# **Supporting Information**

## Highly Efficient White Organic Electroluminescence Device Based on a Phosphorescent Orange Material Doped in a Blue Host Emitter

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*Synthesis:* Materials obtained from commercial suppliers were used without further purification. Anhydrous hexane was distilled with sodium benzophenone ketyl under nitrogen atmosphere, degassed by the freeze-pump-thaw method. All glass wares, syringes, magnetic stirring bars and needles were dried in a convection oven at least 4 hours. Reactions were monitored with thin layer chromatography (TLC). Commercial TLC plates (Silica gel 60 F254, Merck Co.) were developed and the spots were seen under UV light at 254 and 365 nm. Silica column chromatography was done with silica gel 60 G (particle size 5~40  $\mu$ m, Merck Co.). <sup>1</sup>H NMR spectrum was recorded on a Bruker AVANVE 300 MHz spectrometer with tetramethylsilane as an internal standard. Mass spectra were measured on a GC/MS mass spectrometer. Elemental analyses were performed on a flash EA 1112 spectrometer.

[(bzq)<sub>2</sub>Ir( $\mu$ -Cl)]<sub>2</sub> was synthesized according to a modified version of the Nonoyama procedure, by refluxing IrCl<sub>3</sub>.*n*H<sub>2</sub>O (7 mmol, 2.5 g) with 2.5 equiv of the ligand of benzoquinoline (3.2 g) in a 3:1 mixture of 2-methoxyethanol and water for 6-7 h. The reaction mixture was cooled to room temperature, and more water was added to precipitate the product. The resulting mixture was subsequently filtered through a Buchner funnel and then washed with hexane and ethyl ether several times to provide the crude product: [(bzq)<sub>2</sub>Ir( $\mu$ -Cl)]<sub>2</sub>, 82% yield. <sup>S1</sup>

(bzq)<sub>2</sub>Ir(dipba): In a 50-mL flask, a hexane solution of n-BuLi (0.15 mL x 2.6 M) was added to 1-bromobenzene (65 mg, 0.4 mmol) in hexane (10 mL) under argon. The reaction mixture was stirred at room temperature for 1 hour, and was then added dropwise to N,N'-diisopropylcarbodiimide (50 mg, 0.4 mmol). The colorless solution was stirred rapidly for 30 min, and then added dropwise to  $[(bzq)_2Ir(\mu-Cl)]_2$  (230 mg, 0.2 mmol) in hexane solvent (15 mL). After being stirred at 80°C for 8 hours, the reaction mixture was cooled to room temperature. The solvent was evaporated under

Supplementary Material (ESI) for *Journal of Materials Chemistry* This journal is © The Royal Society of Chemistry 2011 vacuum, and the product was washed with Et<sub>2</sub>O (20 mL) three times, giving rise to (bzq)<sub>2</sub>Ir(dipba) (68%).

(bzq)<sub>2</sub>Ir(dipba): MS: m/z 753 (M<sup>+</sup>). Anal. Calcd for C<sub>39</sub>H<sub>36</sub>IrN<sub>4</sub>: C, 62.21; H, 4.82; N, 7.44. Found: C, 62.12; H, 4.78; N, 7.55. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  9.63 (d, J = 5.10, 2H), 8.19 (d, J = 8.1 Hz, 2H), 7.74 (d, J = 9.0 Hz, 2H), 7.62 (t, J = 7.2, 2H), 7.60 (d, J = 9.0 Hz, 2H), 7.44-7.33 (m, 5H), 7.30 (d, J = 8.1 Hz, 2H), 6.91 (t, J = 7.2 Hz, 2H), 6.38 (d, J = 7.2 Hz, 2H), 3.23-3.16 (m, 2H), 0.65 (d, J = 6.0 Hz, 6H), -0.47 (d, J = 6.0 Hz, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  24.04, 24.86, 48.05, 117.01, 120.50, 122.89, 126.01, 128.01, 128.19, 128.62, 129.07, 129.37, 133.76, 134.30, 136.92, 142.04, 149.74, 152.54, 159.66, 175.13.



