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We report a family of sulfur-containing, single-boron multi-resonance thermally activated delayed fluorescence emitters that exhibit narrowband emissions spanning the full visible spectrum from blue to red. Site-specific incorporation of a carbazole unit and ring-fused π -extension with an indolocarbazole fragment enable extensive color tuning while maintaining sharp emission profiles.

Polycyclic aromatic hydrocarbons (PAHs) doped with heteroatoms have emerged as a prominent class of advanced organic functional materials owing to their tunable electronic structures and exceptional optoelectronic properties.^{1–4} Their frontier orbital distributions, energy gaps, and excited-state dynamics can be precisely modulated not only by controlling the size and topology of the π -conjugated framework but also through the deliberate incorporation of heteroatoms such as boron (B), nitrogen (N), oxygen (O), and sulfur (S). A major breakthrough in this field occurred in 2016, when Hatakeyama *et al.* developed B,N-doped PAHs, typified by DABNA, which exhibit narrowband thermally activated delayed fluorescence (TADF) arising from the multi-resonance (MR) effect.^{5,6} Since then, MR-TADF emitters have become key candidates for next-generation organic light-emitting diodes (OLEDs) that combine excellent color purity with high external quantum efficiency (EQE).^{7–11}

With the implementation of the BT.2020¹² wide-color-gamut standard for ultrahigh-definition displays, there has been a growing demand for organic emitters with precisely controlled electroluminescence (EL) spectra. Consequently, the development of narrowband MR-TADF emitters covering the entire visible range, particularly the red region, has become a central challenge in OLED research. Although numerous MR-TADF emitters exhibiting blue to green emissions have been

Full-range luminescence color tuning from blue to red in generic single-boron multi-resonance delayed fluorescence emitters

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reported,^{5–11} efficient red organoboron MR emitters remain scarce^{13–30} (see SI for more details). The reported molecular design strategies for red MR-TADF can be broadly classified into three categories: (i) constructing *para*-D- π -D (D = N, O, S) and *para*-B- π -B architectures,^{13–15,17,18,21–23,29} (ii) introducing strong donor and acceptor substituents at the periphery,^{19,25,28} and (iii) expanding the π -conjugated MR core.^{16,20,26,27} However, these approaches often involve complex multistep synthetic routes and lead to high molecular weights, thereby limiting emitter design diversity.

Herein, we report a universal and synthetically simple design strategy that enables full-range emission color tuning—from blue to red—with a versatile single-boron MR-TADF framework. As the parent MR scaffold, we employed a S-containing MR core (**CzBS**)³¹ in which the S-induced heavy-atom effect facilitates the reverse intersystem crossing (RISC) process.^{31–33} **CzBS** exhibits sky-blue narrowband emission with a high photoluminescence (PL) quantum yield ($\Phi_{PL} = 99\%$) and high RISC rate ($k_{RISC} = 4 \times 10^5 \text{ s}^{-1}$). With this scaffold, **CzBS-Cz1** (**1**) and **CzBS-Cz2** (**2**) were developed by introducing an additional carbazole fragment in the *para*-B- π -N and *para*-N- π -S fashions, respectively (Fig. 1a), leading to hypsochromic and bathochromic spectral shifts.³⁴ Furthermore, **IDCzBS** (**3**) was designed *via* a novel ring-fused π -extension, which induced a further bathochromic shift into the red region. Remarkably, **3** (M.W. = 446) represents the most compact red MR-TADF emitter reported to date (SI), demonstrating that even a minimal single-boron MR core can deliver efficient narrowband red TADF. This conceptually simple yet powerful strategy thus provides a broadly applicable platform for color-tunable MR-TADF emitters compatible with wide-color-gamut OLEDs.

Compounds **1–3** were synthesized in three steps starting from commercially available haloarene (SI). The synthetic sequence comprises: (i) nucleophilic aromatic substitution (S_NAr) to introduce carbazole or indolocarbazole moieties, (ii) sulfidation using benzenethiol *via* S_NAr or Pd-catalyzed C–S cross-coupling,³⁵ and (iii) intramolecular borylation *via* one-pot tandem lithiation–borylation–annulation.^{5,13} Notably, the S_NAr reaction with

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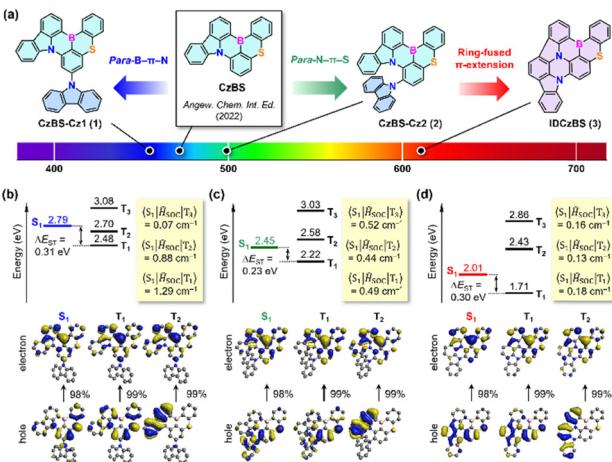


