Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C


# Supporting Information

## Guanidinate Ligated Iridium(III) Complexes with Various Cyclometalated Ligands. Synthesis, Structure, and Highly Efficient Electrophosphorescent Properties with a Wide Range of Emission Colour

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**Figure S1**. Phosphorescence life-times of complexes (**1**-**8**).

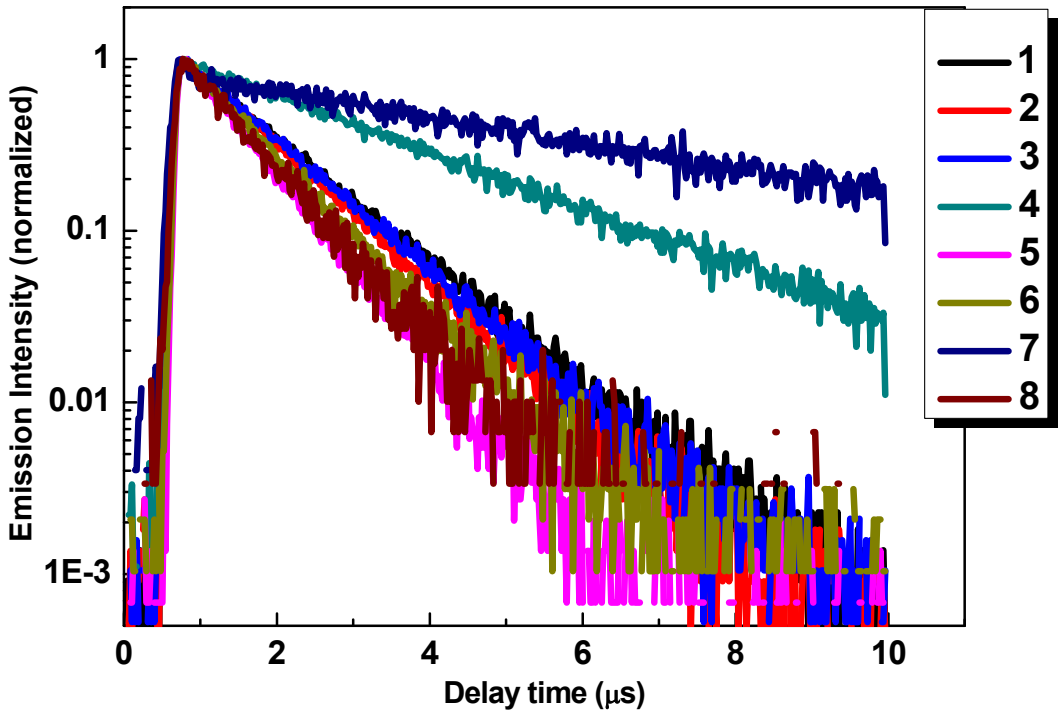
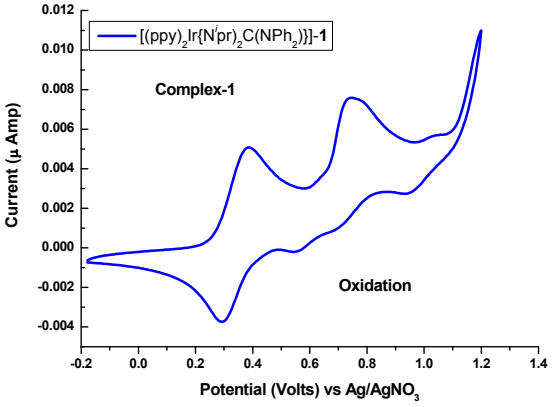
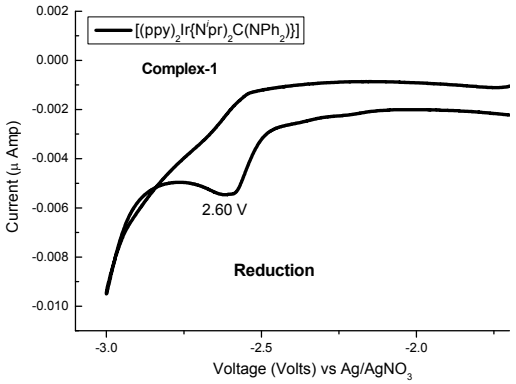
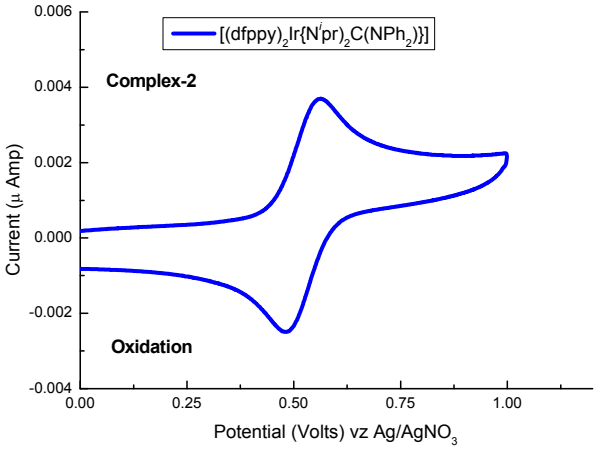
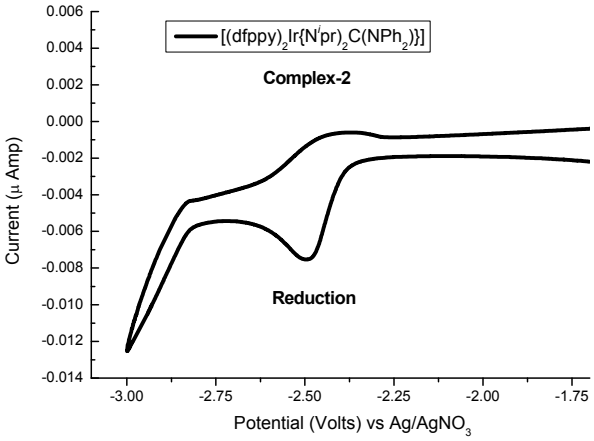


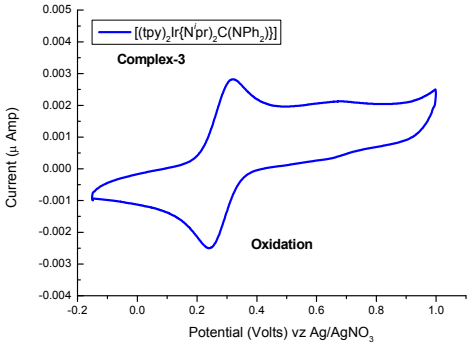
**Figure S2.** Redox Properties of Complexes (**1**-**8**).

