

Supplementary Information

Efficient Single-Layer Electroluminescent Device Based on a Bipolar Emitting Boron-Containing Material

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Synthesis of 1,6-bis(2-hydroxyphenyl)pyridine boron bis(4-n-butyl-phenyl)phenyleneamine

Tris(4-bromo-phenyl)amine (2.5 g, 5.2 mmol) in THF (40 mL) at -78°C was added n-BuLi (6.3 mL, 1.6 M) in hexanes. The solution was stirred at -78°C for 45 min, and then trimethylborate (0.95 mL, 7.9 mmol) was added. After stirring at -78°C for an additional 2 h, the solution was gradually warmed to RT, and stirring was continued overnight. After solvent evaporation in vacuum, the residue was dissolved in 0.1 M HCl (30 mL) and extracted with DCM (2×10 mL). The pH of the aqueous phase was then adjusted to 8 with NaHCO_3 and the solution was extracted with DCM (3×20 mL). The combined organic layers were washed with water and dried over Na_2SO_4 , the solvent was evaporated to give white solid, which was used directly in the subsequent step without further purification. The solid was added to the mixture of H_2dppy (1.42 g, 5.4 mmol) and NEt_3 (2.5 mL) in 30 mL of benzene, and the reaction mixture was heated to reflux for 10 h. After cooled to room temperature, a light yellow solid precipitated from the solution. The solid product was collected by filtration and purified by recrystallization and sublimation to give yellow solid (1.57 g). Yield: 48% ^1H NMR (CDCl_3): $\delta = 8.371$, (t, $J = 8.0$ Hz, 1 H), 8.317, (d, $J = 7.0$ Hz, 2 H), 8.040, (d, $J = 6.5$ Hz, 4 H), 7.398, (m, 4 H), 7.203-7.143, (m, 4 H), 7.035-6.992 (m, 4 H), 6.961-6.929, (m, 4 H), 2.454, (m, $J = 7.0$ Hz, 4 H), 1.478 (m, $J = 4.0$ Hz, 4 H), 0.867, (t, $J = 7.5$ Hz, 6 H). Ms: m/z : 628 $[\text{M}]^+$; element analysis calcd (%) for $\text{C}_{43}\text{H}_{41}\text{BN}_2\text{O}_2$: C, 82.16; H, 6.57; N, 4.46. found: C, 82.05; H, 6.85; N, 4.29. X-ray quality crystals were grown by slow diffusion of diethyl ether vapor into a CHCl_3 solution of (dppy)BTPA

S-Table 1. Crystal data and structure refinement for (dppy)BTPA.

Identification code	(dppy)BTPA
formula	C43 H41 B N2 O2
Formula weight	628.59
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2(1)/c
Unit cell dimensions	$a = 16.815(3)$ Å $\alpha = 90^\circ$. $b = 10.182(2)$ Å $\beta = 99.93(3)^\circ$ $c = 20.772(4)$ Å $\gamma = 90^\circ$
Volume	3503.3(12) Å ³
Z, Calculated density	4, 1.192 Mg/m ³
Absorption coefficient	0.072 mm ⁻¹
$F(000)$	1336
Crystal size	0.31 x 0.10 x 0.10 mm ³
Theta range for data collection	2.35 to 27.48°
Limiting indices	0 ≤ h ≤ 21, 0 ≤ k ≤ 13, -26 ≤ l ≤ 26
Reflections collected / unique	7814/7814 [$R(\text{int}) = 0.089867$]
Completeness to theta = 27.48	97.30%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9928 and 0.9777
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameter	7814/43/415
Goodness-of-fit on F^2	0.775
Final R indices [$I > 2 \sigma(I)$]	$RI = 0.0873$, $wR2 = 0.1871$
R indices (all data)	$RI = 0.3259$, $wR2 = 0.2501$
Largest diff. peak and hole	0.393 and -0.281 e.Å ⁻³

S-Table 2. Bond lengths (Å) and angles (°) for (dppy)BTPA.

