# Electronic Supplementary Information (ESI)

B- and N-embedded color-tunable phosphorescent iridium complexes and B-N lewis adducts with intriguing structural and optical changes

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### General information

Unless noted, all reagents or solvents were obtained from commercial suppliers and used without further purification. All air sensitive experiments were performed in N<sub>2</sub> atmosphere through schlenk technology. Intermediate 2-a was synthesized according to literature procesures<sup>1</sup>. The <sup>1</sup>H and <sup>13</sup>C NMR spectra were measured by using a Bruker 500 MHz spectrometer at room temperature. Mass spectra were conducted at Micromass Q-Tof instrument (ESI) and Agilent Technologies 5973N (EI). A Hitachi F-4600 fluorescence spectrophotometer was used to measure phosphorescence spectral. An Edinburgh FLS-920 spectrometer was used to determine phosphorescence quantum efficiency and lifetimes of the molecules in solution. Elemental analyses for C, H, and N were performed on a Vario MICRO elemental analyzer.

Synthesis and characterization



Fig. S1. Synthesis of ligands L-1, L-2 and L-3.

L-1: 1-a (0.382 g, 2 mmol),  $K_2CO_3$  (1.104 g, 8 mmol) and phenol (0.752 g, 8 mmol) were charged to a 100 mL double-neck reaction bottle, followed by N-Methyl pyrrolidone (10 mL). The mixture was heated to 190 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with ethyl acetate three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by

column chromatography on silica gel with  $CH_2Cl_2$ / petroleum ether 1:1 (v/v) to afford white solid. 576 mg (85 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.64 (ddd, *J* = 4.8, 1.7, 0.9 Hz, 1H), 7.71 (m, 1H), 7.61 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.40 (d, *J* = 2.2 Hz, 2H), 7.35 (m, 4H), 7.22 (ddd, *J* = 7.4, 4.8, 1.1 Hz, 1H), 7.10 (m, 6H), 6.74 (dd, *J* = 3.0, 1.4 Hz, 1H). <sup>13</sup>C NMR(101 MHz, CDCl<sub>3</sub>): 158.98, 156.80, 156.24, 149.67, 142.38, 136.86, 129.89, 129.52, 123.66, 122.68, 120.77, 119.15, 115.52, 112.14, 109.99. EI-MS (*m/z*): 340 (M<sup>+</sup>, 100%).

2-b: 2-a (0.352 g, 1 mmol), Bis(pinacolato)diboron (0.379 g, 1.5 mmol) Pd(dppf)<sub>2</sub>Cl<sub>2</sub>(0.0229 g, 0.03 mmol) and CH<sub>3</sub>COOK (0.9814 g, 10 mmol) were charged to a 100 mL schlenck tube, followed by 1,4-Dioxane (15 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with CH<sub>2</sub>Cl<sub>2</sub>/ petroleum ether 1: 3 (v/v) to afford green solid. 337 mg (85 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.32 (d, *J* = 1.8 Hz, 1H), 7.30 (t, *J* = 3.7 Hz, 1H), 6.95 (s, 2H), 6.89 (m, 6H), 1.33 (s, 12H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 147.22, 144.81, 128.89, 123.91, 123.62, 123.44, 117.53, 117.24, 114.71, 83.89, 25.06, 24.87. EI-MS (*m/z*): 400.02 (M<sup>+</sup>, 100%).

L-2: 2-b (0.4791g, 1.2 mmol), 2-Bromopyridine (0.158 g, 1 mmol),  $Pd[P(C_6H_5)_3]_4$  (0.0115 g, 0.01 mmol) and  $K_2CO_3$  (0.55 g, 4 mmol) were charged to a 100 mL schlenck tube, followed by  $H_2O$  (2 mL) and 1,4-Dioxane (4 mL) . The mixture was heated to 100 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with  $CH_2Cl_2$  three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with  $CH_2Cl_2$ / petroleum ether 2: 1 (v/v) to afford green solid. 316 mg (75 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.63 (d, *J* = 4.3 Hz, 1H), 7.71 (td, *J* = 7.8, 1.5 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 2H), 7.21 (m, 3H), 6.94 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 155.60, 149.47, 146.94, 145.49, 136.83, 135.21, 128.80, 123.64, 122.1, 119.68, 117.58, 114.70, 109.71, 31.45, 30.20, 29.72. EI-MS (*m*/z): 351.04 (M<sup>+</sup>, 100%).

3-a: 2-Bromo-1,3-difluoro-5-iodobenzene (0.319 g, 1 mmol), K<sub>2</sub>CO<sub>3</sub> (0.552 g, 4 mmol) and phenol (0.376 g, 4 mmol) were charged to a 100 mL double-neck reaction bottle, followed by N-Methyl pyrrolidone (10 mL). The mixture was heated to 135 °C for 24 h under N<sub>2</sub>. The resulting solution was separated with water precipitation. The combined cake was dried in vacuum, and target product was purified by recrystallization with CH<sub>2</sub>Cl<sub>2</sub>/ petroleum ether to afford white solid. 20.9 g (90 %).<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.40 (m, 4H), 7.19 (m, 2H), 7.05 (m, 4H), 6.95 (d, *J* = 3.7 Hz, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 156.32, 155.96, 130.08, 124.39, 123.12, 118.98, 107.57, 91.27. EI-MS (*m*/*z*): 467 (M<sup>+</sup>, 100%).