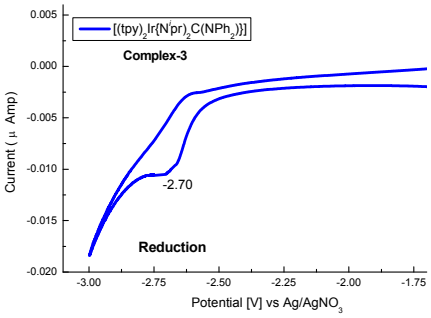


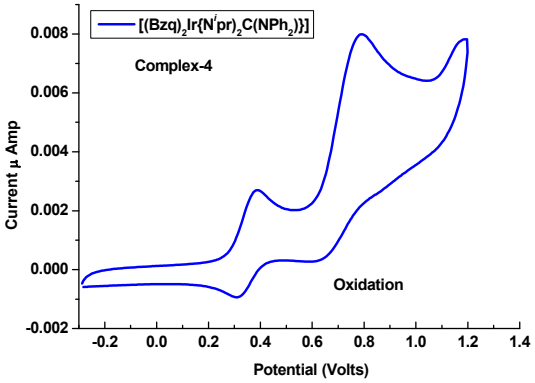



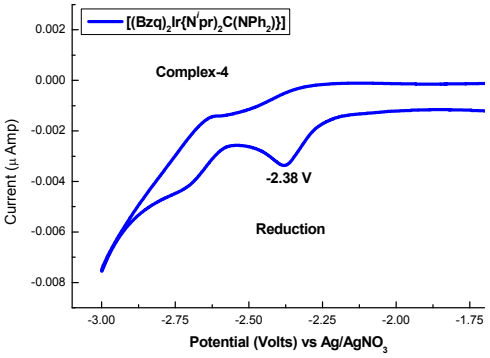



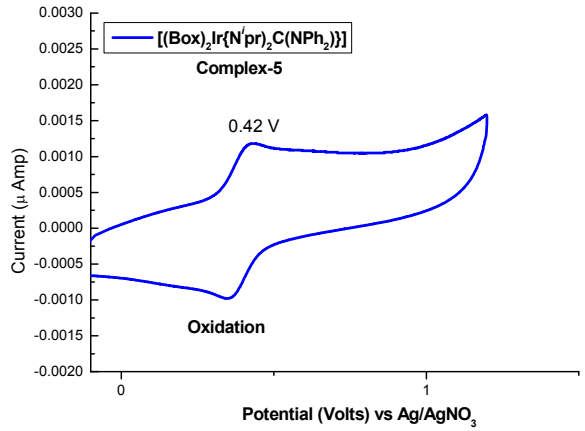



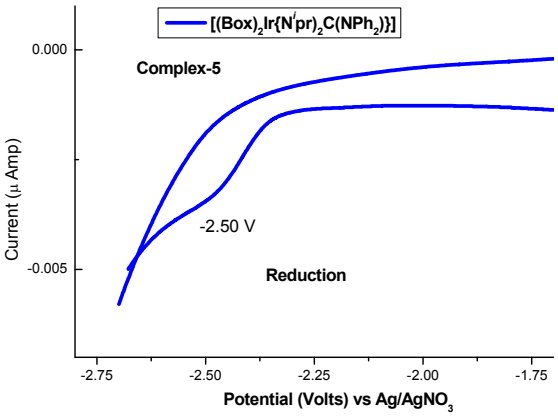

[(tpy)2Ir{N(i)pr)2C(NPh2)}]
Complex-3
Oxidation
Current (μ Amp)
Potential (Volts) vz Ag/AgNO3

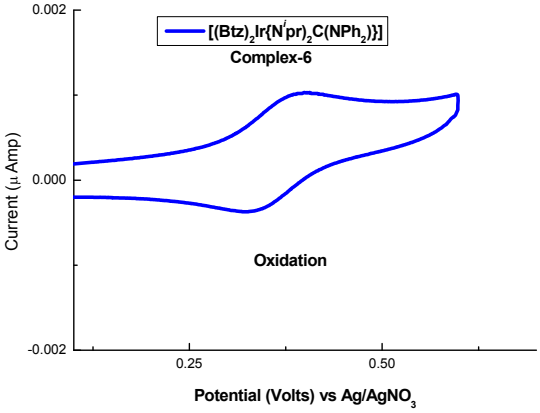

[(tpy)2Ir{N(i)pr)2C(NPh2)}]
Complex-3
-2.70
Reduction
Current ( μ Amp)
Potential [V] vs Ag/AgNO3

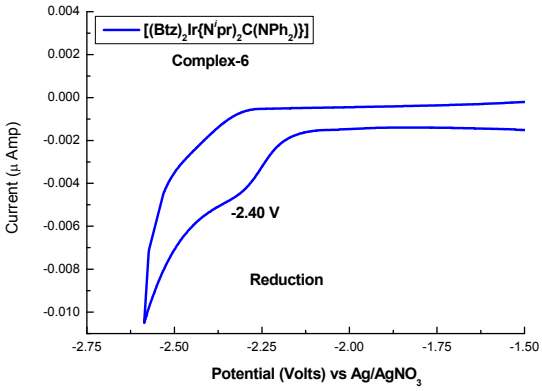

[(Bzq)2Ir{N(i)pr)2C(NPh2)}]
Complex-4
Oxidation
Current μ Amp
Potential (Volts)

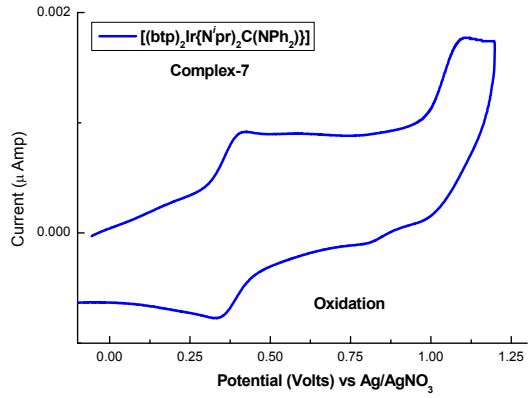

[(Bzq)2Ir{N(i)pr)2C(NPh2)}]
Complex-4
-2.38 V
Reduction
Current (μ Amp)
Potential (Volts) vs Ag/AgNO3

