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SUPPORTING INFORMATION

Diboron complexes with bis-spiro structures as high-performance blue emitters for OLEDs

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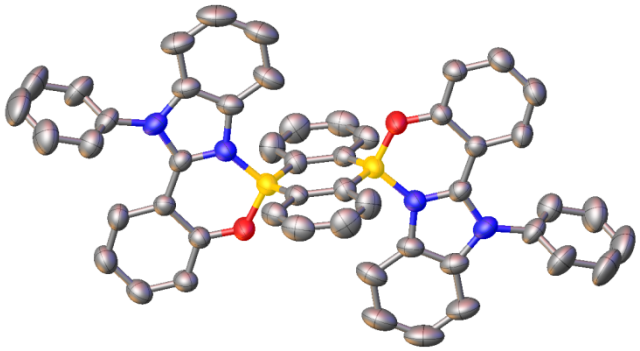

Fig. S1 Molecular structure of **1** as determined by single crystal X-ray diffraction. Atom color code: carbon (gray), boron (yellow), nitrogen (blue), oxygen (red). Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{50}H_{34}B_2N_4O_2$, M = 744.43, monoclinic, *C2/c*, a = 23.440(5) Å, b = 9.4816(19) Å, c = 18.355(4) Å, α = 90°, β = 110.48(3)°, γ = 90°, V = 3821.6(13) Å^3, T = 293(2) K, Z = 4, μ (Mo Kα) = 0.079 mm^{-1}, 17271 reflections measured, 4341 unique. The final wR_2 was 0.1445 (all data) and R_1 was 0.0532 ($I \geq 2\sigma(I)$).

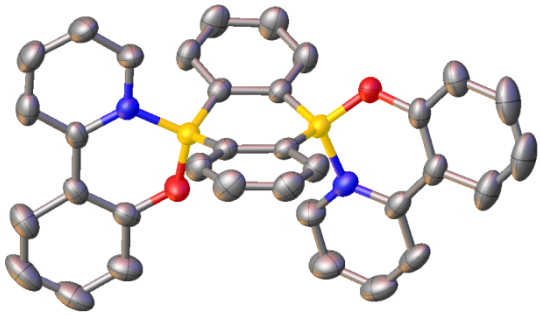

Fig. S2 Molecular structure of **2** as determined by single crystal X-ray diffraction. Atom color code: carbon (gray), boron (yellow), nitrogen (blue), oxygen (red). Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{34}H_{24}B_2N_2O_2$, M = 514.17, monoclinic, *P2(1)/c*, a = 11.169(2) Å, b = 16.752(3) Å, c = 14.317(3) Å, α = 90°, β = 106.57(3)°, γ = 90°, V = 2567.5(9) Å^3, T = 293(2) K, Z = 4, μ (Mo Kα) = 0.082 mm^{-1}, 24493 reflections measured, 5844 unique. The final wR_2 was 0.1157 (all data) and R_1 was 0.0583 ($I \geq 2\sigma(I)$).