**S-Scheme 1.** Synthetic route for the Ir-complex (bzq)<sub>2</sub>Ir(dipba).

*Fabrication of the OLEDs and EL Measurements*: The general architecture of the complex multilayer diodes used in this study is as follows: The ITO (indium-tin oxide) coated glass substrates ( $20\Omega$ /square) were first cleaned in ethanol, acetone, and soap ultrasonic bathes. All organics were purified by gradient sublimation and thermally evaporated at a rate of 1.0 Å s<sup>-1</sup> at a base pressure of around 3.5 x 10<sup>-4</sup> Pa. A LiF layer (0.5 nm) was deposited at a rate of 0.2 Å s<sup>-1</sup>. The finishing Al electrode (cathode) was deposited at a rate of 10 Å s<sup>-1</sup> in another chamber. The active area of the diode segments was 2 x 3 mm<sup>2</sup>. EL spectra and brightness-current density-voltage characteristics of the devices were measured by combining a Spectrascan PR-650 spectrophotometer with a computer-controlled direct-current power supply Keithley model 2400 voltage-current source under ambient condition at room temperature.

Single-carrier devices were fabricated using the following configurations: [Al/active molecular layer (85 nm)/Al] (electron-only device) and [ITO/active molecular layer (85 nm)/Au] (hole-only device). A low work function metal (Al) is used as the electrodes in electron-only devices, whereas a metal (Au) or a metal oxide (ITO) with a high work function is used as the electrodes in hole-only devices.

Absorption, PL and Electrochemical Measurements: Absorption spectrum was obtained using a Shimadzu UV-2550 UV-vis spectrometer. PL spectra were recorded by a Perkin-Elmer LS-55 fluorescence spectrometer with a Xe arc lamp excitation source. All solvents were degassed via three freeze-pump-thaw cycles. The PL quantum yields were measured by use of quinine sulfate in 1 M sulfuric acid as a standard ( $\Phi$ = 0.546).<sup>S2</sup>

Electrochemical measurements were performed with a BAS 100W Bioanalytical electrochemical work station, using Pt working electrode, platinum wire as auxiliary electrode, and a porous glass wick  $Ag/Ag^+$  as reference electrode, standardized against ferrocene/ferrocenium couple, scan rate 100 mV s<sup>-1</sup>. The electrochemical behavior of the corresponding compounds were studied by cyclic voltammetry using ferrocene as an internal standard. Due to the limitation<sup>S3</sup> in measuring reduction potentials in the range of -2.7 V to -3.5 V in CH<sub>2</sub>Cl<sub>2</sub>, we obtained only the oxidation potentials for (bzq)<sub>2</sub>Ir(dipba), and no reduction wave was detected within the electrochemical window of dichloromethane. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy levels of (bt)<sub>2</sub>Ir(dipba) were calculated from the cyclic voltammetry (CV) data together with the absorption spectrum.

The time-of-flight (TOF) technique involves generation of carriers near one electrode with a short pulse of light and observation of the current displaced in the external circuit by the motion of the carriers through the sample. The sample for TOF measurement has been prepared on the glass substrate covered with indium tin oxide (ITO) layer with the structure of  $[(ITO)/(bzq)_2Ir(dipba) (1 \ \mu m)/AI]$ . An intense short duration (5-6 ns) light pulse from a frequency-tripled (355 nm) Nd:YAG laser was incident at one side of the sample to generate photocarriers. The sample was mounted in a vacuum and measurement was made at the electric field of  $6.0 \times 10^{-5}$  V cm<sup>-1</sup> under room temperature (293 K).

Single-Crystal XRD Data of Crystals: Single crystals suitable for X-ray structural analysis were obtained by vacuum sublimation. Diffraction data were collected on a Rigaku R-Axis Rapid diffractometer (Mo K $\alpha$  radiation, graphite monochromator) in

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the  $\psi$  rotation scan mode. The structure determination was performed by direct methods using SHELXTL 5.01v and refinements with full-matrix least squares on  $F^2$ .