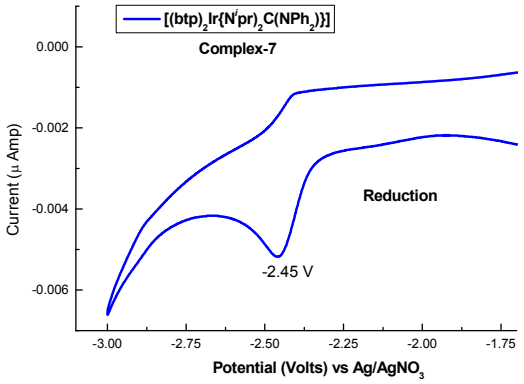


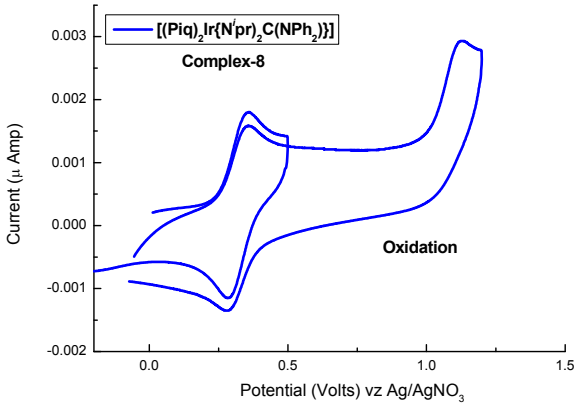



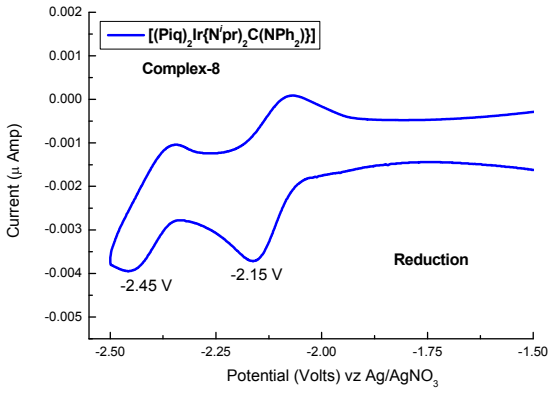




[(btp)2Ir{N^i pr)2C(NPh2)}]
Complex-7
Oxidation
Current (μ Amp)
Potential (Volts) vs Ag/AgNO3
0.002
0.000
0.00
0.25
0.50
0.75
1.00
1.25


[(btp)2Ir{N^i pr)2C(NPh2)}]
Complex-7
Reduction
-2.45 V
Current (μ Amp)
Potential (Volts) vs Ag/AgNO3
0.000
-0.002
-0.004
-0.006
-3.00
-2.75
-2.50
-2.25
-2.00
-1.75


[(Piq)2Ir{N^i pr)2C(NPh2)}]
Complex-8
Oxidation
Current (μ Amp)
Potential (Volts) vz Ag/AgNO3
0.003
0.002
0.001
0.000
-0.001
-0.002
0.0
0.5
1.0
1.5


[(Piq)2Ir{N^i pr)2C(NPh2)}]
Complex-8
Reduction
-2.45 V
-2.15 V
Current (μ Amp)
Potential (Volts) vz Ag/AgNO3
0.002
0.001
0.000
-0.001
-0.002
-0.003
-0.004
-0.005
-2.50
-2.25
-2.00
-1.75
-1.50