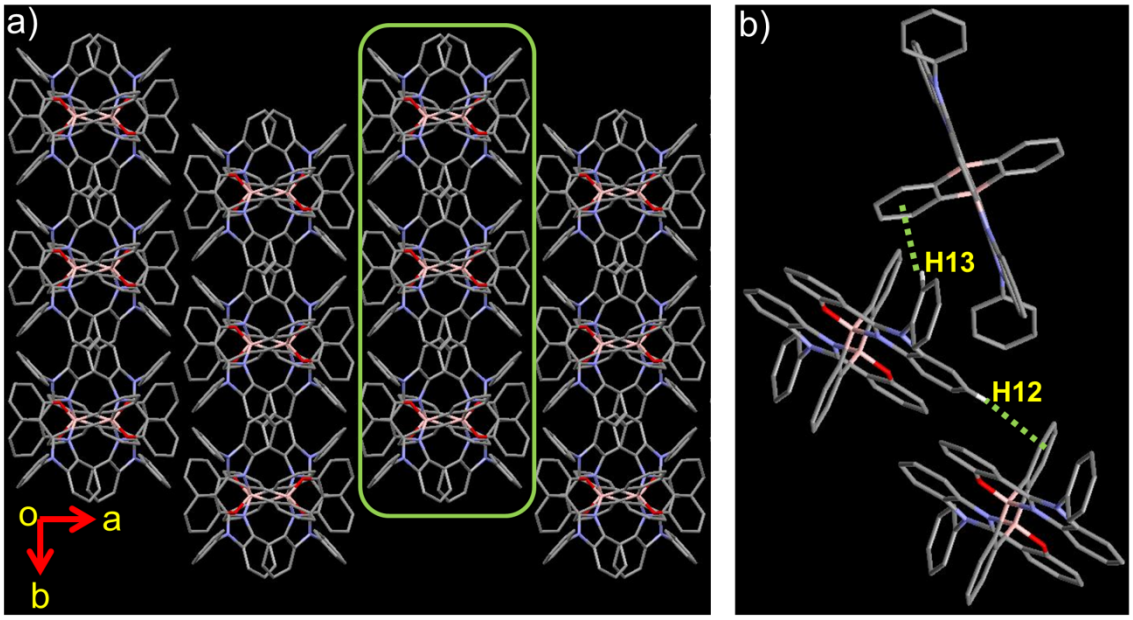

Fig. S3 a) Two dimensional layer structures formed along crystallographic *c*-axis in the crystal of **1**; b) C–H···π interactions (green line) in the layer structures.

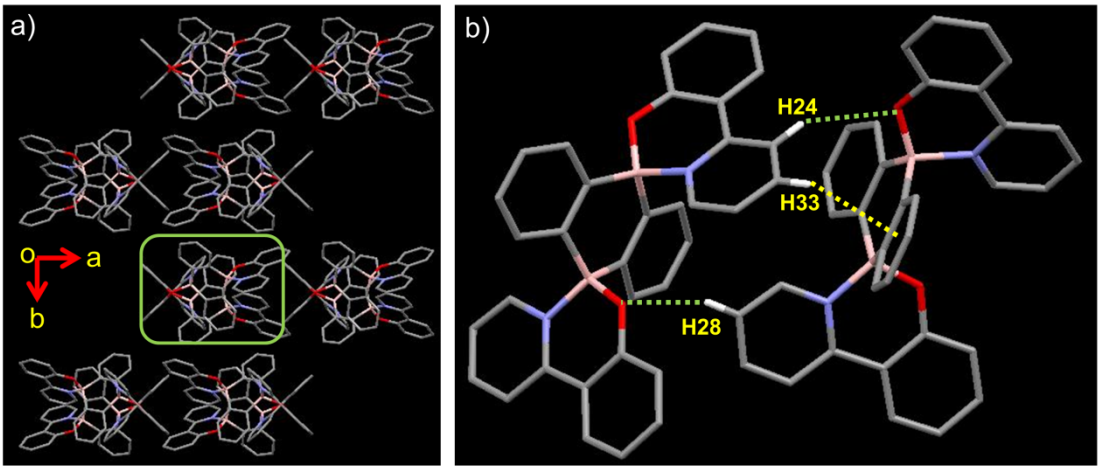

Fig. S4 a) Molecular chains formed along crystallographic *c*-axis in the crystal of **2**; b) C–H···O hydrogen-bonding (green line) and C–H···π (yellow line) interactions in the molecular chains.