C(36)-C(27)	1.580(6)	C(12)-C(13)	1.421(3)
C(36)-C(37)	1.735(5)	C(13)-C(14)	1.367(3)
C(37)-C(38)	1.577(8)	C(14)-C(15)	1.358(3)
C(38)-C(39)	1.666(8)	C(15)-C(16)	1.380(3)
B(1)-O(2)	1.444(3)	C(16)-C(17)	1.371(3)
B(1)-O(1)	1.458(3)	C(18)-C(23)	1.388(3)
B(1)-C(18)	1.598(3)	C(18)-C(19)	1.393(3)
B(1)-N(1)	1.603(3)	C(19)-C(20)	1.383(3)
O(1)-C(1)	1.350(2)	C(20)-C(21)	1.367(3)
O(2)-C(17)	1.342(2)	C(21)-C(22)	1.362(3)
N(1)-C(11)	1.346(2)	C(22)-C(23)	1.370(3)
N(1)-C(7)	1.364(3)	C(24)-C(25)	1.364(3)
N(2)-C(21)	1.413(3)	C(24)-C(29)	1.407(3)
N(2)-C(30)	1.413(3)	C(25)-C(26)	1.357(3)
N(2)-C(24)	1.457(3)	C(26)-C(27)	1.337(4)
C(1)-C(2)	1.385(3)	C(27)-C(28)	1.371(4)
C(1)-C(6)	1.409(3)	C(28)-C(29)	1.353(3)
C(2)-C(3)	1.317(3)	C(30)-C(31)	1.368(4)
C(3)-C(4)	1.365(4)	C(30)-C(35)	1.388(3)
C(4)-C(5)	1.370(3)	C(31)-C(32)	1.407(4)
C(5)-C(6)	1.405(3)	C(32)-C(33)	1.368(5)
C(6)-C(7)	1.468(3)	C(33)-C(34)	1.311(4)
C(7)-C(8)	1.377(3)	C(33)-C(40)	1.520(5)
C(8)-C(9)	1.355(3)	C(34)-C(35)	1.353(4)
C(9)-C(10)	1.373(3)	C(41)-C(40)	1.504(6)
C(10)-C(11)	1.377(3)	C(41)-C(42)	1.636(6)
C(11)-C(12)	1.467(3)	C(42)-C(43)	1.549(6)
C(12)-C(17)	1.380(3)		
C(27)-C(36)-C(37)	113.7(4)	C(15)-C(14)-C(13)	119.6(2)
C(38)-C(37)-C(36)	105.1(4)	C(14)-C(15)-C(16)	120.5(2)
C(37)-C(38)-C(39)	104.5(5)	C(17)-C(16)-C(15)	120.1(2)
O(2)-B(1)-O(1)	105.7(2)	O(2)-C(17)-C(16)	118.2(2)
O(2)-B(1)-C(18)	112.6(2)	O(2)-C(17)-C(12)	120.2 (2)
O(1)-B(1)-C(18)	113.3(2)	C(16)-C(17)-C(12)	121.6(2)
O(2)-B(1)-N(1)	108.5(2)	C(23)-C(18)-C(19)	113.8(2)
O(1)-B(1)-N(1)	107.4(2)	C(23)-C(18)-B(1)	123.2(2)
C(18)-B(1)-N(1)	109.0(2)	C(19)-C(18)-B(1)	122.9(2)
C(1)-O(1)-B(1)	116.6(2)	C(20)-C(19)-C(18)	123.4(2)