3-b: 3-a (0.94 g, 2 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.23 g, 0.2 mmol) and 2-(tributylstannyl)pyridine (0.74 g, 2 mmol) were

charged to a 100 mL double-neck reaction bottle, followed by toluene (50 mL). The mixture was heated to 120 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with dichloromethane three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with  $CH_2CI_2$ / petroleum ether 1: 1 (v/v) to afford yellowish solid. 600 mg (71 %). <sup>1</sup>H NMR (400 MHz, CDCI<sub>3</sub>)  $\delta$  8.58 (dd, *J* = 4.8, 0.8 Hz, 1H), 7.66 (td, *J* = 7.8, 1.8 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.44 (s, 2H), 7.38 (m, 4H), 7.17 (m, 7H). <sup>13</sup>C NMR (101 MHz, CDCI<sub>3</sub>): 156.81, 155.73, 149.75, 140.41, 136.86, 129.95, 123.67, 122.83, 120.41, 118.33, 113.71, 109.22, 31.52, 30.25, 29.73. EI-MS (*m*/*z*): 419 (M<sup>+</sup>, 90%).

L-3: 3-b (0.209 g, 0.5 mmol) was charged to a 100 mL schlenck tube, followed by *m*-xylene (5 mL) under N<sub>2</sub>. *n*-BuLi (0.26 mL, 0.65 mmol) was added at -40 °C, and the resulting mixture was stirred for 1 h at -40 °C. Then, the mixture was warmed up to room temperature and stirred for another 1h. BBr<sub>3</sub> (0.061 mL, 0.65 mmol) was added at -40 °C and the mixture was stirred for 1 h at -40 °C, then the mixture was warmed up to room temperature and stirred for another 1h. BBr<sub>3</sub> (0.061 mL, 0.65 mmol) was added at -40 °C and the mixture was stirred for 1 h at -40 °C, then the mixture was warmed up to room temperature and stirred for another 1 h. Ethyldiisopropylamine (1.03 mmol, 0.175 mL) was added at 0 °C, then the mixture was warmed up to 120 °C and stirred for 12 h. The resulting solution was saturated with sodium acetate solution and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum to afford green solid. 160 mg (92 %). EI-MS (*m/z*): 347 (M<sup>+</sup>, 100%). As the ligand contains Lewis base pyridine unit, B–N interactions can occur, so the ligand cannot be characterized by nuclear magnetic resonance.



Fig. S2. Synthesis of iridium(III) complexes Ir-OO, Ir-ON, Ir-NN, Ir-OB and Ir-BB.

Ir-OO: L-1 (0.0824 g, 0.243 mmol) and IrCl<sub>3</sub> (0.035 g, 0.1 mmol) were charged to a 100 mL double-neck reaction bottle, followed by mixture of 2-ethoxyethanol (9 mL) and H<sub>2</sub>O (3 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. H<sub>2</sub>O (100 mL) was added and the resulting precipitate was filtered. The product has been washed three times with water and dried to give chloro-bridged dimer complex without further purification. The chloro-bridged dimer complex (0.181 g, 0.1 mmol), acetylacetone (0.05 mL, 0.5mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.053 g, 0.5 mmol) were charged to a 100 mL schlenck tube, followed by 2-ethoxyethanol (10 mL). The mixture was heated to 60 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with CH<sub>2</sub>Cl<sub>2</sub>/ petroleum ether 3:2 (v/v) to

afford yellow solid. 116 mg (60 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.30 (d, *J* = 5.0 Hz, 2H), 7.40 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.27 (s, 1H), 7.24 (m, 3H), 6.94 (m, 12H), 6.85 (m, 2H), 6.77 (t, *J* = 7.3 Hz, 2H), 6.17 (dd, *J* = 7.9, 5.0 Hz, 6H), 5.22 (s, 1H), 1.77 (s, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 184.01, 166.88, 163.01, 158.57, 157.89, 151.88, 149.42, 147.97, 135.60, 129.38, 128.21, 127.29, 121.92, 120.87, 120.54, 118.18, 117.38, 116.95, 113.09, 111.55, 100.17, 29.66, 28.51. C<sub>51</sub>H<sub>39</sub>IrN<sub>2</sub>O<sub>6</sub>•CHCl<sub>3</sub> calcd: C, 57.38; N, 2.57; H, 3.67. Found: C, 57.26; N, 2.55; H, 3.74. HR-MS: *m/z* calcd for C<sub>51</sub>H<sub>39</sub>IrN<sub>2</sub>O<sub>6</sub> [M]<sup>+</sup>: 968.2437. Found: 968.2494.

