

SUPPORTING INFORMATION

2-(2-Hydroxyphenyl)imidazole-based four-coordinate organoboron compounds with efficient deep blue photoluminescence and electroluminescence

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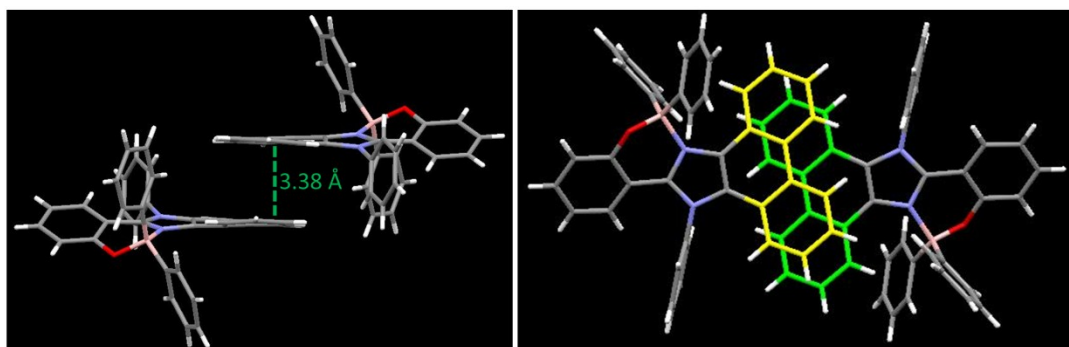


Fig. S1 The distance (left) and overlapping area (right) of the $\pi\cdots\pi$ interactions observed in the crystal of **3**.

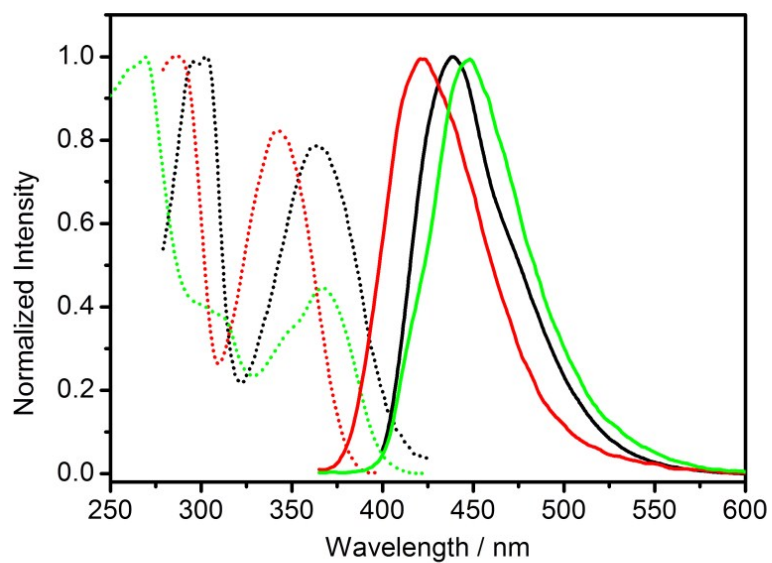


Fig. S2 Normalized absorption (dashed lines) and emission (solid lines) spectra of **1** (black), **2** (red) and **3** (green) measured with thin films. The spectra of **1** were reported previously, and they are given here for a clear comparison.