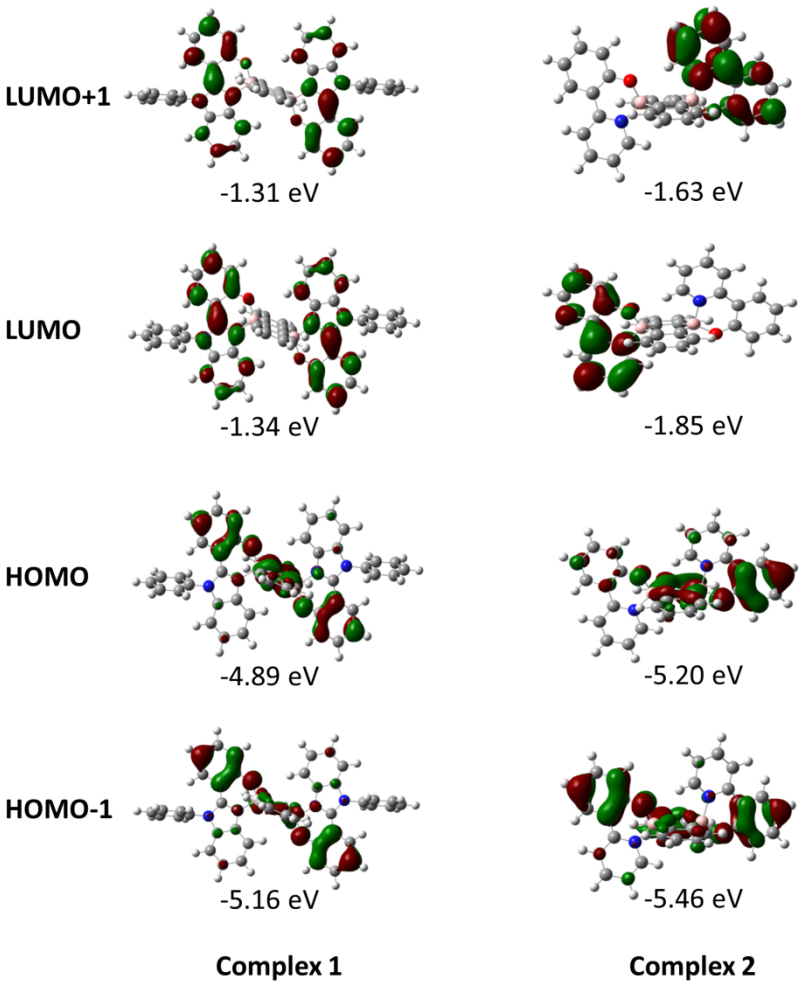

Fig. S5 DFT-calculated molecular orbital distributions and energy levels of **1** and **2**.

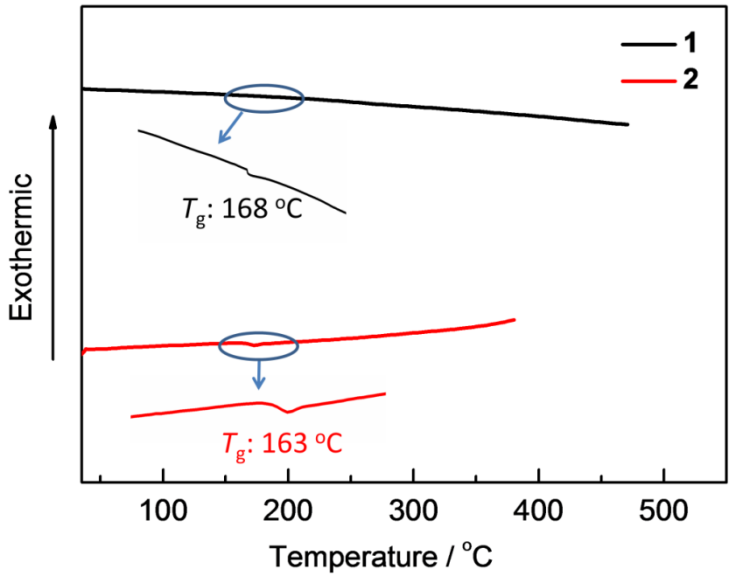

Fig. S6 DSC curves of **1** and **2** (the second heating cycle).