Ir-ON: L-2 (0.102 g, 0.3 mmol), L-1 (0.104 g, 0.3 mmol) and IrCl<sub>3</sub> (0.087 g, 0.25 mmol) were charged to a 100 mL double-neck reaction bottle, followed by mixture of 2-ethoxyethanol (15 mL) and H<sub>2</sub>O (5 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. H<sub>2</sub>O (100 mL) was added and the resulting precipitate was filtered. The product has been washed three times with water and dried to give chloro-bridged dimer complex without further purification. The chloro-bridged dimer complex (0.183 g, 0.1 mmol), acetylacetone (0.05 mL, 0.5 mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.053 g, 0.5 mmol) were charged to a 100 mL schlenck tube, followed by 2ethoxyethanol (10 mL). The mixture was heated to 60 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with CH<sub>2</sub>Cl<sub>2</sub>/ petroleum ether 3:1 (v/v) to afford orange solid. 78 mg (40 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.49 (d, J = 5.3 Hz, 1H), 8.15 (d, J = 5.5 Hz, 1H), 7.83 (m, 2H), 7.35 (m, 3H), 7.17 (m, 6H), 6.90 (m, 8H), 6.73 (t, J = 7.4 Hz, 2H), 6.58 (m, 2H), 6.14 (m, 3H), 5.53 (d, J = 7.9 Hz, 1H), 5.20 (s, 1H), 1.75 (d, J = 17.7 Hz, 6H). <sup>13</sup>C NMR(101 MHz, CDCl<sub>3</sub>): 184.22, 167.38, 158.87, 152.66, 149.33, 148.97, 148.02, 147.67, 136.51, 130.36, 128.90, 122.97, 122.18, 121.56, 121.32, 120.96, 120.47, 118.78, 116.62, 114.68, 114.22, 111.92, 107.48, 100.46, 29.70, 28.63. C<sub>51</sub>H<sub>36</sub>IrN<sub>3</sub>O<sub>6</sub> calcd: C, 62.56; N, 4.29; H, 3.71. Found: C, 62.41; N, 4.26; H, 3.82. HR-MS: *m*/z calcd for C<sub>51</sub>H<sub>36</sub>IrN<sub>3</sub>O<sub>6</sub> [M]<sup>+</sup>: 979.2233. Found: 979.2212.

Ir-OB: L-3 (0.104 g, 0.3 mmol), L-1 (0.104 g, 0.3 mmol) and IrCl<sub>3</sub> (0.087 g, 0.25 mmol) were charged to a 100 mL double-neck reaction bottle, followed by mixture of 2-ethoxyethanol (15 mL) and H<sub>2</sub>O (5 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. H<sub>2</sub>O (100 ml) was added and the resulting precipitate was filtered. The product has been washed three times with water and dried to give chloro-bridged dimer complex without further purification. The chloro-bridged dimer complex (0.182 g, 0.1 mmol), acetylacetone (0.05 mL, 0.5 mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.053 g, 0.5 mmol) were charged to a 100 mL schlenck tube, followed by 2-ethoxyethanol (10 mL). The mixture was heated to 60 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and

target product was purified by column chromatography on silica gel with  $CH_2CI_2$ / petroleum ether 3:2 (v/v) to afford red solid. 79 mg (40 %).<sup>1</sup>H NMR (400 MHz,  $d^6$ -DMSO)  $\delta$  8.63 (m, 1H), 8.57 (dd, J = 7.8, 1.5 Hz, 1H), 8.49 (d, J = 4.9 Hz, 1H), 8.37 (d, J = 8.2 Hz, 1H), 8.25 (d, J = 5.8 Hz, 1H), 8.10 (m, 2H), 7.72 (m, 2H), 7.61 (s, 1H), 7.53 (m, 2H), 7.44 (m, 2H), 7.35 (t, J = 7.4 Hz, 1H), 7.22 (m, 3H), 7.06 (m, 1H), 6.96 (t, J = 7.4 Hz, 1H), 6.82 (m, 4H), 6.71 (t, J = 7.3 Hz, 1H), 5.91 (m, 2H), 5.76 (m, 2H), 5.29 (s, 1H), 1.75 (s, 3H), 1.64 (s, 3H). <sup>13</sup>C NMR(101 MHz, d<sup>6</sup>-DMSO): 183.94, 183.75, 167.32, 166.90, 163.00, 162.50, 160.59, 159.95, 157.86, 157.26, 153.90, 152.93, 152.13, 149.96, 148.70, 148.03, 137.74, 137.13, 134.60, 134.10, 133.70, 133.35, 129.75, 128.47, 127.75, 122.47, 122.21, 121.01, 120.06, 119.83, 118.61, 117.74, 117.49, 117.31, 116.35, 114.35, 111.54, 111.04, 104.22, 100.33, 28.31, 28.12. C<sub>51</sub>H<sub>36</sub>BIrN<sub>2</sub>O<sub>6</sub>•CHCl<sub>3</sub> calcd: C, 56.97; N, 2.55; H, 3.37. Found: C, 56.86; N, 2.53; H, 3.48. HR-MS: *m*/z calcd for C<sub>51</sub>H<sub>36</sub>BlrN<sub>2</sub>O<sub>6</sub> [M]<sup>+</sup>: 976.2296. Found: 976.2280. Ir-NN: L-2 (0.085 g, 0.243 mmol) and IrCl<sub>3</sub> (0.035 g, 0.1 mmol) were charged to a 100 mL double-neck reaction bottle, followed by mixture of 2-ethoxyethanol (9 mL) and H<sub>2</sub>O (3 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. H<sub>2</sub>O (100 mL) was added and the resulting precipitate was filtered. The product has been washed three times with water and dried to give chloro-bridged dimer complex without further purification. The chloro-bridged dimer complex (0.185 g, 0.1 mmol), acetylacetone (0.05 mL, 0.5 mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.053 g, 0.5 mmol) were charged to a 100 mL schlenck tube, followed by 2-ethoxyethanol (10 mL). The mixture was heated to 60 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with  $CH_2Cl_2$ / petroleum ether 3.1 (v/v) to afford red solid. 149 mg (75 %).<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.37 (d, J = 5.5 Hz, 2H), 7.74 (m, 4H), 7.16 (m, 2H), 7.09 (dd, J = 8.0, 1.3 Hz, 2H), 7.03 (m, 2H), 6.98 (s, 2H), 6.81 (qd, J = 5.9, 4.1 Hz, 6H), 6.68 (td, J = 7.8, 1.4 Hz, 2H), 6.57 (td, J = 7.8, 1.3 Hz, 2H), 5.47 (dd, J = 8.0, 1.3 Hz, 2H), 5.20 (s, 1H), 1.75 (s, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): 184.35, 168.24, 151.16, 148.67, 147.97, 147.63, 142.13, 141.10, 136.26, 129.47, 128.94, 122.87, 122.76, 122.62, 122.18, 121.74, 120.09, 117.91, 117.00, 116.74, 114.63, 114.25, 107.40, 100.48, 29.71, 28.65. C<sub>51</sub>H<sub>33</sub>IrN<sub>4</sub>O<sub>6</sub>•2(CH<sub>2</sub>Cl<sub>2</sub>) calcd: C, 54.83; N, 4.82; H, 3.19. Found: C, 54.72; N, 4.79; H, 3.32. HR-MS: *m*/z calcd for C<sub>51</sub>H<sub>33</sub>IrN<sub>4</sub>O<sub>6</sub> [M]<sup>+</sup>: 990.2029. Found: 990.2002.