## OLEDs Characterization of complexes (2-8).

**Figure S3**. Electroluminescence spectra of complex-**2** at different concentration: inset OLED photograph at 9 volt.

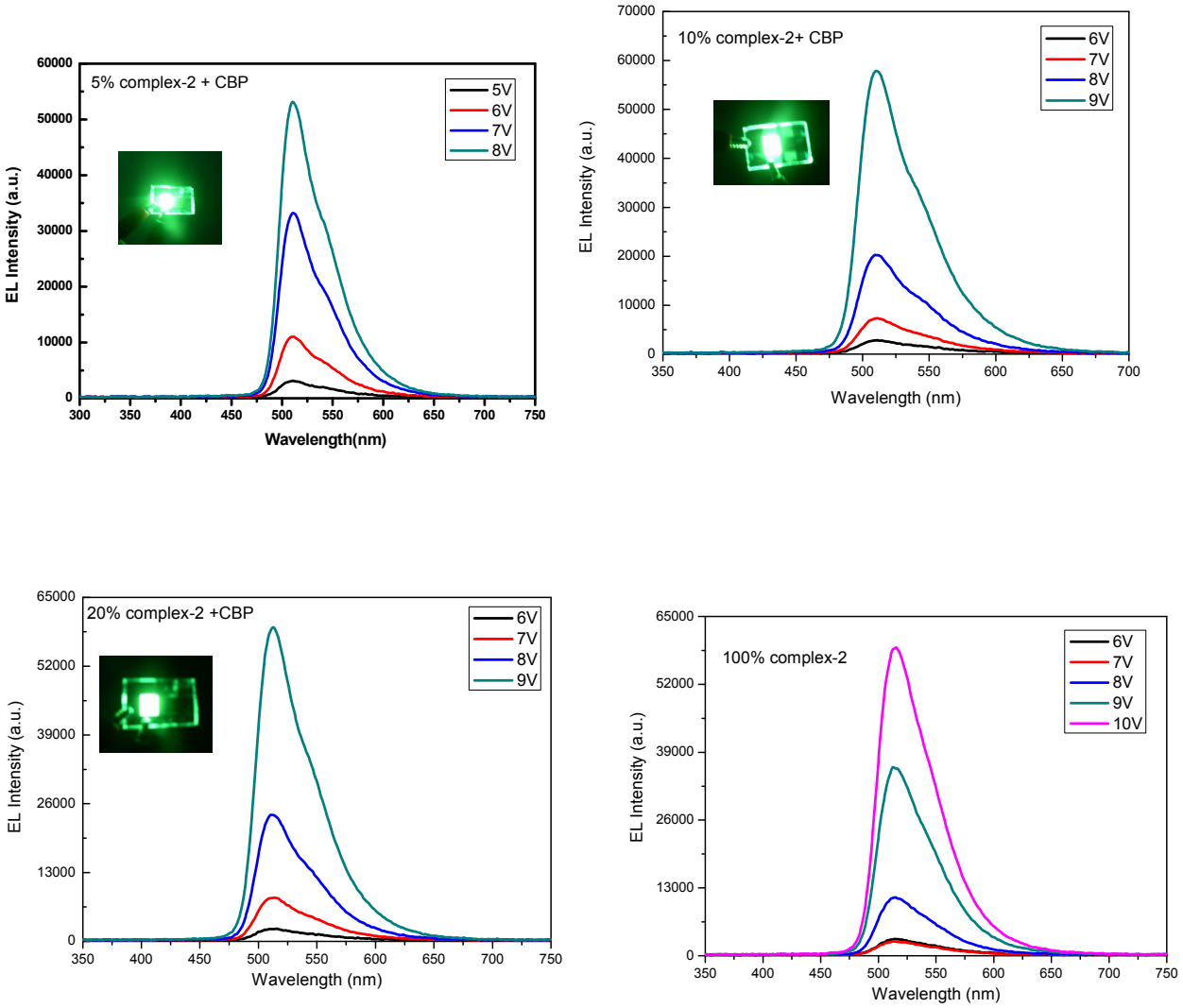


**Figure S4**. Electroluminescence spectra of complex-**3** at different concentration: inset OLED photograph at 9 volt.

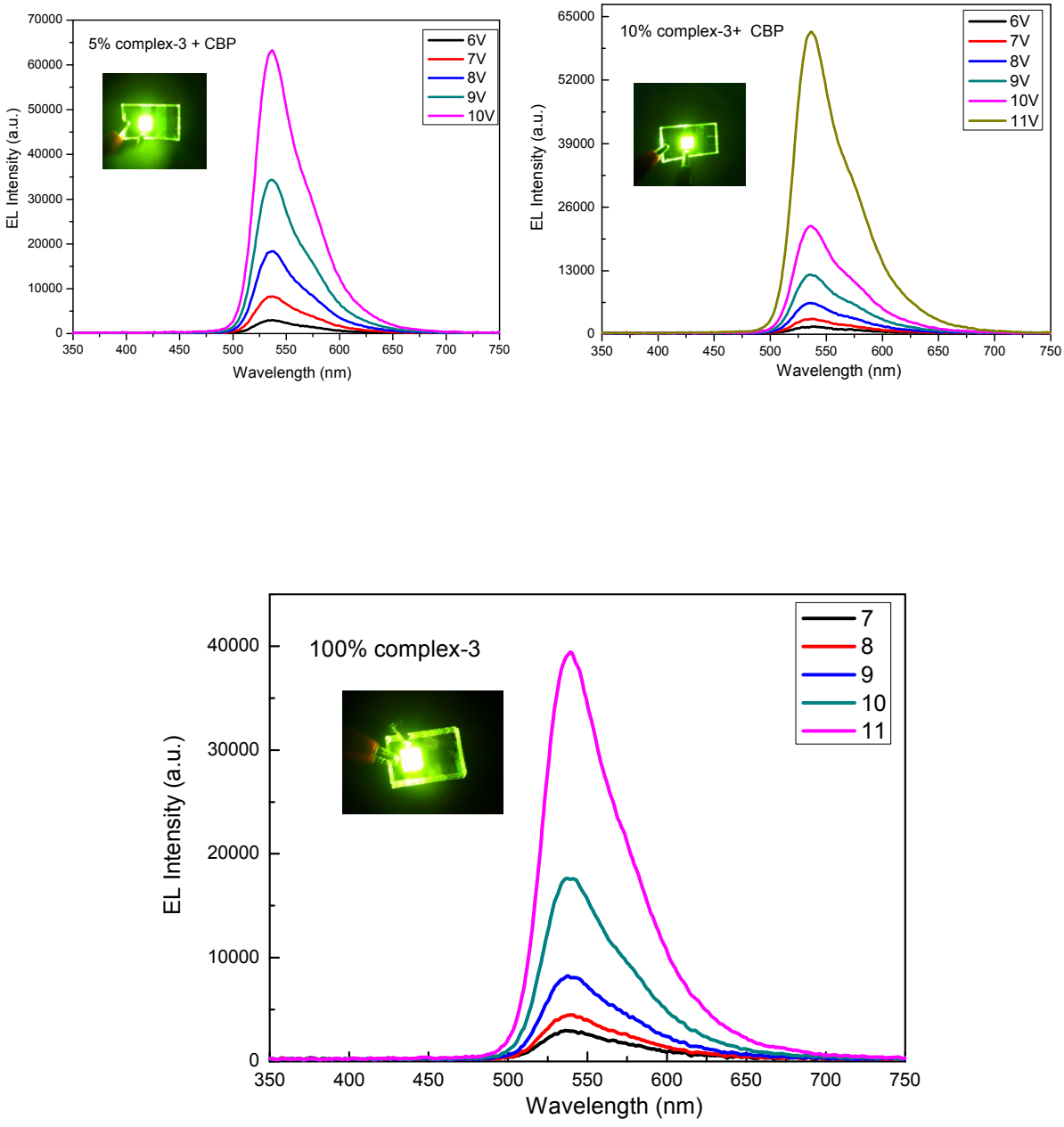
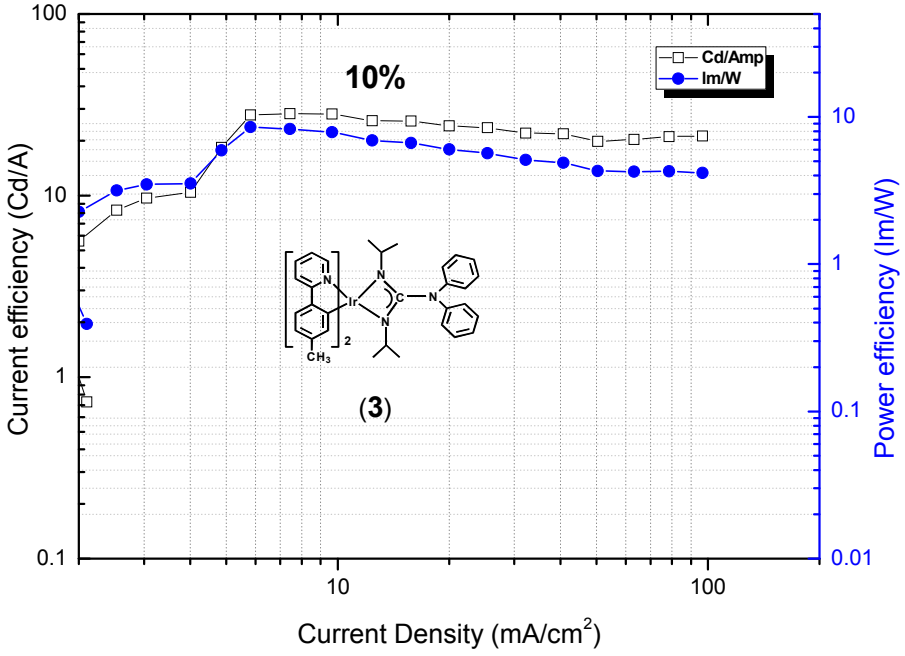