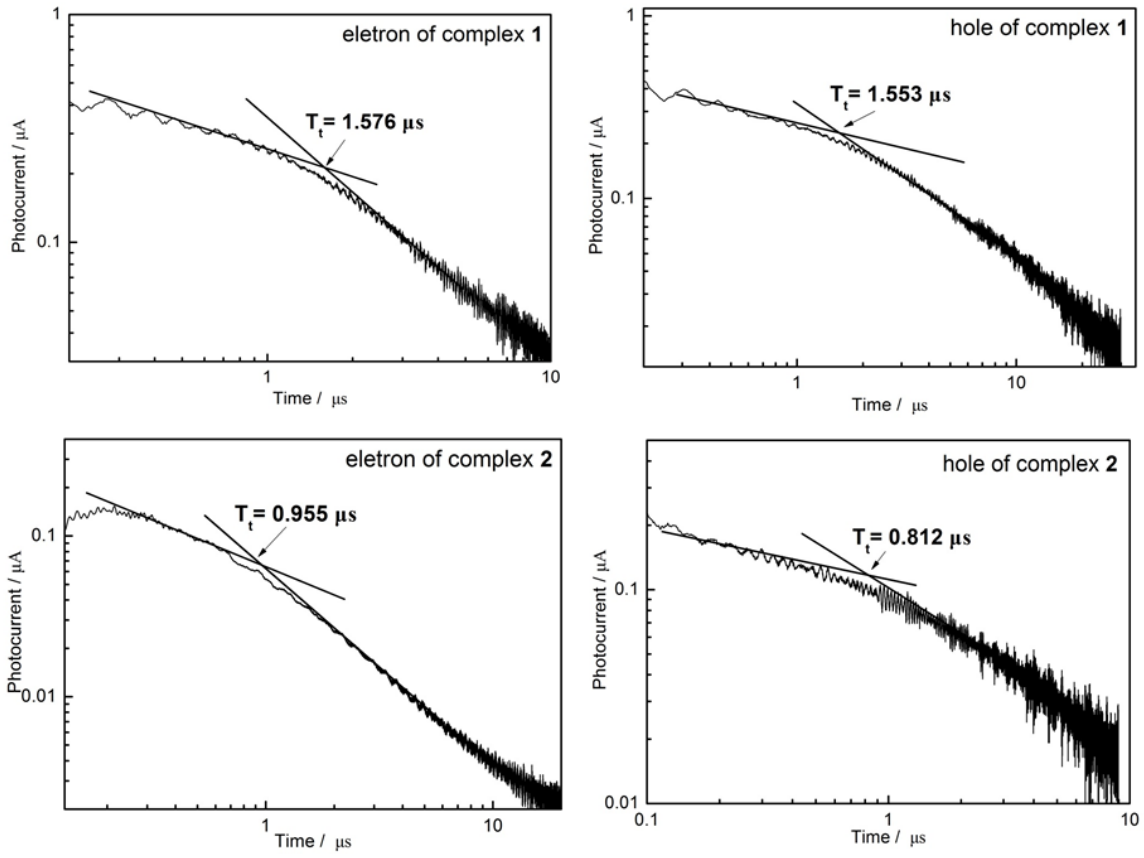

Fig. S7 Time-of-flight transients for hole and electron mobilities of **1** and **2**. The carrier mobilities were estimated based on the equation of $\mu = D/ET_t$, where D is the thickness of the transporting layer (for **1**, D = 1.1 μm; for **2**, D = 1.2 μm), E is the strength of electrical field (6.25×10^5 V cm^{-1}), and T_t is the transit time.