Ir-BB: L-2 (0.085 g, 0.243 mmol) and IrCl<sub>3</sub> (0.035 g, 0.1 mmol) were charged to a 100 mL double-neck reaction bottle, followed by mixture of 2-ethoxyethanol (9 mL) and H<sub>2</sub>O (3 mL). The mixture was heated to 110 °C for 24 h under N<sub>2</sub>. H<sub>2</sub>O (100 mL) was added and the resulting precipitate was filtered. The product has been washed three times with water and dried to give chloro-bridged dimer complex without further

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purification. The chloro-bridged dimer complex (0.184 g, 0.1 mmol), acetylacetone (0.05 mL, 0.5 mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.053 g, 0.5 mmol) were charged to a 100 mL schlenck tube, followed by 2-ethoxyethanol (10 mL). The mixture was heated to 60 °C for 24 h under N<sub>2</sub>. The resulting solution was saturated with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The combined organic phase was dried and concentrated in vacuum, and target product was purified by column chromatography on silica gel with CH<sub>2</sub>Cl<sub>2</sub>/ petroleum ether 3:2 (v/v) to afford red solid. 127 mg (65 %).<sup>1</sup>H NMR (400 MHz, *d*<sup>6</sup>-DMSO)  $\delta$  8.72 (d, *J* = 8.1 Hz, 2H), 8.55 (t, *J* = 6.7 Hz, 4H), 8.49 (d, *J* = 7.7 Hz, 2H), 8.22 (t, *J* = 7.7 Hz, 2H), 8.06 (s, 2H), 7.68 (t, *J* = 7.7 Hz, 2H), 7.47 (m, 6H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 7.4 Hz, 2H), 5.75 (m, 2H), 5.31 (s, 1H), 1.70 (s, 6H). <sup>13</sup>C NMR(101 MHz, *d*<sup>6</sup>-DMSO): 184.10, 167.41, 162.67, 160.44, 159.87, 153.61, 152.98, 148.96, 138.07, 134.58, 134.09, 133.73, 133.41, 130.11, 123.42,122.50, 122.24, 121.68, 120.88, 119.62, 118.48, 117.67, 117.20, 104.50, 100.39, 29.01, 28.21. C<sub>51</sub>H<sub>33</sub>B<sub>2</sub>IrN<sub>2</sub>O<sub>6</sub>•CH<sub>2</sub>Cl<sub>2</sub> calcd: C, 58.39; N, 2.62; H, 3.27. Found: C, 58.31; N, 2.59; H, 3.38. HR-MS: *m*/z calcd for C<sub>51</sub>H<sub>33</sub>B<sub>2</sub>IrN<sub>2</sub>O<sub>6</sub> [M]<sup>+</sup>: 984.2154. Found: 984.2185.

Ir-OB·Pyridine: <sup>1</sup>H NMR (400 MHz, *d*<sup>6</sup>-DMSO) δ 8.57 (m, 2H), 8.46 (d, *J* = 5.0 Hz, 1H), 8.24 (d, *J* = 8.1 Hz, 1H), 8.16 (d, *J* = 5.7 Hz, 2H), 8.01 (m, 3H), 7.78 (tt, *J* = 7.7, 1.8 Hz, 1H), 7.58 (dt, *J* = 7.6, 4.3 Hz, 2H), 7.47 (d, *J* = 2.2 Hz, 1H), 7.38 (ddd, *J* = 7.6, 4.3, 1.5 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.17 (m, 6H), 6.98 (m, 4H), 6.77 (m, 5H), 5.91 (d, *J* = 8.0 Hz, 2H), 5.77 (t, *J* = 3.4 Hz, 1H), 5.52 (d, *J* = 7.9 Hz, 1H), 5.27 (s, 1H), 1.72 (s, 3H), 1.65 (s, 3H).

Ir-OB·DMAP: <sup>1</sup>H NMR (400 MHz,  $d^{6}$ -DMSO)  $\delta$  8.47 (d, J = 5.0 Hz, 1H), 8.19 (m, 2H), 8.02 (m, 2H), 7.87 (m, 2H), 7.69 (d, J = 8.3 Hz, 1H), 7.54 (m, 1H), 7.47 (d, J = 2.3 Hz, 1H), 7.39 (s, 1H), 7.18 (m, 3H), 7.03 (m, 3H), 6.95 (t, J = 7.4 Hz, 1H), 6.86 (m, 3H), 6.78 (m, 4H), 6.71 (t, J = 7.2 Hz, 1H), 6.56 (d, J = 6.2 Hz, 2H), 5.95 (d, J = 7.4 Hz, 2H), 5.77 (m, 1H), 5.44 (s, 1H), 5.28 (s, 1H), 2.93 (s, 6H), 1.72 (s, 3H), 1.66 (s, 3H).

