were applied in both cases.⁷¹ The structures were solved and refined with the SHELX suite of programs.⁷² All non-hydrogen atoms were refined with anisotropic displacement coefficients. The H atoms were placed at calculated positions and were refined as riding atoms. Crystallographic data for the structures of 2a and 2c have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1044387 and 1044388.

DFT calculations were performed with the Gaussian03 program.⁷³ The structures were optimized using 6-31G(d) (B3LYP) as the basis set. The input files were generated using X-ray data. Excitation data were determined using TD-DFT (B3LYP) calculations.

Cyclic voltammetry measurements were performed with a conventional three electrode cell using an electrochemical workstation (CH Instrument, Model: 1100A) The three-electrode system consisted of a glassy carbon working electrode, a Pt wire as the secondary electrode, and a Ag wire as the reference electrode. The voltammograms were recorded with *ca*. 1.0×10^{-3} M solution in DMF containing Bu₄NPF₆ (0.1 M) as the supporting electrolyte. The scans were reference after the addition of a small amount of ferrocene as the internal stan-

dard. Thermogravimetric analyses (TGA) were recorded using a PerkinElmer Pyris 6 TGA model in a nitrogen atmosphere at a heating rate of 20 °C min⁻¹. Differential scanning calorimetric (DSC) analyses were recorded using a PerkinElmer Pyris 6 DSC model in a nitrogen atmosphere at a heating rate of 10 °C min⁻¹. Electroluminescence properties were measured using a Minolta CS-100A instrument. The *I*–*V* and *L*–*V* characteristics of the devices were measured by integrating a Keithley 2400 source-meter as the voltage and current source and a Minolta CS100A instrument as the Luminance detector. All of the measurements and device fabrications were performed at room temperature in a dust-controlled environment.

Device fabrication

The indium-tin oxide (ITO) glass plates were cleaned by sonication and rinsed in a series of solvents: deionized water, Triton-100 water solution, deionized water, acetone, and then methanol. The solution composed of poly(ethylenedioxythiophene):poly(styrene sulfonic acid) (PEDOT:PSS) with Triton-100 (10:1 vol%) was spin-coated (5000 rpm, 60 s) on top of the ITO substrates to form ca. 30 nm layer. The samples were then baked for 30 min at 130 °C under vacuum. Thin films of the emitting layer (EML) were made by spin-casting the compounds dissolved in chloroform (10 mg mL $^{-1}$). These solutions were filtered using a membrane filter with the pore size of 0.45 µm. The thin film samples were then thermally annealed in a vacuum at 80 °C for 5 min. After cooling down to the room temperature, the substrate was transferred into a vacuum thermal evaporator. A 2 nm thick layer of Mg was deposited at a pressure below 2×10^{-6} torr through a mask. Another layer of 100 nm thick Ag was deposited as a protecting layer for Mg. The deposition rates for Mg and Ag cathodes were 1 and 4 Å s^{-1} , respectively, to form the active layer with an area of 0.126 cm². The thickness for each layer was measured by an Alpha step instrument.

General procedure for the synthesis of imidazole boron difluoride complexes

To a solution of imidazole (1 equiv.) in anhydrous 1,2-dichloroethane under nitrogen, $BF_3 \cdot Et_2O$ (6 equiv.) was added. After 5 minutes, diisopropylethylamine (DIEA) (6 equiv.) was added and the resulting mixture was stirred at 40 °C for 1 h. The crude solution was filtered through a column of basic Al_2O_3 , eluting with CH_2Cl_2 . The resulting solid was recrystallized using CH_2Cl_2 /hexane or CH_3CN to obtain the pure product.

Synthesis of boron difluoride complex 2a

The quantities involved are as follows: compound **1a** (2.00 g, 5.15 mmol), BF₃·Et₂O (3.8 mL, 30.90 mmol) and diisopropylethylamine (5.34 mL, 30.90 mmol). Yield: 1.80 g (80%). mp: 301 °C. ¹H NMR (400 MHz, CDCl₃): δ = 6.44 (d, 1H, *J* = 8 Hz, ArH), 6.56 (t, 1H, *J* = 8 Hz, ArH), 6.93 (d, 2H, *J* = 8 Hz, ArH), 7.12–7.22 (m, 4H, ArH), 7.27–7.34 (m, 6H, ArH), 7.47–7.57 (m, 5H, ArH) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 109.85, 119.15, 120.55, 124.87, 126.74, 128.24, 128.37, 128.44, 128.56, 129.01, 129.15, 130.47, 130.56, 130.75, 131.23, 132.42, 132.50, 133.13, 135.23, 156.81 ppm. ¹⁹F NMR (376 MHz, CDCl₃): δ = -138.22 ppm. ¹¹B NMR (128 MHz, CDCl₃): δ = 1.17 (s) ppm. HR-MS (ESI): calcd for C₂₇H₁₉B₁F₂N₂O₁ ([M]⁺): 436.1558, found: 436.1519. Elemental analysis calcd (%) for C₂₇H₁₉B₁F₂N₂O₁: C 74.33, H 4.39, N 6.42; found: C 74.20, H 4.28, N 6.29. IR (KBr): ν (cm⁻¹) = 3056 (s), 1570 (m), 1503 (s), 1311 (m), 1266 (m), 1165 (m), 1150 (m), 1086 (m), 1053 (s), 921 (m), 905 (s), 864 (m), 757 (m), 718 (m), 705 (m), 540 (m).