Fig. 1 (a) Molecular design strategy for achieving blue-to-red narrow-band emissions based on the single-boron MR framework of **CzBS**. (b)-(d) Simulated energy-level diagrams and natural transition orbital (NTO) representations of the excited singlet (S_1) and triplet (T_1 - T_3) states for (b) **1**, (c) **2**, and (d) **3**, calculated using TDDFT at the PBE0/DZP level.

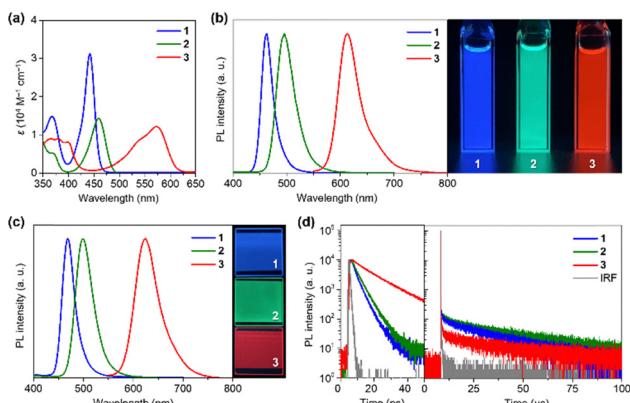


Fig. 2 (a) UV-vis absorption and (b) PL spectra with corresponding emission photographs of **1-3** in toluene (10^{-5} M). (c) Steady-state PL spectra and emission photographs, and (d) transient PL decay curves of the doped films of **1-3** in mCBP host matrices at a doping concentration of 1 wt%. IRF denotes the instrument response function.

dihydroindolo[2,3-*a*]carbazole in the synthesis of **3** proceeded smoothly, affording a highly π -extended PAH framework incorporating two adjacent N atoms. Thermogravimetric analysis revealed high thermal decomposition temperatures (T_d , 5% weight loss) of 419, 394, and 449 °C for **1-3**, respectively, confirming their excellent thermal stability and suitability for vacuum thermal evaporation in OLED fabrication.

Time-dependent density functional theory (TDDFT) calculations predicted the lowest-excited singlet (S_1) energies of **1-3** to be 2.79, 2.45, and 2.01 eV, respectively (Fig. 1b-d), indicating that their emission color can be tuned from blue to red. The corresponding spin-orbit coupling (SOC) matrix element ($\langle S_1 | \hat{H}_{SOC} | T_1 \rangle$), which plays a pivotal role in governing the spin-flip RISC process, was calculated to be 1.29, 0.49, and 0.18 cm^{-1} for **1-3**, respectively. The relatively large SOC values for **1** and **2** can be attributed to the S-induced heavy-atom effect, suggesting efficient RISC processes comparable to those of the parent **CzBS**.³¹ In contrast, the π -extension in **3** attenuated the S-induced electronic perturbation, resulting in a reduced SOC value.

Subsequently, the photophysical properties of **1-3** were examined in dilute toluene solutions and in doped films employing 3,3'-di(carbazol-9-yl)-1,1'-biphenyl (mCBP) as the host matrix (Fig. 2 and Table 1). As expected, the absorption and emission maxima ($\lambda_{\text{abs}}/\lambda_{\text{PL}}$) in solution exhibited systematic bathochromic shifts in the order of **1** (442/463 nm), **2** (459/495 nm), and **3** (573/612 nm), corresponding to blue, green, and red emissions, respectively (Fig. 2a and b). The Φ_{PL} values in toluene were 95%, 90%, and 73% for **1-3**, respectively. The lower Φ_{PL} observed for **3** was attributed to enhanced nonradiative decay pathways associated with the energy-gap law.^{36,37} In the doped films, the PL spectra of **1-3** (Fig. 2d) showed modest bathochromic shifts (by 4–13 nm) and slightly broader full width at half maximum (FWHMs) relative to their solution states, likely because of host–guest electronic interactions. The Φ_{PL} values of **1** and **2** remained high (>90%), whereas that of **3** was somewhat decreased, presumably because of incomplete excited energy transfer from the host to the emitter. The singlet–triplet energy gaps (ΔE_{ST}) of **1-3**, estimated from their fluorescence and phosphorescence spectra, were comparably small (0.12–0.15 eV, Table 1 and SI), confirming the feasibility of the RISC process.