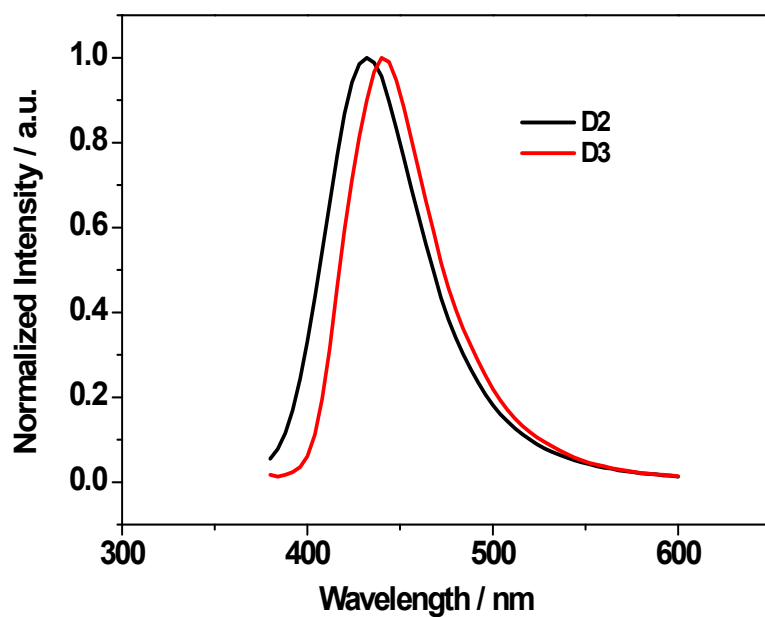


Fig. S3 EL spectra of devices **D2** and **D3** recorded at 100 cd/m².

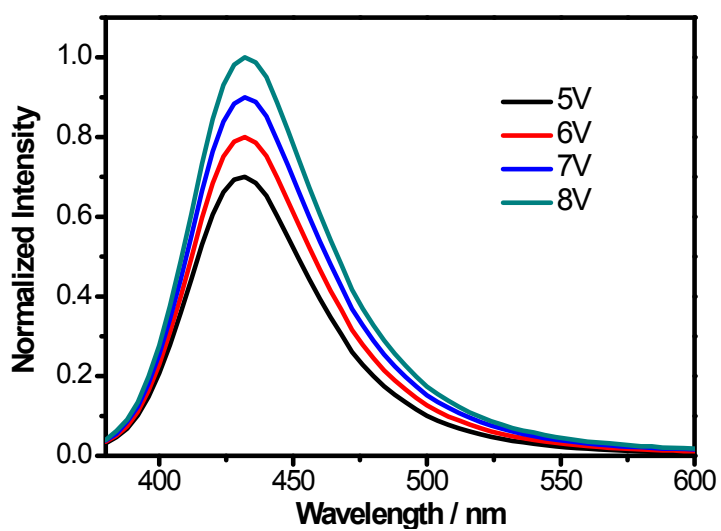


Fig. S4 EL spectra of device **D2** recorded at different driving voltages.

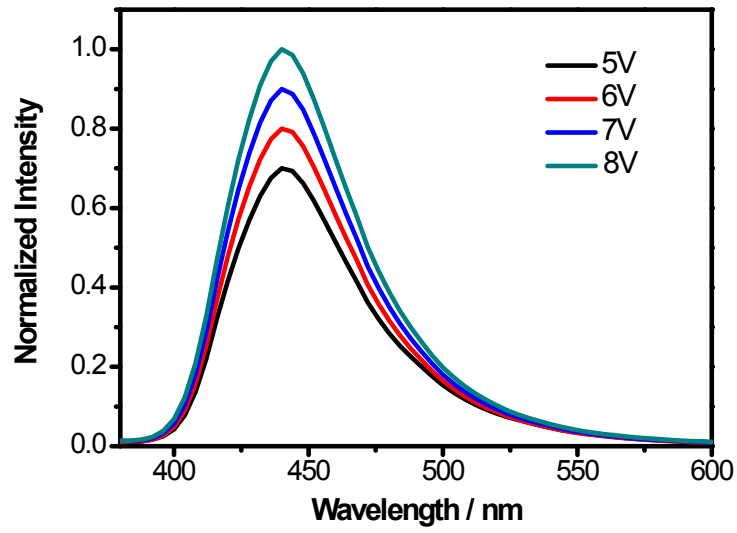


Fig. S5 EL spectra of device D3 recorded at different driving voltages.