Synthesis of boron difluoride complex 2b

The quantities involved are as follows: compound 1b (1.50 g, 3.73 mmol), BF3·Et2O (2.76 mL, 22.38 mmol) and diisopropylethylamine (3.87 mL, 22.38 mmol). Yield: 1.31 g (78%). mp: 274 °C. ¹H NMR (400 MHz, CDCl₃): δ = 2.44 (s, 1H, CH₃), 6.49 (d, 1H, J = 8 Hz, ArH), 6.58 (t, 1H, J = 8 Hz, ArH), 6.93 (d, 2H, J = 8 Hz, ArH), 7.12–7.24 (m, 6H, ArH), 7.28–7.33 (m, 6H, ArH), 7.50–7.53 (m, 2H, ArH). ¹³C NMR (100 MHz, $CDCl_3$): δ = 21.40, 109.83, 118.99, 120.35, 124.79, 126.72, 128.09, 128.39, 128.82, 128.94, 130.44, 130.93, 131.11, 132.18, 132.43, 132.46, 132.91, 140.93, 141.38, 156.64 ppm. ¹⁹F NMR (376 MHz, CDCl₃): δ = -138.24 ppm. ¹¹B NMR (128 MHz, CDCl₃): $\delta = 1.16$ (s) ppm. HR-MS (ESI): calcd for $C_{28}H_{21}B_1F_2N_2O_1$ ([M]⁺): 450.1714, found: 450.1687. Elemental analysis calcd (%) for C28H21B1F2N2O1: C 74.69, H 4.70, N 6.22; found: C 74.55, H 4.55, N 6.04. IR (KBr): ν (cm⁻¹) = 3040 (m), 1610 (m), 1570 (m), 1497 (s), 1311 (m), 1267 (m), 1172 (m), 1051 (s), 904 (s), 855(m), 699 (m), 540 (m).

Synthesis of boron difluoride complex 2c

The quantities involved are as follows: compound 1c (1.60 g, 3.51 mmol), BF3·Et2O (2.60 mL, 21.06 mmol) and diisopropylethylamine (3.64 mL, 21.06 mmol). Yield: 1.21 g (69%). mp: 288 °C. ¹H NMR (400 MHz, CDCl₃): δ = 6.42 (d, J = 8 Hz, 1H, ArH), 6.63 (t, J = 8 Hz, 1H, ArH), 6.94 (d, J = 8 Hz, 2H, ArH), 7.19 (t, J = 8 Hz, 3H, ArH), 7.27-7.37 (m, 5H, ArH), 7.45-7.52 (m, 4H, ArH), 7.78 (d, J = 8 Hz, 2H) ppm. ¹³C NMR (100 MHz, $CDCl_3$): $\delta = 109.46$, 119.34, 120.72, 121.92, 124.60, 126.23, 127.57, 127.61, 128.09, 128.24, 128.79, 129.13, 129.51, 130.45, 131.20, 132.33, 132.76, 132.97, 133.43, 138.34, 141.54, 156.85. ppm. ¹⁹F NMR (376 MHz, CDCl₃): $\delta = -63.73$ (s, CF3), -138.30 (BF₂), ppm. ¹¹B NMR (128 MHz, CDCl₃): $\delta = 0.90$ (s) ppm. HR-MS (ESI): calcd for C₂₈H₁₈B₁F₅N₂O₁ ([M]⁺): 504.1432, found: 504.1391. Elemental analysis calcd (%) for C₂₈H₁₈B₁F₅N₂O₁: C 66.69, H 3.60, N 5.56; found: C 66.53, H 3.48, N 5.50. IR (KBr): ν (cm⁻¹) = 3057 (s), 1615 (m), 1575(m), 1502 (m), 1459(m), 1419 (m), 1386(m), 1323 (m), 1289 (m), 1266(s), 1154 (m), 907(m), 858 (m), 753 (m), 705 (m), 526 (m).

Conclusion

In summary, we have synthesized 2-(4,5-diphenyl-1*-p*-aryl-1*H*imidazol-2-yl)phenol-based boron complexes (**2a**–**2c**) from the excited-state intramolecular, proton-transfer process celebrated tetraphenylimidazoles. We studied their photophysical, electrochemical and electroluminescence properties. All three new boron compounds showed good quantum yields in solution and one electron electrochemical irreversible reduction. Furthermore, they also showed high thermal stability. Single layer organic light emitting devices were fabricated using these boron compounds as the electron-transporting materials. With a doping concentration of 16 wt% (Ir(ppy)₃), compound 2a showed a maximum brightness as high as 6450 cd m⁻² at 12.5 V. We expect that our boron compounds have the potential to serve as electron-transporting material for further OLED applications. Further studies to improve the brightness and efficiency by modification of boron compounds and optimization of the electroluminescence device are in progress in our laboratories.

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