Table 1 Photophysical data of MR-TADF emitters **1-3**

Emitter	State ^a	λ_{PL}^b (nm)	FWHM ^c (nm eV ⁻¹)	Φ_{PL}^d (%)	Φ_p^e (%)	Φ_d^e (%)	τ_p^f (ns)	τ_d^f (μs)	k_r^g (10^7 s ⁻¹)	k_{ISC}^h (10^7 s ⁻¹)	k_{RISC}^i (10^5 s ⁻¹)	ΔE_{ST}^j (eV)
1	Sol	463	25/0.15	95	23	72	2.9	37	8.0	27	1.1	0.13
	Film	468	30/0.17	91	23	68	3.4	25	6.7	23	1.6	0.14
2	Sol	495	39/0.20	90	24	66	3.0	25	8.1	25	1.4	0.13
	Film	499	41/0.21	91	20	71	4.0	31	5.1	20	1.4	0.15
3	Sol	612	46/0.15	73	73	~0	9.8	—	7.5	—	—	0.12
	Film	625	55/0.17	53	34	19	13	46	2.6	5.0	0.18	0.12

^a Sol = deoxygenated toluene solution (10^{-5} M); film = 1 wt%-doped film in an mCBP host matrix. ^b PL emission maximum. ^c Full width at half-maximum of the PL spectrum given in wavelength and energy. ^d Absolute PL quantum yield evaluated using an integrating sphere. ^e Fractional quantum yields for prompt fluorescence (Φ_p) and delayed fluorescence (Φ_d); $\Phi_p + \Phi_d = \Phi_{\text{PL}}$. ^f Emission lifetimes for prompt fluorescence (τ_p) and delayed fluorescence (τ_d). ^g Rate constant of fluorescence radiative decay ($S_1 \rightarrow S_0$); $k_r = \Phi_p/\tau_p$. ^h Rate constant of ISC ($S_1 \rightarrow T_1$); $k_{\text{ISC}} = (1 - \Phi_p)/\tau_p$. ⁱ Rate constant of RISC ($T_1 \rightarrow S_1$); $k_{\text{RISC}} = \Phi_d/(k_{\text{ISC}} \tau_p \tau_d \Phi_p)$. ^j Singlet–triplet energy gap estimated from the λ_{PL} positions of fluorescence and phosphorescence spectra.

Transient PL decay profiles of **1–3** in the doped films revealed distinct TADF behavior, featuring nanosecond-scale prompt and microsecond-scale delayed emission components (Fig. 2d). From these data, the photophysical rate constants for radiative decay (k_r), intersystem crossing (k_{ISC}), and RISC (k_{RISC}) were determined (Table 1). Owing to the MR effect, all emitters exhibited large k_r values exceeding 10^7 s^{-1} . Compounds **1** and **2** showed relatively high k_{RISC} values on the order of 10^5 s^{-1} , consistent with the enhanced SOC induced by the heavy-atom effect. In contrast, **3** exhibited a k_{RISC} value approximately one order of magnitude lower than those of **1** and **2**, reflecting its reduced SOC (Fig. 1b).

To evaluate the EL performance of **1–3** as MR-TADF emitters, OLEDs were fabricated with the configuration: indium tin oxide (ITO, 50 nm)/2,3,6,7,10,11-hexacyano-1,4,5,8,9,12-hexaazatriphenylene (HAT-CN, 10 nm)/1,1-bis[(di-4-tolylamino)phenyl]-cyclohexane (TAPC, 40 nm)/1,3-bis(1,8-dimethylcarbazol-9-yl)-benzene (mMCP, 5 nm)/1 wt%-emitter: mCBP (30 nm)/2,8-bis(diphenylphosphinyl)dibenzo[b,d]furan (PPF, 5 nm)/1,3-bis[3,5-di(pyridin-3-yl)phenyl]benzene (B3PyPB, 40 nm)/8-quinolinolato lithium (LiQ, 1 nm)/Al (100 nm).³¹ The molecular structures of these materials and corresponding energy-level diagram of the devices are shown in the SI.