Ir-BB·Pyridine: <sup>1</sup>H NMR (400 MHz, *d*<sup>6</sup>-DMSO) δ 8.54 (m, 4H), 8.51 (d, *J* = 6.1 Hz, 2H), 8.40 (d, *J* = 8.4 Hz, 2H), 8.25 (d, *J* = 6.6 Hz, 2H), 8.07 (m, 4H), 7.78 (tt, *J* = 7.7, 1.8 Hz, 2H), 7.65 (s, 2H), 7.41 (m, 4H), 7.37 (ddd, *J* = 7.6, 4.3, 1.4 Hz, 4H), 7.15 (m, 6H), 6.98 (t, *J* = 7.3 Hz, 2H), 5.63 (d, *J* = 8.1 Hz, 2H), 5.34 (s, 1H), 1.71 (s, 6H).

Ir-BB·DMAP: <sup>1</sup>H NMR (400 MHz, *d*<sup>6</sup>-DMSO) δ 8.58 (d, *J* = 5.5 Hz, 2H), 8.09 (d, *J* = 5.5 Hz, 4H), 7.91 (m, 3H), 7.67 (d, *J* = 6.7 Hz, 2H), 7.47 (t, *J* = 6.3 Hz, 2H), 7.33 (s, 2H), 7.22 (t, *J* = 7.7 Hz, 3H), 7.09 (t, *J* = 7.1 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.78 (m, 6H), 6.57 (d, *J* = 5.7 Hz, 4H), 5.51 (d, *J* = 7.6 Hz, 2H), 5.32 (s, 1H), 2.94 (s, 12H), 1.77 (s, 6H).

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### UV/visible absorption spectra



Fig. S3. UV/visible absorption spectra of iridium complexes (Ir-OO, Ir-ON, Ir-OB, Ir-NN and Ir-BB) and corresponding ligands (L-1, L-2 and L-3) in degassed CH<sub>2</sub>Cl<sub>2</sub>.

### X-ray crystal structure analysis

Single-crystals of Ir-NN, Ir-BB and Ir-ON were all obtained by slow diffusion of ethanol to their  $CH_2CI_2$  solutions, respectively. Single-crystals of Ir-OB and Ir-OO were both obtained by slow diffusion of ethanol to their  $CHCI_3$  solutions, respectively. Single-crystals of Ir-BB·Pyridine and Ir-BB·DMAP were both obtained by slow diffusion of hexane to toluene/pyridine and toluene/DMAP solutions of Ir-BB, respectively. The X-ray diffraction data were collected on a Bruker Smart CCD Apex DUO diffractometer with graphite monochromated Mo K $\alpha$  radiation ( $\lambda$  = 0.71073 Å) using the  $\omega$ -20 scan mode. All crystal datas are deposited in The Cambridge Crystallographic Data Centre (CCDC: 1832468 for Ir-NN, 1832469 for Ir-OB, 1832470 for Ir-OO, 1860053 for Ir-ON, 1860052 for Ir-BB, 1860054 for Ir-BB+Pyridine, 1860055 for Ir-BB+DMAP).



Fig. S4. Crystal and packing structures of Ir-OO, the hydrogen atoms have been omitted for clarity, selected bond lengths (Å) and angles (°): Ir01–N1 2.038(3), Ir01–N2B 2.033(3), Ir01–C00U 1.999(3), Ir01–C00I 2.002(3), Ir01–O006 2.144(2), Ir01–O007 2.134(2); N1–Ir01–N2B 178.71(11), N1–Ir01–C00U 80.23(11), N1–Ir01–C00I 100.76(11), O006–Ir01–O007 88.59(9).



Fig. S5. Crystal and packing structures of Ir-ON, the hydrogen atoms have been omitted for clarity, selected bond lengths (Å) and angles (°): Ir1–N2 2.035(9), Ir1–N3 2.017(9), Ir1–C27 2.017(9), Ir1–C4 2.014(9), Ir1–O5 2.137(6), Ir1–O6 2.144(6); N2–Ir1–N3 178.9(3), N2–Ir1–C27 99.9(4), N2–Ir1–C4 79.7(4), O5–Ir1–O6 89.2(2).



Fig. S6. Crystal and packing structures of Ir-OB, the hydrogen atoms have been omitted for clarity, selected bond lengths (Å) and angles (°): Ir1–N1 2.050(5), Ir1–N2 2.044(5), Ir1–C10 2.019(5), Ir1–C8 2.021(6), Ir1–O5 2.121(3), Ir1–O6 2.138(4); N1–Ir1–N2 178.55(19), N1–Ir1–C10 100.8(2), N1–Ir1–C8 80.1(2), O5–Ir1–O6 89.76(13).



Fig. S7. Crystal and packing structures of Ir-BB, the hydrogen atoms have been omitted for clarity, selected bond lengths (Å) and angles (°): Ir01–N00C 2.030(5), Ir01–N00A 2.042(5), Ir01–C4D 2.024(5), Ir01–C6E 2.012(5), Ir01–O1 2.155(4), Ir01–O2 2.149(4); N00C–Ir01–N00A 177.2(2), N00C–Ir01–C4D 100.5(2), N00C–Ir01–C6E 80.2(2), O1–Ir01–O2 89.83(15).