The crystal structure and crystal packing diagram of  $(bzq)_2Ir(dipba)$  were given in S-Fig. 1 and 2, and the corresponding crystal data were listed in S-Table 1, 2, 3 and 4. CCDC reference number 714888.



S-Fig. 1 Thermal ellipsoid (ORTEP) plot of (bzq)<sub>2</sub>Ir(dipba).



S-Fig. 2 Crystal packing diagram of (bzq)<sub>2</sub>Ir(dipba).

**S-Fig. 2** revealed that there is only a very little parallel overlap between the bzq aromatic rings of two adjacent molecules in the solid state of  $(bzq)_2Ir(dipba)$ , with the shortest face-to-face separation being ca. 3.3 Å, suggesting that there is almost no intermolecular  $\pi$ - $\pi$  interaction between the ppy groups. The lack of intermolecular  $\pi$ - $\pi$  interaction could help prevent the undesired triplet-triplet annihilation in the solid state of these materials, especially in  $(bzq)_2Ir(dipba)$ .



**S-Fig. 3** Current density-electric field characteristics of the single-carrier devices based on neat  $(bzq)_2Ir(dipba)$  film (top) and  $(bzq)_2Ir(dipba)$  doped in Bepp<sub>2</sub> film with the concentration of 2 mol % (bottom) as the active molecular layer.



**S-Fig. 4** EL spectra of Device I [ITO/NPB (30 nm)/(bzq)<sub>2</sub>Ir(dipba) (20 nm)/Bepp<sub>2</sub> (35 nm)/LiF (0.5 nm)/Al] and the single layer device [ITO/(bzq)<sub>2</sub>Ir(dipba) (85 nm)/LiF (0.5 nm)/Al] at the driving voltage of 6 V.



**S-Fig. 5** Current density and brightness-voltage curves of device I [ITO/NPB (30 nm)/(bzq)<sub>2</sub>Ir(dipba) (20 nm)/Bepp<sub>2</sub> (35 nm)/LiF (0.5 nm)/Al] (top) and the single layer device [ITO/(bzq)<sub>2</sub>Ir(dipba) (85 nm)/LiF (0.5 nm)/Al] (bottom).



**S-Fig. 6** Luminous efficiency, external quantum efficiency and power efficiency-brightness curves (top). Luminous efficiency, external quantum efficiency and power efficiency-current density curves (bottom) of Device II.



**S-Fig. 7** PL decay characteristics for Bepp<sub>2</sub> at 300 K in THF solution (top) and in solid state (bottom).



**S-Fig. 8** Time dependent emission spectra (top) and images in THF solution (77 K) (bottom).

Identification code	(bzq) <sub>2</sub> Ir(dipba)
Empirical formula	C <sub>39</sub> H <sub>35</sub> Ir N <sub>4</sub>
Formula weight	751.91
Temperature, K	293(2)
Wavelength, Å	0.71073
Crystal system	Monoclinic
space group	C2/c
Unit cell dimensions	
a (Å)	13.245(3)
b (Å)	16.006(3)
c (Å)	29.949(6)
α (deg)	90
β(deg)	93.84(3)
γ (deg)	90
Volume, Å <sup>3</sup>	6335(2)
Z	8
Calculated density, g/cm <sup>3</sup>	1.577
Abs coeff, mm <sup>-1</sup>	4.249
F(000)	2992
Crystal size, mm	0.20 x 0.19 x 0.16
Theta range for	3.08 to 27.48
data collection, deg.	
Limiting indices	-17<=h<=16,
	-20<=k<=20,
	-38<=1<=38
Reflections collected / unique	26545 / 7190 [R(int) = 0.0431]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	7190 / 0 / 401
GOF on $F^2$	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0373, $wR2 = 0.0627$
R indices (all data)	R1 = 0.0492, $wR2 = 0.0661$

S-Table 1 Crystal data and structure refinement for (bzq)<sub>2</sub>Ir(dipba).