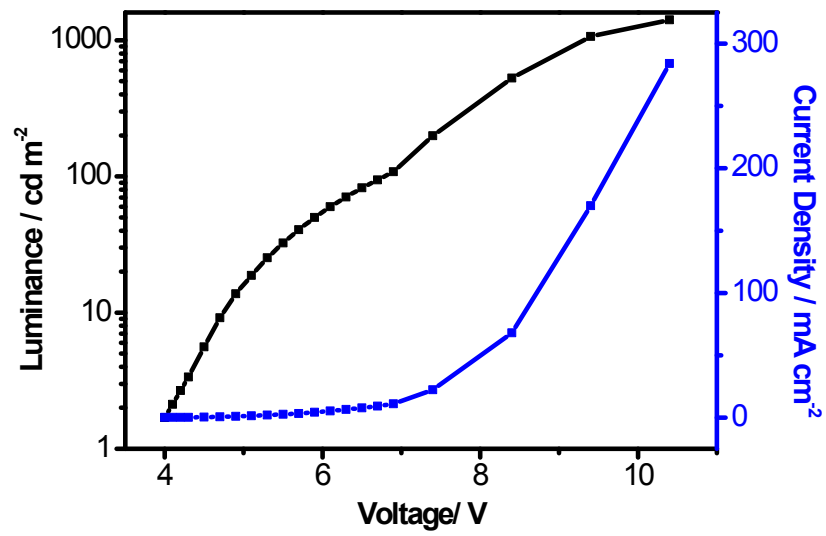


Fig. S6 The luminance-voltage-current density characteristics of device D2.

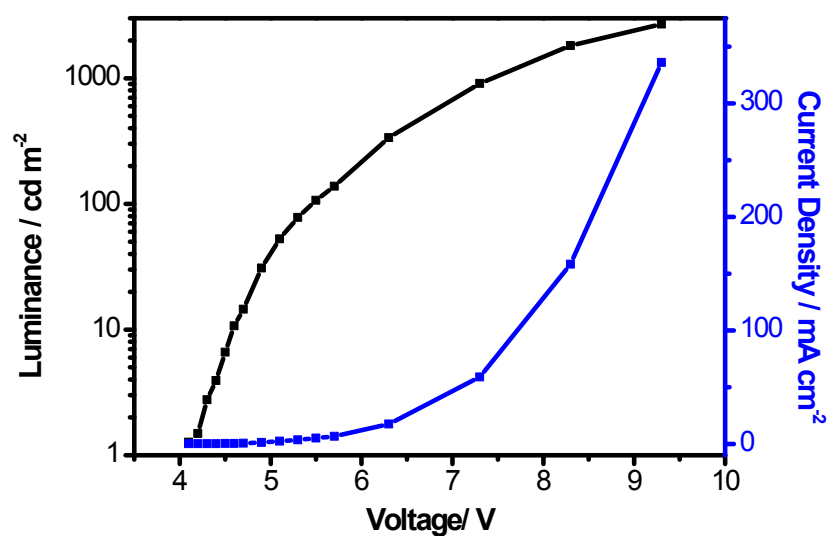


Fig. S7 The luminance-voltage-current density characteristics of device D3.

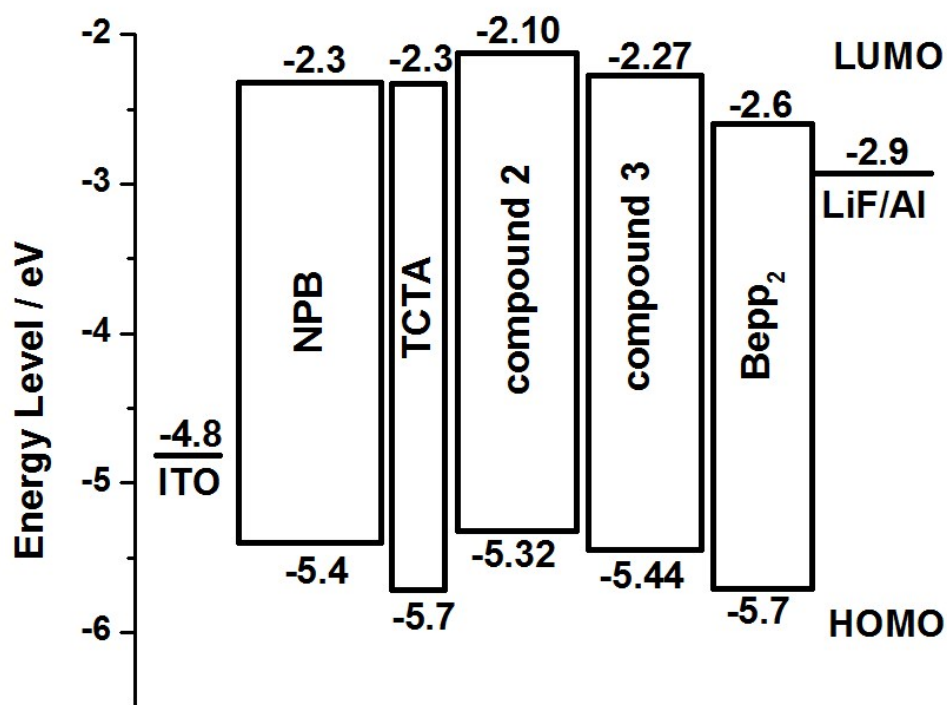


Fig. S8 Energy level diagram for the EL devices.