**Figure S5.** Current density vs current and power efficiency graph of 10% and non-doped(100%) devices of complex (**3**):



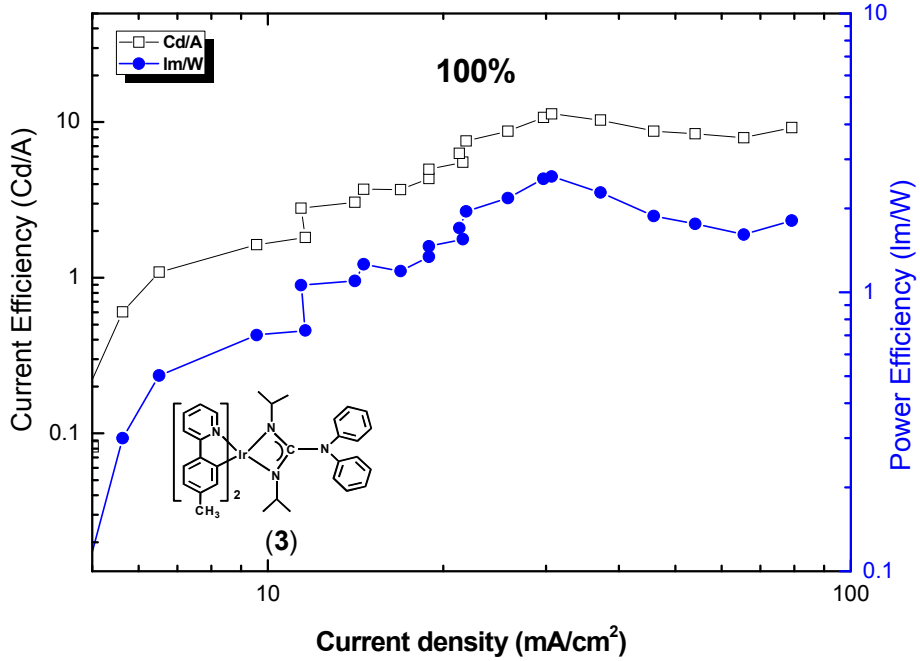



**Figure S6.** Electroluminescence spectra of complex-**4** at 5% doping concentration in CBP at different voltages: inset OLED photograph at 9 volt.

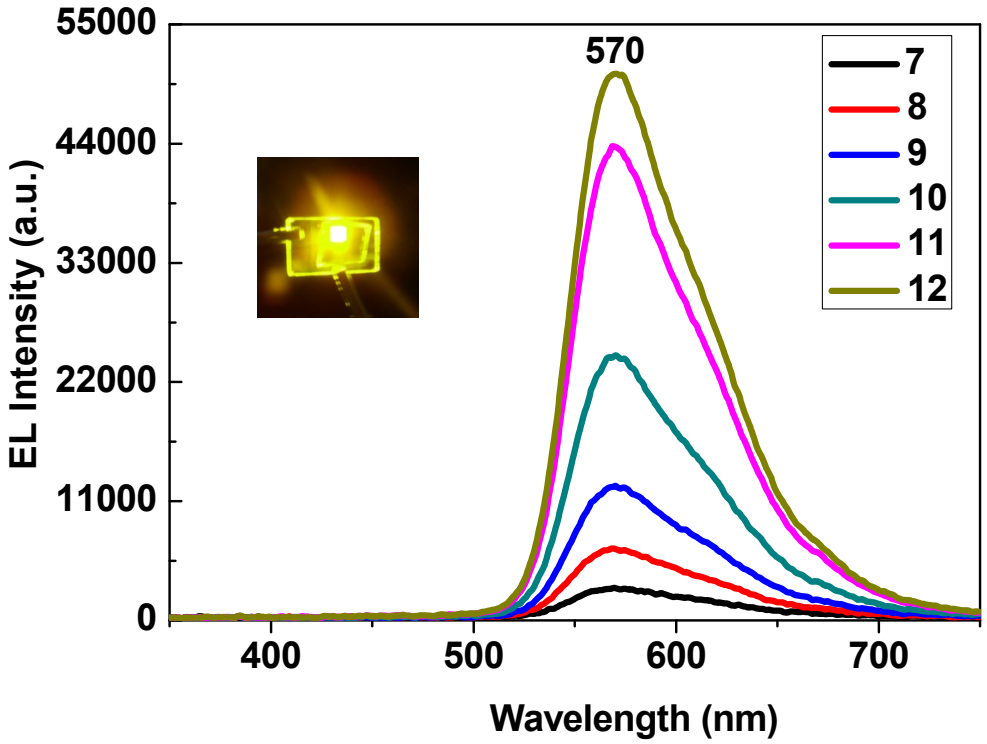


**Figure S7.** Electroluminescence spectra of complex-**5** at 5% doping concentration in CBP at different voltages: inset OLED photograph at 9 volt.

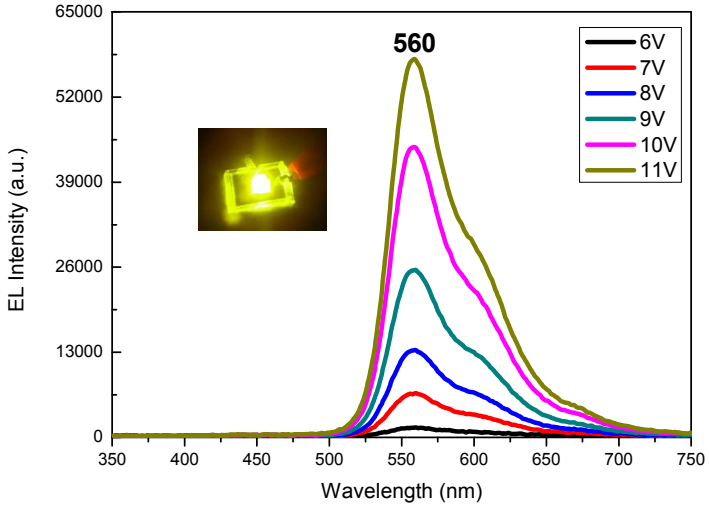



**Figure S8.** Voltage, current density and luminance (J-V-L) characteristics of device with 5% doping of complex (**5**):