**S-Table 2** Atomic coordinates  $(x \ 10^4)$  and equivalent isotropic displacement parameters  $(\text{\AA}^2 x \ 10^3)$  for  $(\text{bzq})_2 \text{Ir}(\text{dipba})$ . U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	Х	у	Z	U(eq)
C(1)	5597(3)	4851(3)	8243(2)	45(1)
Ir(1)	7322(1)	5628(1)	8816(1)	29(1)
N(1)	5902(2)	5220(2)	8625(1)	34(1)
C(2)	4596(4)	4590(3)	8149(2)	55(1)
N(2)	8758(2)	5961(2)	9044(1)	33(1)
C(3)	3898(4)	4719(3)	8458(2)	55(1)
N(3)	7165(3)	6683(2)	8364(1)	39(1)
C(4)	4183(3)	5105(3)	8864(2)	43(1)
N(4)	7872(3)	5530(2)	8147(1)	37(1)
C(5)	3523(3)	5288(3)	9213(2)	53(1)
C(6)	3865(3)	5674(3)	9594(2)	53(1)
C(7)	4901(3)	5926(3)	9672(1)	41(1)
C(8)	5298(4)	6339(3)	10054(2)	51(1)
C(9)	6304(4)	6560(3)	10089(1)	49(1)
C(10)	6959(3)	6381(3)	9753(1)	41(1)
C(11)	6615(3)	5964(2)	9364(1)	32(1)
C(12)	5576(3)	5749(2)	9337(1)	33(1)
C(13)	5203(3)	5346(2)	8939(1)	35(1)
C(14)	9216(3)	6691(3)	8997(1)	41(1)
C(15)	10227(3)	6819(3)	9139(2)	50(1)
C(16)	10783(3)	6179(3)	9328(2)	47(1)
C(17)	10336(3)	5399(3)	9384(1)	38(1)
C(18)	10828(3)	4676(3)	9581(2)	45(1)
C(19)	10328(3)	3949(3)	9625(2)	46(1)
C(20)	9277(3)	3867(3)	9484(1)	38(1)
C(21)	8706(4)	3143(3)	9542(2)	47(1)
C(22)	7701(4)	3130(3)	9411(2)	50(1)
C(23)	7214(3)	3825(3)	9203(1)	38(1)
C(24)	7735(3)	4557(2)	9126(1)	29(1)
C(25)	8767(3)	4561(2)	9287(1)	31(1)
C(26)	9311(3)	5318(2)	9241(1)	31(1)
C(27)	7590(3)	6300(3)	8035(1)	35(1)
C(28)	7768(3)	6687(3)	7591(1)	39(1)
C(29)	7155(4)	6496(4)	7219(2)	66(2)
C(30)	7332(6)	6841(4)	6809(2)	84(2)
C(31)	8119(6)	7378(4)	6772(2)	83(2)
C(32)	8721(5)	7575(4)	7137(2)	85(2)
C(33)	8554(4)	7237(4)	7549(2)	64(2)

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C(34)	6579(4)	7455(3)	8308(2)	49(1)		
C(35)	6804(6)	8023(4)	8704(2)	89(2)		
C(36)	5464(5)	7269(4)	8253(3)	108(3)		
C(37)	8577(3)	5038(3)	7893(1)	42(1)		
C(38)	8188(5)	4158(4)	7832(3)	105(3)		
C(39)	9623(4)	5034(5)	8120(2)	81(2)		