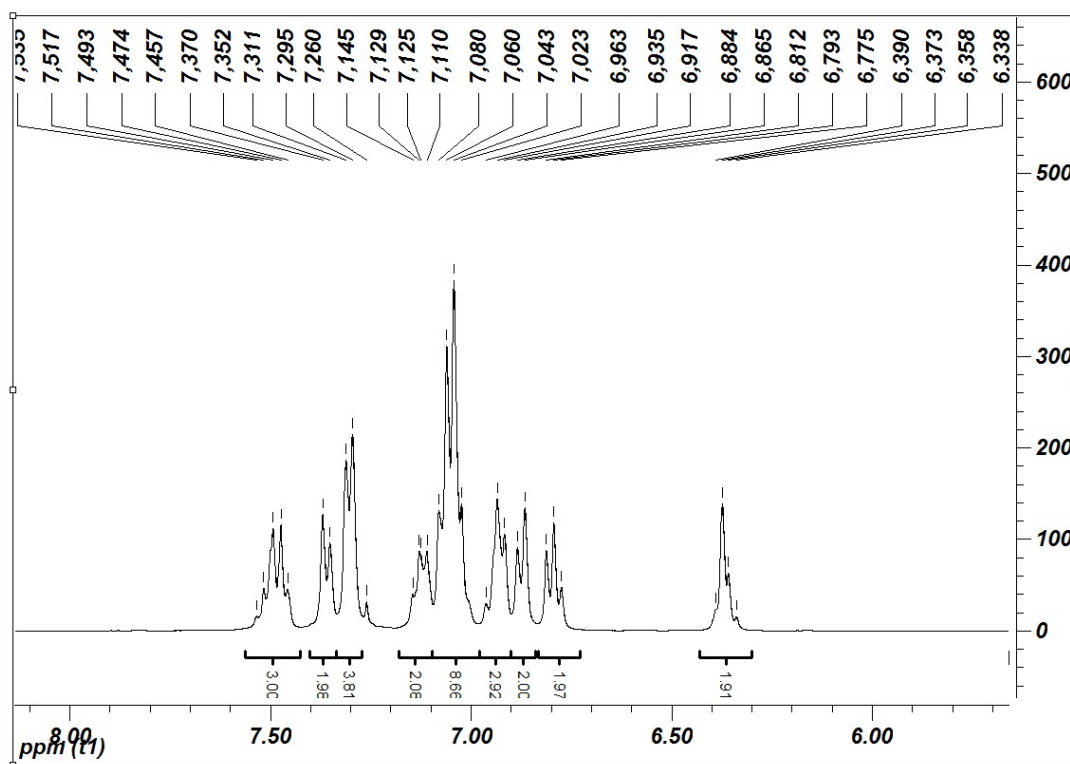


Fig. S9 ^1H NMR spectrum of compound **2** measured in CDCl_3 (400 MHz).