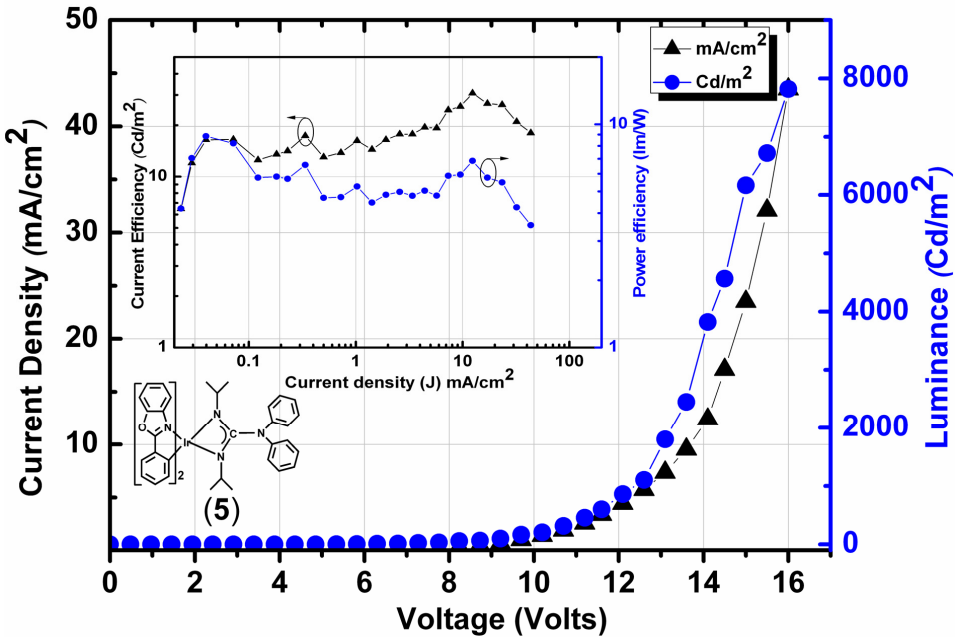


**Figure S9.** Electroluminescence spectra of complex-**6** at 5% doping concentration in CBP at different voltages: inset OLED photograph at 9 volt.

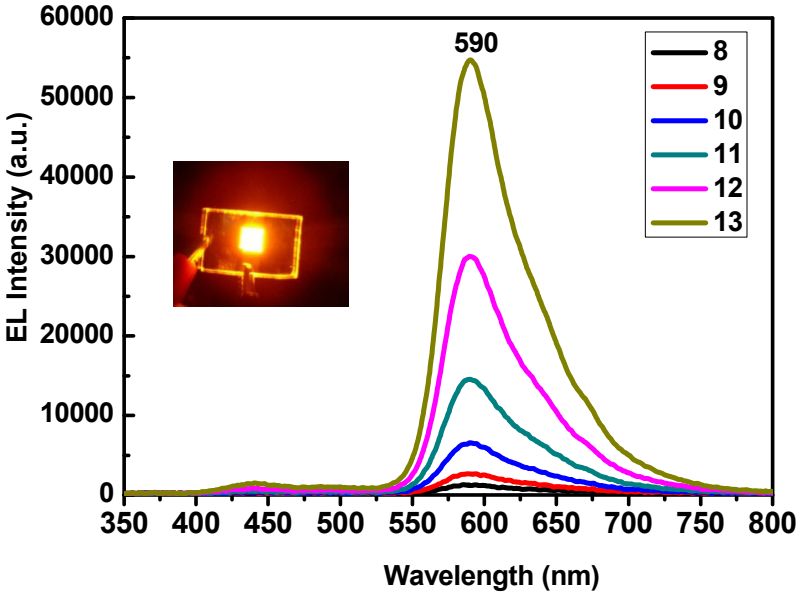



**Figure S10.** Voltage, current density and luminance (*J-V-L*) characteristics of device with 5% doping of complex (**6**)

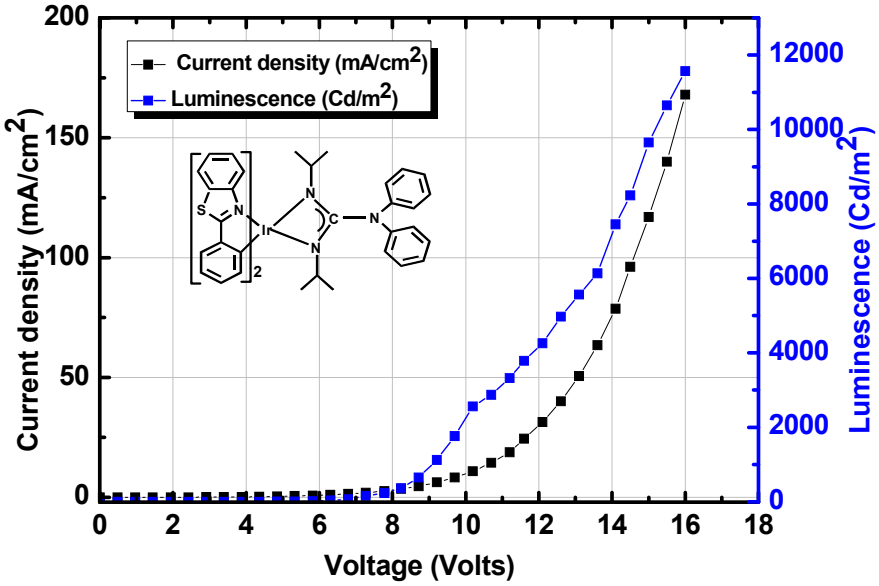


**Figure S11.** Current and power efficiency graph of device with 5% doping concentration of complex (**6**)

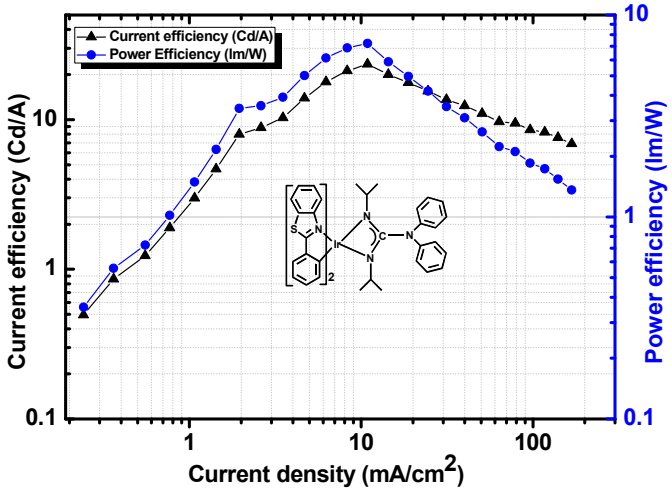



**Figure S12.** Electroluminescence spectra of complex-**7** at 5% doping concentration in CBP at different voltages: inset OLED photograph at 9 volt.