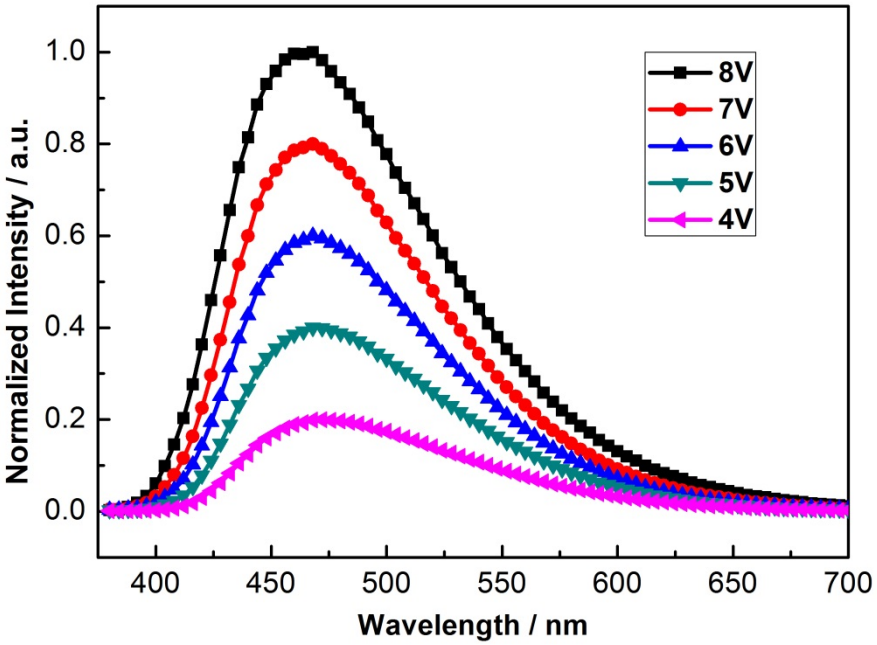

Fig. S8 EL spectra of **D1** at different driving voltages.

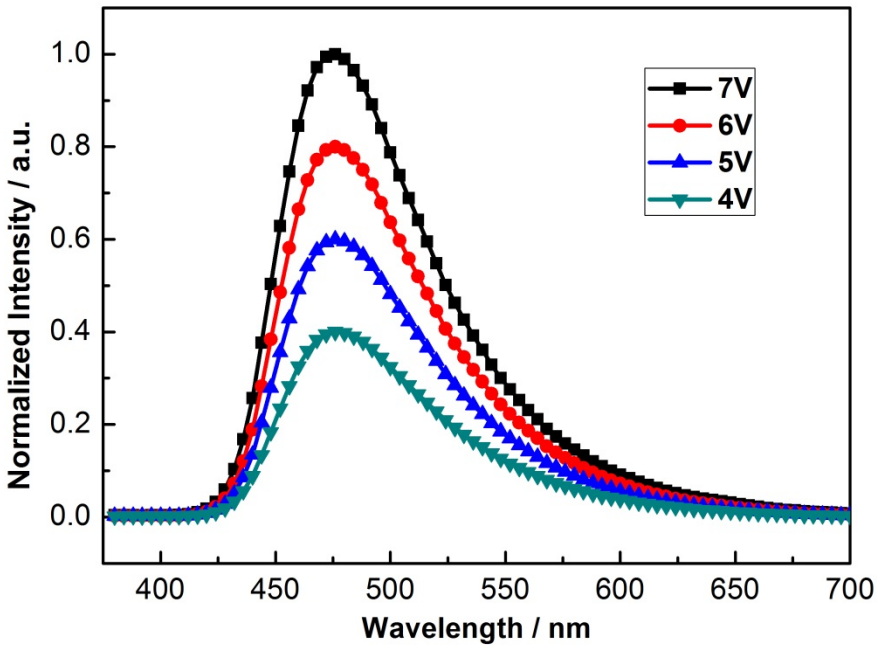

Fig. S9 EL spectra of **D2** at different driving voltages.

Table S1. Cyclic voltammetric data measured in dichloromethane,[a] and related experimental and DFT-calculated (B3LYP/6-31G(d,p)) HOMO and LUMO energies.

			Electrochemical[b]		**DFT**	
	E_{ox}^{onset} / V	E_{red}^{onset} / V	HOMO / eV	LUMO / eV	HOMO / eV	LUMO / eV
1	+0.81	–2.04	–5.61	–2.76	–4.89	–1.34
2	+0.87	–1.99	–5.67	–2.81	–5.20	–1.85

[a] Potentials are given *vs.* ferrocene/ferrocenium (Fc/Fc^+). [b] Estimated assuming that the HOMO of Fc lies 4.8 eV below the vacuum level.