Fig. S8. Crystal and packing structures of Ir-NN, the hydrogen atoms have been omitted for clarity, selected bond lengths (Å) and angles (°): Ir1–N2A 2.042(3), Ir1–N2B 2.027(4), Ir1–C8B 2.007(4), Ir1–C8A 2.015(4), Ir1–O3 2.138(3), Ir1–O4 2.148(3); N2A–Ir1–N2B 177.41(12), N2A–Ir1–C8B 100.88(15), N2A–Ir1–C8A 80.76(14), O3–Ir1–O4 88.95(11).



Fig. S9. (a) Crystal structure of Ir-BB-Pyridine, selected bond lengths (Å) and angles (°): Ir1–N2 2.048(5), Ir1–N1 2.025(5), Ir1–C16 2.025(6), Ir1–C8 2.022(5), Ir1–O5 2.138(4), Ir1–O6 2.157(4); N1–Ir1–N2 175.93(17), N2–Ir1–C16 102.3(2), N2–Ir1–C8 80.41(19), O5–Ir1–O6 88.39(15). (b) Crystal structure of Ir-BB-DMAP, selected bond lengths (Å) and angles(°): Ir1–N2 2.015(2), Ir1–N1 2.032(2), Ir1–C41 1.983(3), Ir1–C11 2.021(3), Ir1–O5 2.125(2), Ir1–O6 2.1321(19); N1–Ir1–N2 178.23(10), N1–Ir1–C41 101.71(9), N1– Ir1–C11 77.86(10), O5–Ir1–O6 88.19(8).

Complex	Ir-00	Ir-OB	Ir-NN	Ir-ON	Ir-BB
	$C_{51}H_{39}IrN_2O_6$	$C_{51}H_{36}BIrN_2O_6$	$C_{51}H_{33}\text{lr}N_4O_6$	$C_{51}H_{36}IrN_3O_6$	$C_{51}H_{33}B_2IrN_2O_6$
chemical formula	·CHCl <sub>3</sub>	.CHCl³	<sup>·</sup> 2(CH <sub>2</sub> Cl <sub>2</sub> )		·CH <sub>2</sub> Cl <sub>2</sub>
formula weight	1087.43	1095.22	1159.87	979.03	1068.56
crystal size (mm)	0.19 ×0.22 × 0.23	0.19 × 0.21 × 0.22	0.17 × 0.20 × 0.22	0.02 × 0.04 × 0.30	0.17 × 0.19 × 0.21
temperature (K)	296	296	293	173	296
radiation	0.71073	0.71073	0.71073	0.71073	0.71073
crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic
space group	P21/n	P21/c	P-1	P-1	P-1
a(Å)	10.3303(7)	14.7106(11)	9.758(3)	12.8021(14)	12.9285(11)
b(Å)	31.873(2)	23.3274(17)	13.838(4)	13.4779(14)	13.0934(11)
<i>c</i> (Å)	13.6751(9)	12.5713(10)	18.798(5)	13.5356(13)	15.0271(12)
α(°)	90	90	103.599	71.759	107.392
<b>β</b> (°)	95.520	90.352	104.123	73.179	96.416
γ(°)	90	90	101.639	63.251	111.677
V(Å <sup>3</sup> )	4481.8(5)	4313.9(6)	2300.4(11)	1950.2(4)	2183.9(3)
Z	4	4	2	2	2
ρ( <sub>calc</sub> ) (g/cm <sup>3</sup> )	1.612	1.686	1.674	1.667	1.625
F (000)	2168	2176	1152	976	1060
absorp.coeff. (mm⁻ ¹)	3.212	3.338	3.192	3.483	3.235
θ range (deg)	1.6 to 25.0	1.7 to 25.0	2.5 to 26.0	3.0 to 25.0	2.6 to 25.0
	32297	7556	35318	15739	7623
refins collected	(R <sub>int</sub> = 0.031)	(R <sub>int</sub> = 0.010)	(R <sub>int</sub> = 0.057)	(R <sub>int</sub> = 0.101)	(R <sub>int</sub> = 0.000)
indep. reflns	7867	7556	8968	6734	7623
Refns obs. [ <i>I ≥2σ(I)</i> ]	7208	6306	7206	4729	6708
data/restr/paras	7867/0/579	7556/0/588	8968/0/727	6734/0/581	7623 /0/ 588

## Table S1. Crystallographic Data for Ir-OO, Ir-ON, Ir-NN, Ir-OB and Ir-BB.

GOF	1.07	1.16	1.02	1.05	1.13
R₁/wR₂[ <i>l≥</i> 2σ( <i>l</i> )]	0.0234/0.0501	0.0397/0.1049	0.0346/0.0560	0.0565 / 0.0971	0.0367 / 0.1004
R <sub>1</sub> /wR <sub>2</sub> (all data)	0.0273/0.0536	0.0507/0.1107	0.0534/0.0594	0.0998 / 0.1116	0.0439 / 0.1036
larg peak and	0.00/ 0.00	2.49/-1.65	1.12/-0.74	1.95/–2.64	2.04 /0.99
hole(e/Å <sup>3</sup> )	0.88/-0.82				