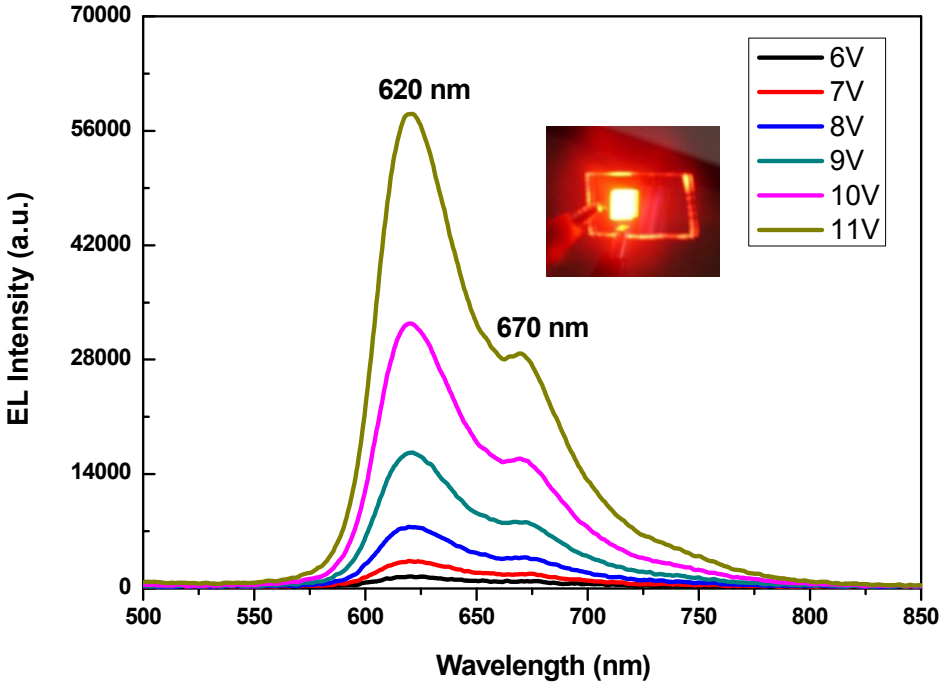


**Figure S13.** Electroluminescence spectra of complex-**8** at 5% doping concentration in $Alq_3$ at different voltages: inset OLED photograph at 9 volt.

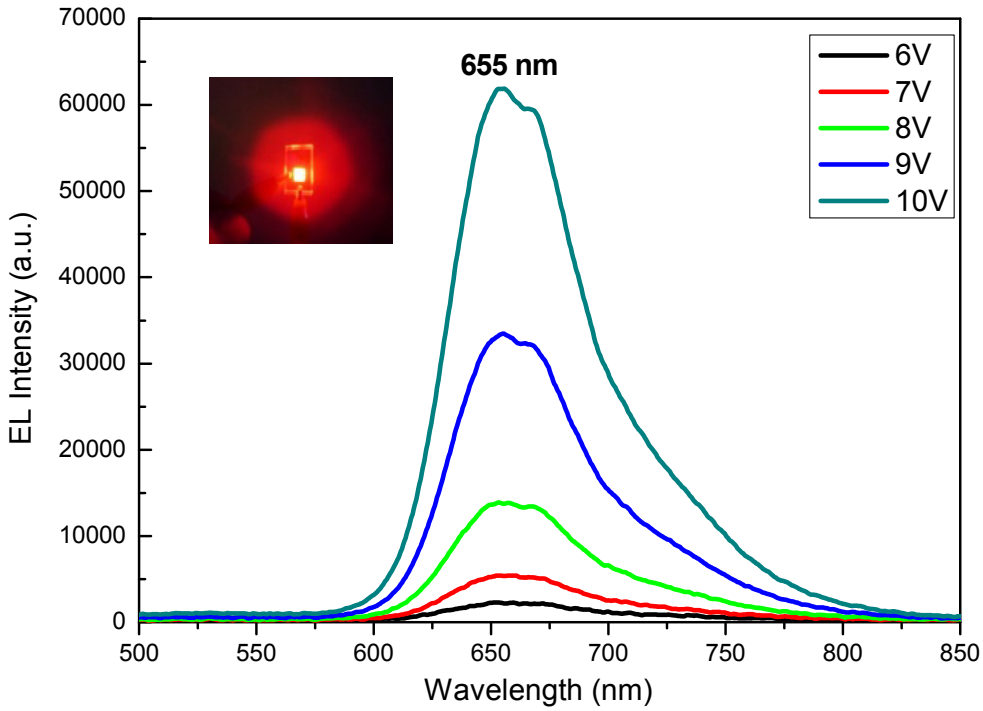


**Figure S14.** Current density, voltage and luminance (*J-V-L*) characteristics of device with 5% doping of complex (**8**)