**S-Table 3** Bond lengths [Å] and angles [°] for (bzq)<sub>2</sub>Ir(dipba).

C(1)-N(1)	1.327(5)	C(18)-C(19)	1.350(6)
C(1)-C(2)	1.400(6)	C(19)-C(20)	1.433(6)
Ir(1)-C(24)	2.008(4)	C(20)-C(21)	1.400(6)
Ir(1)-C(11)	2.016(4)	C(20)-C(25)	1.409(5)
Ir(1)-N(1)	2.037(3)	C(21)-C(22)	1.363(6)
Ir(1)-N(2)	2.049(3)	C(22)-C(23)	1.410(6)
Ir(1)-N(3)	2.165(3)	C(23)-C(24)	1.387(5)
Ir(1)-N(4)	2.183(3)	C(24)-C(25)	1.419(5)
Ir(1)-C(27)	2.620(4)	C(25)-C(26)	1.421(5)
N(1)-C(13)	1.377(5)	C(27)-C(28)	1.497(5)
C(2)-C(3)	1.366(7)	C(28)-C(29)	1.369(6)
N(2)-C(14)	1.328(5)	C(28)-C(33)	1.376(6)
N(2)-C(26)	1.373(5)	C(29)-C(30)	1.383(7)
C(3)-C(4)	1.395(7)	C(30)-C(31)	1.360(9)
N(3)-C(27)	1.320(5)	C(31)-C(32)	1.347(9)
N(3)-C(34)	1.463(5)	C(32)-C(33)	1.380(7)
C(4)-C(13)	1.409(6)	C(34)-C(36)	1.506(8)
C(4)-C(5)	1.435(6)	C(34)-C(35)	1.510(7)
N(4)-C(27)	1.325(5)	C(37)-C(39)	1.501(7)
N(4)-C(37)	1.470(5)	C(37)-C(38)	1.508(7)
C(5)-C(6)	1.348(7)		
C(6)-C(7)	1.435(7)	N(1)-C(1)-C(2)	122.3(4)
C(7)-C(8)	1.393(6)	C(24)-Ir(1)- $C(11)$	88.71(15)
C(7)-C(12)	1.415(5)	C(24)-Ir(1)-N(1)	94.20(14)
C(8)-C(9)	1.376(7)	C(11)-Ir(1)-N(1)	80.96(15)
C(9)-C(10)	1.403(6)	C(24)-Ir(1)-N(2)	81.33(14)
C(10)-C(11)	1.393(6)	C(11)-Ir(1)-N(2)	97.51(15)
C(11)-C(12)	1.415(6)	N(1)-Ir(1)-N(2)	175.33(13)
C(12)-C(13)	1.414(6)	C(24)-Ir(1)-N(3)	165.17(14)
C(14)-C(15)	1.392(6)	C(11)-Ir(1)-N(3)	105.70(14)
C(15)-C(16)	1.363(7)	N(1)-Ir(1)-N(3)	91.57(13)
C(16)-C(17)	1.396(6)	N(2)-Ir(1)-N(3)	93.09(13)
C(17)-C(26)	1.402(6)	C(24)-Ir(1)-N(4)	105.41(13)
C(17)-C(18)	1.435(6)	C(11)-Ir(1)-N(4)	165.51(14)