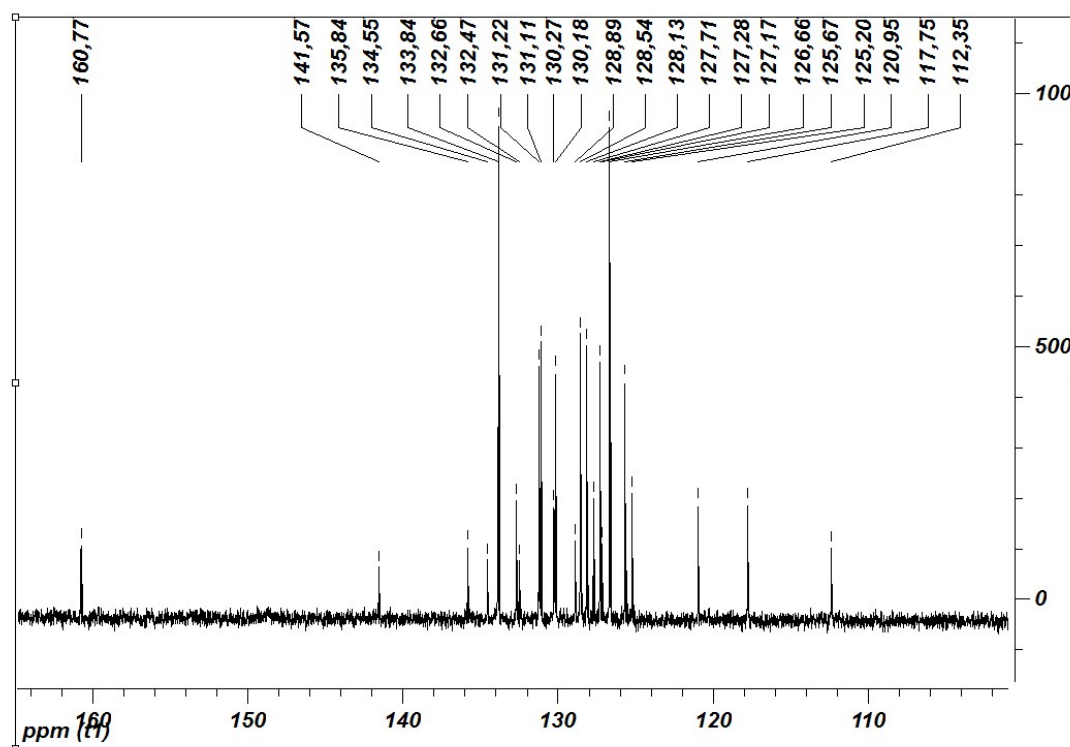


Fig. S10 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2** measured in CDCl_3 (100 MHz).

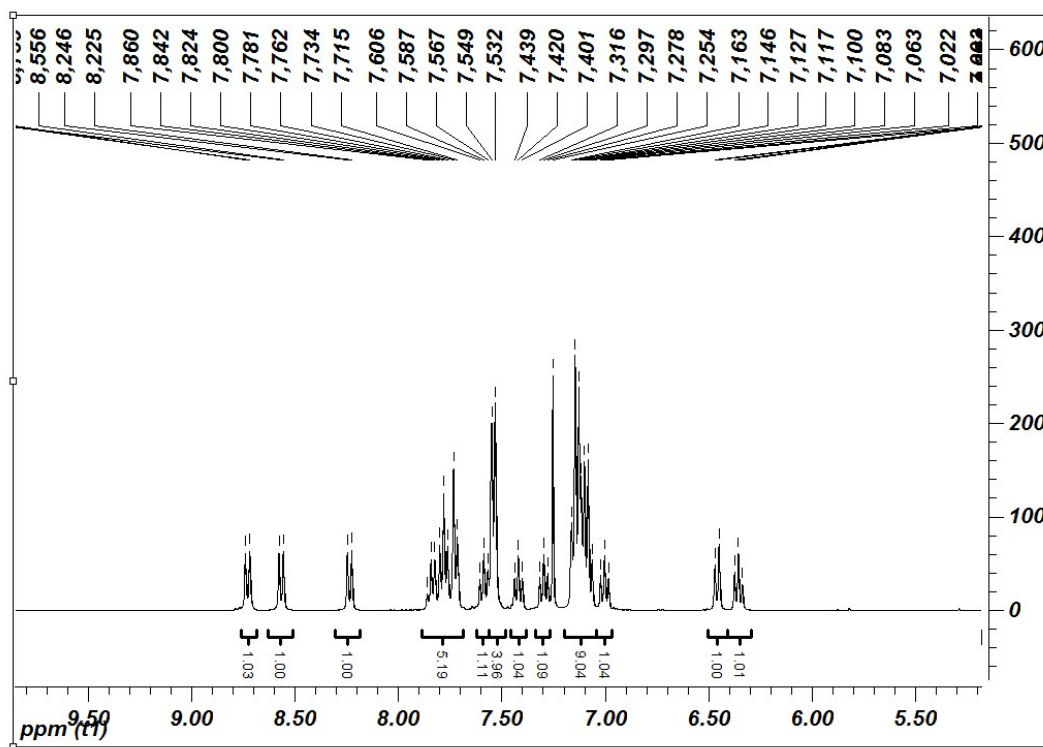


Fig. S11 ^1H NMR spectrum of compound **3** measured in CDCl_3 (400 MHz).