The OLEDs incorporating **1–3** exhibited sharp EL emissions with narrow FWHMs of 0.16–0.21 eV, corresponding to blue ($\lambda_{EL} = 464 \text{ nm}$), green (493 nm), and red (617 nm) emissions, respectively (Fig. 3a). The Commission Internationale de l'Éclairage (CIE) chromaticity coordinates were (0.13, 0.08) for **1**, (0.11, 0.43) for **2**, and (0.64, 0.35) for **3**, demonstrating full-color tunability even at the device level (Fig. 3b). The OLEDs achieved maximum EQE (EQE_{max}) of 21.4%, 20.7%, and 11.9% for **1–3**, respectively (Fig. 3c and d, and Table 2), consistent with their ϕ_{PL} values and TADF properties in the doped films. At a luminance of 1000 cd m⁻², the corresponding EQE₁₀₀₀ values

Table 2 OLED performance data

Emitter	1	2	3
λ_{EL}^a (nm)	464	493	617
FWHM ^b (nm eV ⁻¹)	28/0.16	42/0.21	64/0.21
V_{on}^c (V)	4.8	4.6	5.6
EQE _{max} ^d (%)	21.4	20.7	11.9
EQE _{100/1000} ^e (%)	19.3/12.0	18.5/12.7	7.2/2.1
CIE (x, y) ^f	(0.13, 0.08)	(0.11, 0.43)	(0.64, 0.35)
CE ^g (cd A ⁻¹)	15.8	44.5	15.6
PE ^h (lm W ⁻¹)	10.0	27.7	8.5

^a EL emission maximum at 1 mA cm⁻². ^b Full width at half-maximum of the EL spectrum given wavelength and energy. ^c Turn-on voltage at a luminance above 1 cd m⁻². ^d Maximum external EL quantum efficiency. ^e External EL quantum efficiencies at luminances of 100 and 1000 cd m⁻². ^f CIE chromaticity coordinates. ^g Maximum current efficiency. ^h Maximum power efficiency.

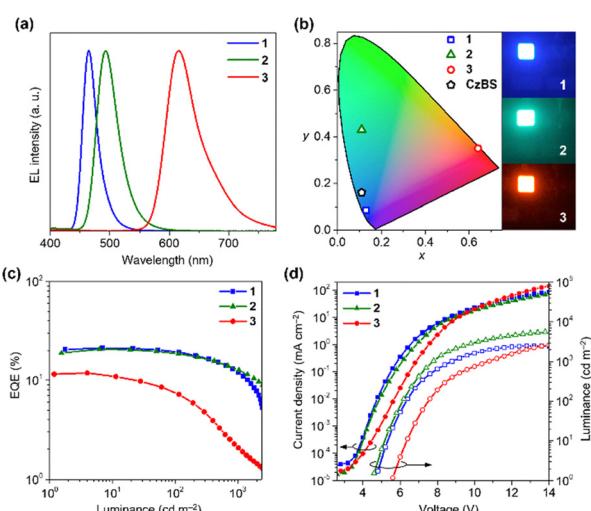


Fig. 3 OLED characteristics of the CzBS-derived MR-TADF emitters **1–3**. (a) EL spectra recorded at 1 mA cm⁻², (b) EL emission images and corresponding CIE chromaticity coordinates. (c) External quantum efficiency–luminance (EQE–L) plots, and (d) current density–voltage–luminance (J–V–L) characteristics.

were 12.0%, 12.7%, and 2.1%, representing roll-off ratios of approximately 44%, 39%, and 82%, respectively. The smaller efficiency roll-offs observed for **1** and **2** are attributed to their relatively high k_{RISC} values, comparable to that of **CzBS**. In contrast, the pronounced roll-off in the **3**-based device likely originates from its lower k_{RISC} . In this case, a large accumulation of triplet excitons occurs at high excitation densities, leading to detrimental exciton losses *via* triplet–triplet annihilation (TTA) and singlet–triplet annihilation (STA).³⁸ This issue can potentially be mitigated by optimizing the emission layer through the introduction of a suitable TADF or phosphorescent sensitizer.³⁹

Conclusions

In summary, we developed a series of S-containing, single-boron MR-TADF emitters that exhibited narrowband emissions spanning the entire visible range from blue to red. Notably, the ring-fused π -extension approach proved highly effective in inducing pronounced bathochromic shifts toward the red region, even within a structurally simple single-boron MR framework. This molecular design strategy provides valuable guidance for accessing low-energy narrowband emitters—an area long considered challenging—and expands the structural design landscape for red and near-infrared MR-TADF materials. We anticipate that further molecular refinements and device engineering will enable high-performance red narrowband OLEDs that combine exceptional color purity with high EL efficiency.

Author contributions

Daiki Endo: conceptualization, investigation, writing – original draft, review & editing. Takuma Yasuda: conceptualization, project management, supervision, resources, writing – original draft, review & editing.

Conflicts of interest

There are no conflicts to declare.



Data availability

The data supporting this article have been included within the manuscript and its supplementary information (SI). Supplementary information: synthetic procedures, characterization data, supplementary figures, and detailed information. See DOI: <https://doi.org/10.1039/d5tc04007h>.

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