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N(1)-Ir(1)-N(4)	94.52(13)	N(2)-C(14)-C(15)	122.3(4)
N(2)-Ir(1)-N(4)	88.01(13)	C(16)-C(15)-C(14)	119.9(4)
N(3)-Ir(1)-N(4)	60.45(12)	C(15)-C(16)-C(17)	120.0(4)
C(24)-Ir(1)-C(27)	135.59(13)	C(16)-C(17)-C(26)	117.1(4)
C(11)-Ir(1)-C(27)	135.70(14)	C(16)-C(17)-C(18)	125.8(4)
N(1)-Ir(1)-C(27)	93.42(13)	C(26)-C(17)-C(18)	117.0(4)
N(2)-Ir(1)-C(27)	90.74(13)	C(19)-C(18)-C(17)	121.5(4)
N(3)-Ir(1)-C(27)	30.15(12)	C(18)-C(19)-C(20)	121.6(4)
N(4)-Ir(1)-C(27)	30.31(12)	C(21)-C(20)-C(25)	117.2(4)
C(1)-N(1)-C(13)	118.4(4)	C(21)-C(20)-C(19)	124.2(4)
C(1)-N(1)-Ir(1)	127.3(3)	C(25)-C(20)-C(19)	118.6(4)
C(13)-N(1)-Ir(1)	114.3(3)	C(22)-C(21)-C(20)	120.1(4)
C(3)-C(2)-C(1)	119.7(4)	C(21)-C(22)-C(23)	121.6(4)
C(14)-N(2)-C(26)	118.1(4)	C(24)-C(23)-C(22)	121.5(4)
C(14)-N(2)-Ir(1)	127.9(3)	C(23)-C(24)-C(25)	115.2(4)
C(26)-N(2)-Ir(1)	113.9(3)	C(23)-C(24)-Ir(1)	132.5(3)
C(2)-C(3)-C(4)	120.1(4)	C(25)-C(24)-Ir(1)	112.3(3)
C(27)-N(3)-C(34)	123.7(3)	C(20)-C(25)-C(24)	124.3(4)
C(27)-N(3)-Ir(1)	94.4(2)	C(20)-C(25)-C(26)	118.8(4)
C(34)-N(3)-Ir(1)	139.4(3)	C(24)-C(25)-C(26)	117.0(3)
C(3)-C(4)-C(13)	117.4(4)	N(2)-C(26)-C(17)	122.6(4)
C(3)-C(4)-C(5)	125.7(4)	N(2)-C(26)-C(25)	114.9(3)
C(13)-C(4)-C(5)	116.9(4)	C(17)-C(26)-C(25)	122.4(4)
C(27)-N(4)-C(37)	123.0(3)	N(3)-C(27)-N(4)	111.7(3)
C(27)-N(4)-Ir(1)	93.4(2)	N(3)-C(27)-C(28)	124.8(4)
C(37)-N(4)-Ir(1)	140.8(3)	N(4)-C(27)-C(28)	123.4(4)
C(6)-C(5)-C(4)	121.5(4)	N(3)-C(27)-Ir(1)	55.4(2)
C(5)-C(6)-C(7)	121.9(4)	N(4)-C(27)-Ir(1)	56.3(2)
C(8)-C(7)-C(12)	117.1(4)	C(28)-C(27)-Ir(1)	178.7(3)
C(8)-C(7)-C(6)	124.8(4)	C(29)-C(28)-C(33)	118.7(4)
C(12)-C(7)-C(6)	118.1(4)	C(29)-C(28)-C(27)	120.6(4)
C(9)-C(8)-C(7)	119.7(4)	C(33)-C(28)-C(27)	120.7(4)
C(8)-C(9)-C(10)	122.3(4)	C(28)-C(29)-C(30)	120.5(6)
C(11)-C(10)-C(9)	121.0(4)	C(31)-C(30)-C(29)	120.1(6)
C(10)-C(11)-C(12)	115.3(4)	C(32)-C(31)-C(30)	119.9(5)
C(10)-C(11)-Ir(1)	131.6(3)	C(31)-C(32)-C(33)	120.8(6)
C(12)-C(11)-Ir(1)	113.1(3)	C(28)-C(33)-C(32)	120.0(6)
C(13)-C(12)-C(7)	119.1(4)	N(3)-C(34)-C(36)	110.7(4)
C(13)-C(12)-C(11)	116.2(3)	N(3)-C(34)-C(35)	110.0(4)
C(7)-C(12)-C(11)	124.6(4)	C(36)-C(34)-C(35)	110.2(5)
N(1)-C(13)-C(4)	122.2(4)	N(4)-C(37)-C(39)	111.6(4)
N(1)-C(13)-C(12)	115.4(4)	N(4)-C(37)-C(38)	109.8(4)
C(4)-C(13)-C(12)	122.4(4)	C(39)-C(37)-C(38)	110.3(5)

**S-Table 4** Anisotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for (bzq)<sub>2</sub>Ir(dipba). The anisotropic displacement factor exponent takes the form:  $-2\pi^2$ [ h<sup>2</sup> a\*<sup>2</sup>U<sup>11</sup> + ... + 2 h k a\* b\* U<sup>12</sup> ]