## Table S2. Crystallographic Data for Ir-BB·Pyridine and Ir-BB·DMAP.

Complex	Ir-BB·Pyridine	Ir-BB·DMAP
chemical formula	$C_{61}H_{43}B_2IrN_4O_6$	$C_{65}H_{55}B_2IrN_6O_6$
formula weight	1141.84	1229.99
crystal size (mm)	0.20 ×0.22 × 0.25	0.18 ×0.20 ×0.22
temperature (K)	293	296
radiation	0.71073	0.71073
crystal system	Monoclinic	Monoclinic
space group	C2/c	P21/n
a(Å)	34.306(9)	16.7138(5)
b(Å)	16.952(5)	25.8579(4)
<i>c</i> (Å)	28.450(6)	16.5041(5)
α(°)	90	90
β(°)	126.132	103.462
γ(°)	90	90
V(Å <sup>3</sup> )	13363(6)	6936.8(3)
Z	8	4
$ ho(_{calc})$ (g/cm <sup>3</sup> )	1.135	1.178
F (000)	4576	2488
absorp.coeff. (mm <sup>-1</sup> )	2.042	1.973
θ range (deg)	1.4 to 25.0	1.5 to 27.9
<b>a</b>	22834	84639
retins collected	(R <sub>int</sub> = 0.057)	(R <sub>int</sub> = 0.098)

indep. reflns	11751	16178
Refns obs.	0200	12057
[ <i>l</i> >2 <i>σ(l</i> )]	9200	12057
data/restr/paras	11751/0/ 669	16178/0/ 727
GOF	1.02	1.07
R <sub>1</sub> /wR <sub>2</sub> [ <i>l</i> >2σ( <i>l</i> )]	0.0386/0.1145	0.0375/0.0760
R <sub>1</sub> /wR <sub>2</sub> (all data)	0.0490/0.1193	0.0558/0.0805
larg peak and hole(e/Å <sup>3</sup> )	1.17/–1.63	1.22/-1.58

## Cyclic voltammetry

The experiments for cyclic voltametric were performed by using three electrode cell assemblies from an IM6ex instrument (Zahner). A one-compartment cell equipped with a platinum wire counter electrode, a  $Ag/Ag^{+}$  reference electrode, and a glassy-carbon working electrode was used for all measurements with a scan rate of 100 mVs<sup>-1</sup>. The concentration of tetrabutylammonium hexafluorophosphate (Bu<sub>4</sub>NPF<sub>6</sub>) in dichloromethane solution was 0.10 molL<sup>-1</sup> and used as supporting electrolyte.



Fig. S10. Cyclic voltammograms of Ir-OO, Ir-ON, Ir-NN, Ir-OB and Ir-BB in degassed CH<sub>2</sub>Cl<sub>2</sub> under the scan rate of 100 mV s<sup>-1</sup>.

### OLED device characterization

The prepatterned indium tin oxide (ITO) substrates were cleaned by ultrasonic acetone bath, followed by ethanol bath. Afterwards, the substrates were dried with N<sub>2</sub> and then loaded into a UV-Ozone chamber. After UV-Ozone treatment, The PEDOT: PSS layer was spin-coated on the ITO substrate as the hole-injecting layer, and then annealed at 120 °C for 10 min inside the N<sub>2</sub>-filled glove-box. The emitter layer was also prepared by spin-coating directly on the hole-injecting layer, and then annealed at 50 °C for 10 min. The electron-transporting material and the cathode material were thermally evaporated onto the emitter layer in a vacuum chamber. Before taken out of the glove-box, the devices were encapsulated with UV-curable epoxy. The voltage-current-luminance characteristics and the EL spectra were simultaneously measured with PR735 Spectra Scan Photometer and Keithley 2400 sourcemeter unit under ambient atmosphere at room temperature.



Fig. S11. Configuration of the OLEDs and chemical structures for the materials involved.



Fig. S12. The J–V–L characteristics for devices of Ir-OO, Ir-ON, Ir-NN, Ir-OB and Ir-BB.

complexes	$V_{\rm on}{}^{\rm a}$	EQE <sub>max</sub> /CE <sub>max</sub> /PE <sub>max</sub> <sup>b</sup>	EQE <sub>100</sub> /CE <sub>100</sub> /PE <sub>100</sub> <sup>c</sup>	$\lambda_{ems}^{d}$	CIE <sup>e</sup>	FWHM <sup>f</sup>
	[V]	[%/cd A <sup>-1</sup> /lm W <sup>-1</sup> ]	[%/cd A <sup>-1</sup> /lm W <sup>-1</sup> ]	[nm]	(x, y)	[cm <sup>-1</sup> ]
Ir-OO	2.9	7.5/25/23	3.5/12/4.3	538	(0.40, 0.57)	2819
Ir-ON	2.9	5.2/15/9.4	2.6/7.2/2.8	568	(0.50, 0.49)	2416
Ir-NN	3.0	5.1/12/11	1.8/4.2/1.7	578	(0.55, 0.44)	2385
Ir-OB	3.4	5.4/6.2/6.5	2.0/2.2/0.7	620	(0.64, 0.34)	1741
Ir-BB	3.3	6.2/4.2/4.4	1.8/1.2/0.4	638	(0.67, 0.31)	1211

Table S3. Comparison of the EL performances of the devices

<sup>a</sup> Voltage in the luminance of 10 cd/m<sup>2</sup>. <sup>b</sup> Maximum external quantum efficiency (EQE<sub>max</sub>), maximum current efficiency (CE<sub>max</sub>), maximum power efficiency (PE<sub>max</sub>). <sup>c</sup> EQE, CE, PE at 100 mA cm<sup>-2</sup>. <sup>d</sup> Maximum emission wavelength of the EL spectra. <sup>e</sup> The Commission Internationale de l'Eclairage (CIE) coordinates. <sup>f</sup> The full width at half maximum.