C(17)-O(2)-B(1)	120.8(12)	C(21)-C(20)-C(19)	119.5(2)
C(11)-N(1)-C(7)	121.7(2)	C(22)-C(21)-C(20)	119.5(2)
C(11)-N(1)-B(1)	120.2(2)	C(22)-C(21)-N(2)	120.8(2)
C(7)-N(1)-B(1)	118.0(2)	C(20)-C(21)-N(2)	119.5(2)
C(21)-N(2)-C(30)	119.8(2)	C(21)-C(22)-C(23)	119.7(2)
C(21)-N(2)-C(24)	118.2(2)	C(22)-C(23)-C(18)	124.1(2)
C(30)-N(2)-C(24)	121.3(2)	C(25)-C(24)-C(29)	118.1(2)
O(1)-C(1)-C(2)	120.7(2)	C(25)-C(24)-N(2)	122.8(2)
O(1)-C(1)-C(6)	120.7(2)	C(29)-C(24)-N(2)	119.1(2)
C(2)-C(1)-C(6)	118.7(2)	C(26)-C(25)-C(24)	120.9(2)
C(3)-C(2)-C(1)	122.1(2)	C(27)-C(26)-C(25)	120.5(2)
C(2)-C(3)-C(4)	120.9(2)	C(26)-C(27)-C(28)	120.9(2)
C(3)-C(4)-C(5)	120.4(2)	C(26)-C(27)-C(36)	115.4(3)
C(4)-C(5)-C(6)	120.0(2)	C(28)-C(27)-C(36)	123.1(3)
C(5)-C(6)-C(1)	118.0(2)	C(29)-C(28)-C(27)	119.5(2)
C(5)-C(6)-C(7)	122.3(2)	C(28)-C(29)-C(24)	120.2(2)
C(1)-C(6)-C(7)	119.5(2)	C(31)-C(30)-C(35)	118.0(2)
N(1)-C(7)-C(8)	119.2(2)	C(31)-C(30)-N(2)	121.3(2)
N(1)-C(7)-C(6)	117.4(2)	C(35)-C(30)-N(2)	120.8(2)
C(8)-C(7)-C(6)	123.4(2)	C(30)-C(31)-C(32)	119.2(3)
C(9)-C(8)-C(7)	119.2(2)	C(33)-C(32)-C(31)	120.1(3)
C(8)-C(9)-C(10)	121.2(2)	C(34)-C(33)-C(32)	119.6(3)
C(9)-C(10)-C(11)	119.1(2)	C(34)-C(33)-C(40)	119.8(3)
N(1)-C(11)-C(10)	119.4(2)	C(32)-C(33)-C(40)	120.6(3)
N(1)-C(11)-C(12)	117.5(2)	C(33)-C(34)-C(35)	122.1(3)
C(10)-C(11)-C(12)	123.0(2)	C(34)-C(35)-C(30)	120.8(2)
C(17)-C(12)-C(13)	116.5(2)	C(40)-C(41)-C(42)	107.2(4)
C(17)-C(12)-C(11)	121.2(2)	C(43)-C(42)-C(41)	104.8(3)
C(13)-C(12)-C(11)	122.3(2)	C(41)-C(40)-C(33)	115.8(4)
C(14)-C(13)-C(12)	121.7(2)		

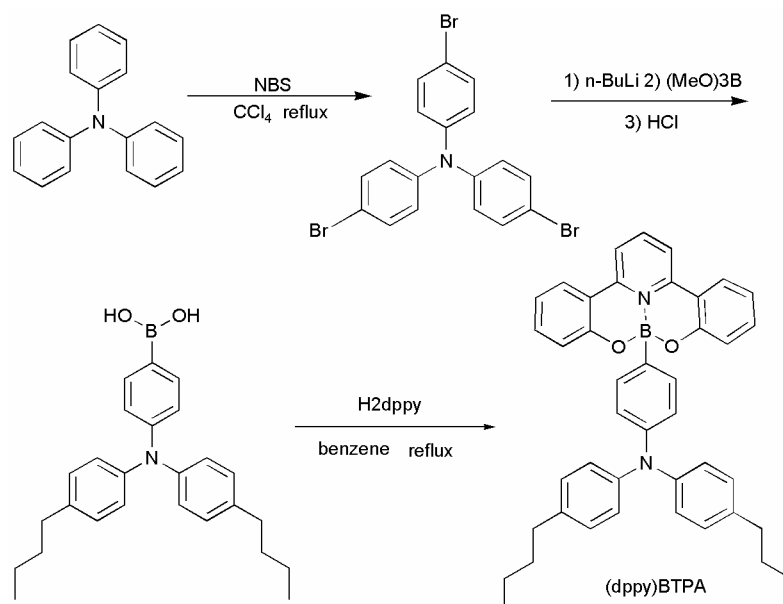
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S-Scheme 1 Synthetic steps for (dppy)BTPA.