	U11	U22	U33	U23	U13	U12
C(1)	41(3)	52(3)	41(2)	-6(2)	3(2)	2(2)
Ir(1)	28(1)	30(1)	30(1)	2(1)	5(1)	-1(1)
N(1)	33(2)	36(2)	34(2)	2(1)	5(1)	1(2)
C(2)	43(3)	67(3)	53(3)	-14(2)	-9(2)	-5(2)
N(2)	30(2)	35(2)	34(2)	-1(1)	6(1)	-5(2)
C(3)	32(3)	61(3)	69(3)	-3(3)	-5(2)	-7(2)
N(3)	47(2)	34(2)	36(2)	6(1)	6(2)	7(2)
C(4)	29(2)	44(3)	56(3)	6(2)	6(2)	1(2)
N(4)	40(2)	35(2)	35(2)	3(1)	10(2)	2(2)
C(5)	28(2)	61(3)	70(3)	9(3)	14(2)	1(2)
C(6)	39(3)	61(3)	60(3)	10(2)	23(2)	12(2)
C(7)	46(3)	37(2)	41(2)	8(2)	12(2)	9(2)
C(8)	64(3)	52(3)	38(2)	2(2)	21(2)	15(2)
C(9)	65(3)	48(3)	34(2)	-5(2)	6(2)	6(2)
C(10)	42(3)	42(2)	38(2)	0(2)	2(2)	1(2)
C(11)	34(2)	30(2)	33(2)	3(2)	6(2)	4(2)
C(12)	37(2)	29(2)	35(2)	6(2)	10(2)	4(2)
C(13)	33(2)	34(2)	37(2)	6(2)	6(2)	3(2)
C(14)	37(2)	34(2)	52(3)	1(2)	7(2)	-8(2)
C(15)	45(3)	43(3)	62(3)	-5(2)	12(2)	-17(2)
C(16)	28(2)	58(3)	55(3)	-7(2)	5(2)	-11(2)
C(17)	29(2)	48(3)	38(2)	-2(2)	8(2)	-2(2)
C(18)	24(2)	64(3)	46(2)	1(2)	0(2)	6(2)
C(19)	41(3)	51(3)	46(3)	9(2)	1(2)	10(2)
C(20)	40(2)	39(2)	36(2)	1(2)	3(2)	5(2)
C(21)	56(3)	33(2)	50(3)	8(2)	-4(2)	4(2)
C(22)	56(3)	37(2)	54(3)	11(2)	-6(2)	-15(2)
C(23)	39(2)	35(2)	39(2)	2(2)	-4(2)	-9(2)
C(24)	31(2)	28(2)	29(2)	1(1)	7(2)	-1(2)
C(25)	31(2)	34(2)	27(2)	0(1)	5(2)	-2(2)
C(26)	27(2)	37(2)	29(2)	-2(2)	5(2)	-2(2)
C(27)	35(2)	36(2)	34(2)	5(2)	3(2)	-2(2)
C(28)	44(2)	40(2)	36(2)	7(2)	8(2)	7(2)
C(29)	76(4)	74(4)	46(3)	6(3)	-2(3)	-17(3)
C(30)	113(6)	95(5)	41(3)	6(3)	-3(3)	6(5)
C(31)	102(5)	96(5)	56(4)	38(3)	36(4)	43(4)
C(32)	64(4)	91(5)	101(5)	57(4)	24(4)	5(3)

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C(33)	48(3)	75(4)	68(3)	30(3)	1(3)	-14(3)
C(34)	57(3)	37(3)	52(3)	9(2)	10(2)	11(2)
C(35)	128(6)	50(3)	86(4)	-11(3)	-3(4)	34(4)
C(36)	57(4)	72(5)	191(9)	15(5)	-22(5)	21(3)
C(37)	46(3)	43(3)	39(2)	2(2)	15(2)	5(2)
C(38)	98(5)	56(4)	168(8)	-43(4)	61(5)	-4(4)
C(39)	58(4)	122(6)	64(4)	-22(4)	14(3)	27(4)

# Supplementary Material (ESI) for Journal of Materials Chemistry

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