<sup>1</sup>H NMR changes, optical response and binding constant for Ir-OB



Fig. S13. Titrations of Ir-OB in *d*<sup>6</sup>-DMSO with excess pyridine (a) and DMAP (b) monitored by <sup>1</sup>H NMR spectra.



Fig. S14. Titrations of Ir-OB in DMSO ([Ir-OB]<sub>0</sub> =  $3 \times 10^{-5}$  M) with pyridine (a, c) and DMAP (b, d) monitored by UV-vis absorption (a, b) and phosphorescence ( $\lambda_{ex}$  = 370 nm) spectroscopies (c, d).



Fig. S15. UV-vis absorption titration plot of Ir-OB with pyridine. The absorbance at 522 nm of DMSO solution of Ir-OB (3 ×10<sup>-5</sup> M) was monitored during the titration with pyridine (black dots). The fitting curve was delineated for the determination of the binding constant of Ir-OB toward pyridine (blue line). The binding constant  $K_{pyridine}$  was calculated to be 19.6 (±0.00016) M<sup>-1</sup>.



Fig. S16. UV-vis absorption titration plot of Ir-OB with pyridine. The absorbance at 522 nm of DMSO solution of Ir-OB (3 ×10<sup>-5</sup> M) was monitored during the titration with DMAP (black dots). The fitting curve was delineated for the determination of the binding constant of Ir-OB toward DMAP (blue line). The binding constant  $K_{DMAP}$  was calculated to be 8.0 (±0.012)×10<sup>3</sup> M<sup>-1</sup>.

### **DFT** calculation

DFT method was used to optimize the geometries all the complexes. The electronic transition energies and electron correlation effects were also calculated by (TD)-DFT method with the B3LYP functional (TD-B3LYP). The LANL2DZ basis set was used to treat with the iridium atom, and the 6–31G(d) basis set was used to treat with all other atoms. All calculations were carried out according to the Gaussian 09 program.<sup>1</sup>



Fig. S17. Scheme caption. The optimized geometries and main orbital transitions of Ir-OO, Ir-ON, Ir-NN, Ir-OB and Ir-BB at the lowest triplet excited state  $(T_1)$ .



Fig. S18. Calculated HOMO and LUMO at the ground state for iridium complexes and comparison with the experimental energy levels. Black (experimental) and blue (calculated).



Figure S19. The optimized geometries of (a) Ir-OB-Pyridine and (b) Ir-OB-DMAP at the lowest triplet excited state ( $T_1$ ).

Complex	State	E (eV) (nm)	Main configurations	Character
Ir-00	S1	2.7638 (448nm)	HOMO→LUMO (0.69)	MLCT/ILCT
	T1	1.8867 (657nm)	HOMO→LUMO (0.66)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT
Ir-ON	S1	2.5107 (493nm)	HOMO→LUMO (0.70)	LLCT
	T1	1.7222 (719nm)	HOMO→LUMO (0.63)	<sup>3</sup> LLCT/ <sup>3</sup> ILCT
lr-NN	S1	2.5890 (478nm)	HOMO→LUMO (0.68)	ILCT
	T1	1.7132 (723nm)	HOMO→LUMO (0.66)	<sup>3</sup> ILCT
lr-OB	S1	2.4331 (509nm)	HOMO→LUMO (0.69)	MLCT/ILCT/LLCT
	T1	1.6351 (758nm)	HOMO→LUMO (0.68)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT/ <sup>3</sup> LLCT
lr-BB	S1	2.2299 (556nm)	HOMO→LUMO (0.69)	MLCT/ILCT/LLCT
	T1	1.6023 (773nm)	HOMO→LUMO (0.67)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT/ <sup>3</sup> LLCT

Table S4. Calculated energies for lowest-energy singlet (S1) and triplet (T1) transitions of all Iridium(III) complexes.

Table S5. Calculated energies for lowest-energy singlet (S1) and triplet (T1) transitions of all B-N Lewis adducts.

Complex	State	E (eV) (nm)	Main configurations	Character
Ir-OB · Pyridine	S1	2.2407 (553nm)	HOMO→LUMO (0.70)	MLCT/ILCT
	T1	1.6196 (765nm)	HOMO→LUMO (0.68)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT
Ir-OB.DMAP	S1	2.3147 (535nm)	HOMO→LUMO (0.69)	MLCT/ILCT
	T1	1.8727 (662nm)	HOMO $\rightarrow$ LUMO (0.56)	<sup>3</sup> MLCT/ <sup>3</sup> LLCT
			HOMO→LUMO+1 (0.40)	3MLC1/3ILC1
Ir-BB·Pyridine	S1	1.9161 (647nm)	HOMO→LUMO (0.69)	MLCT/ILCT
	T1	1.3684 (906nm)	HOMO→LUMO (0.69)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT
Ir-BB.DMAP	S1	2.4934 (497nm)	HOMO→LUMO (0.68)	MLCT/ILCT
	T1	1.8322 (676nm)	HOMO→LUMO (0.66)	<sup>3</sup> MLCT/ <sup>3</sup> ILCT

## NMR spectra



Fig. S20. <sup>1</sup>H NMR spectra of Ir-BB-Pyridine.



Fig. S21. <sup>1</sup>H NMR spectra of Ir-BB-DMAP.



Fig. S22. <sup>1</sup>H NMR spectra of Ir-OB-Pyridine.



Fig. S23. <sup>1</sup>H NMR spectra of Ir-OB-DMAP.

## TG analysis



Fig. S24. TG thermograms of all iridium complexes (Ir-OO, Ir-ON, Ir-OB, Ir-NN and Ir-BB).

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