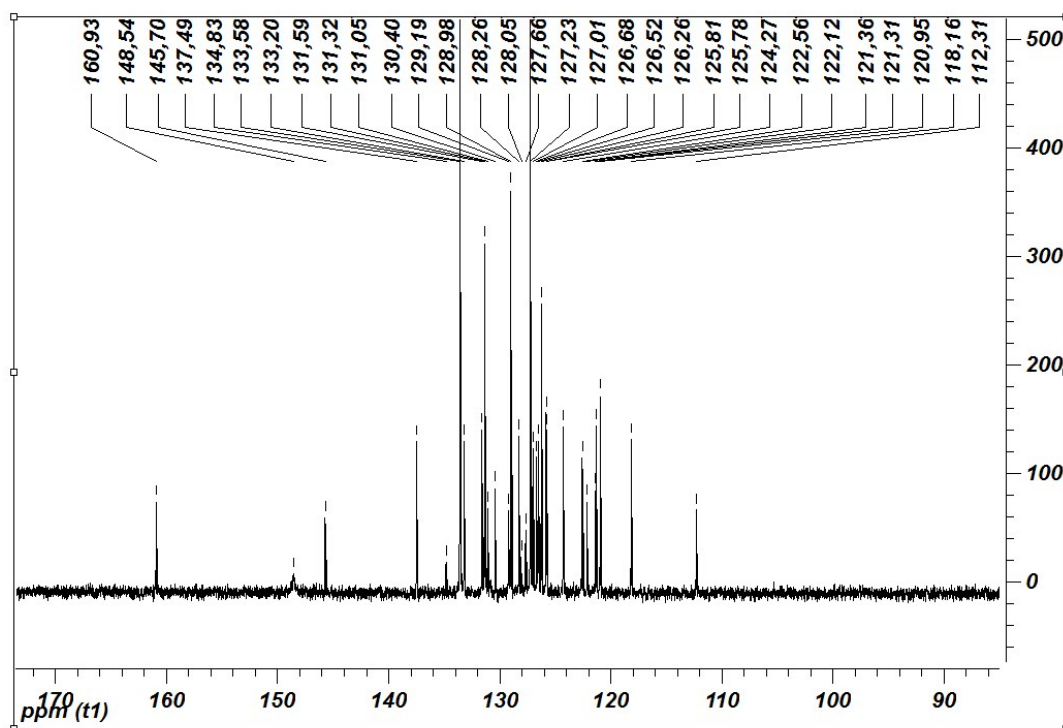


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3** measured in CDCl_3 (100 MHz).

Table S1 Crystal data for **2** and **3**.

	2	3
chemical formula	C ₃₉ H ₂₉ BN ₂ O	C ₃₉ H ₂₇ BN ₂ O
formula weight	552.45	550.44
temperature	293(2)	293(2)
radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)
crystal system	triclinic	Monoclinic
space group	P-1	P2(1)/n
<i>a</i> (Å)	10.144(2)	9.4745(19)
<i>b</i> (Å)	11.510(2)	16.609(3)
<i>c</i> (Å)	14.188(3)	18.798(4)
α (deg)	77.15(3)	90.00
β (deg)	77.52(3)	99.49(3)
γ (deg)	69.49(3)	90.00
<i>V</i> (Å ³)	1495.1(5)	2917.6(10)
<i>Z</i>	2	4
calculated density (g cm ⁻³)	1.227	1.253
F(000)	580	1152
θ range (deg)	3.14–27.48	3.08–24.99
reflections collected	14740	19865
independent reflections	6776	4933
reflections [<i>I</i> > 2 σ (<i>I</i>)]	4569	2659
GOF	1.053	1.007
R1/WR2 [<i>I</i> > 2 σ (<i>I</i>)]	0.0505/0.1233	0.0658/0.1686
R1/WR2 (all data)	0.0756/0.1336	0.1297/0.2146

Table S2. Photophysical data of compounds **1–3**.

Compound	media	$\lambda_{\text{abs}} / \text{nm}$	$\lambda_{\text{em}} / \text{nm}$	Φ_{F}
1 ^a	CH ₂ Cl ₂	356	435	0.73
	thin film	363	440	0.47
2	CH ₂ Cl ₂	341	423	0.64
	thin film	341	421	0.52
3	CH ₂ Cl ₂	333, 364	469	0.69
	thin film	367	448	0.60

^a The data for compound **1** are previously reported by us (*Inorg. Chem.* 2015, 54, 2652.)