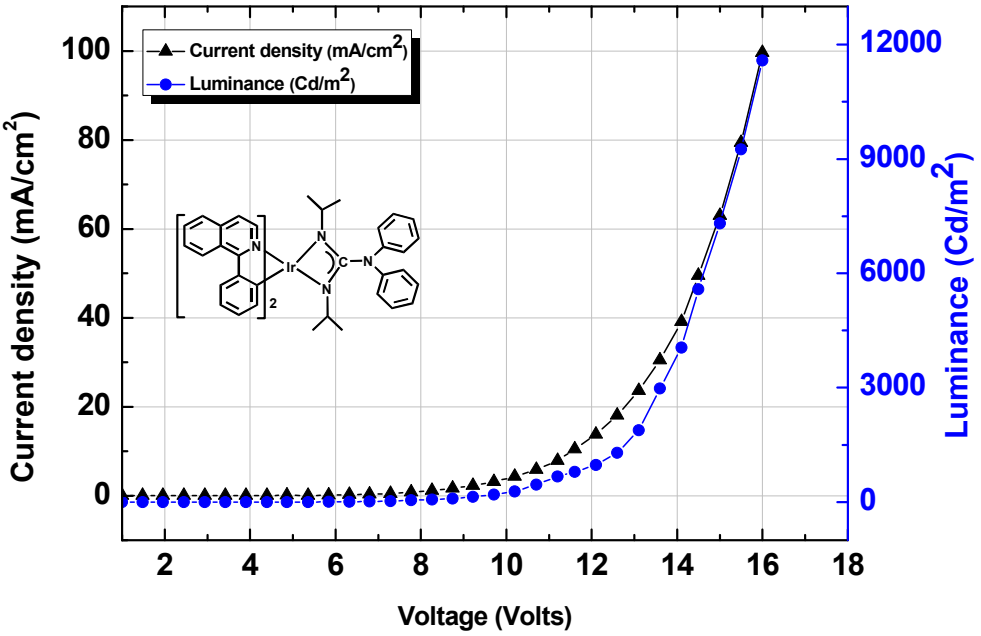



**Figure S15.** Current and power efficiency graph of device with 5% doping concentration of complex-**8**

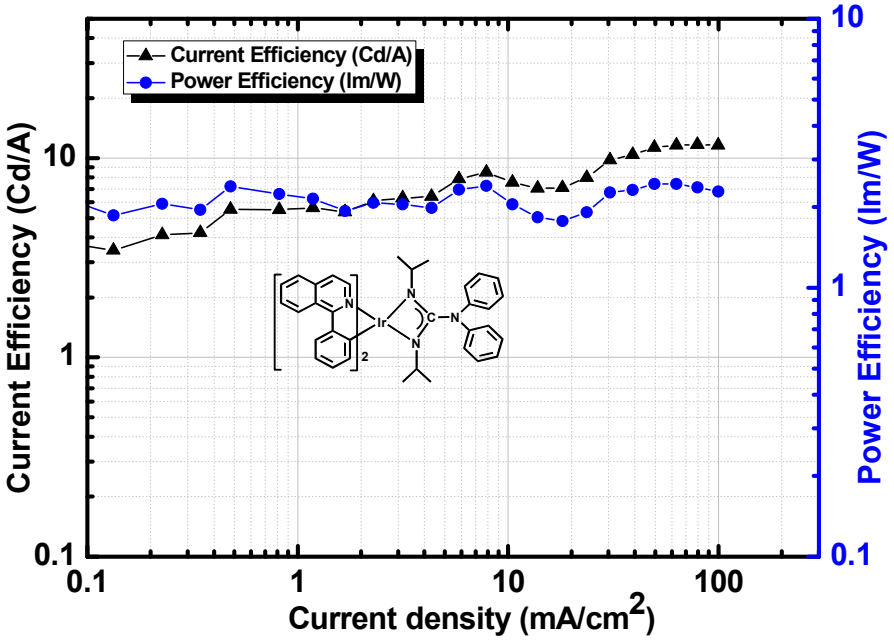


**Figure S16.** ORTEP diagrams of Complex **8**.

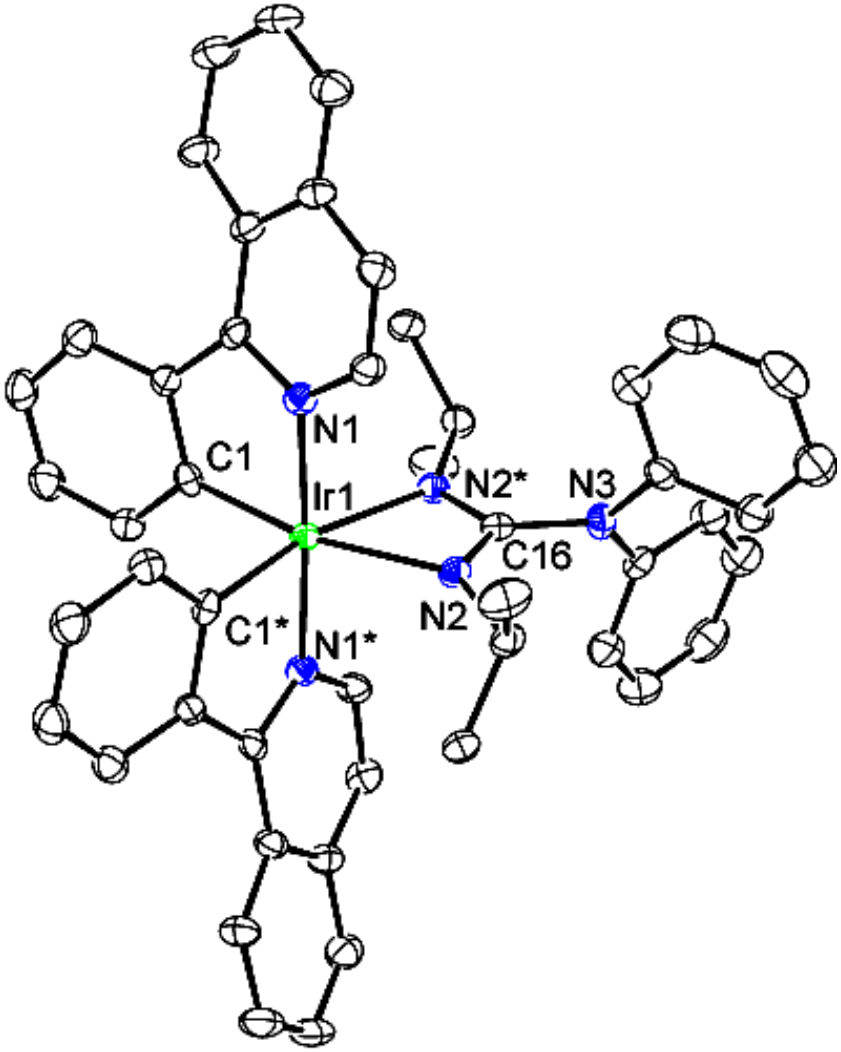


Table-SI-1 Summary of Crystallographic Data of **1,2,4-8.**

| | **1** | **2** | **4** | **5** | **6** | **7·toluene** | **8·toluene** |
|---|---|---|---|---|---|---|---|
| Empirical formula | $C_{41}H_{40}IrN_5$ | $C_{41}H_{36}F_4IrN_5$ | $C_{45}H_{40}IrN_5$ | $C_{45}H_{40}IrN_5O_2$ | $C_{45}H_{40}IrN_5S_2$ | $C_{52}H_{48}IrN_5S_2$ | $C_{56}H_{52}IrN_5$ |
| fw | 794.98 | 866.95 | 843.02 | 875.02 | 907.14 | 907.23 | 987.23 |
| Temp(K) | 173 | 173 | 173 | 173 | 173 | 173 | 173 |
| Cryst syst | monoclinic | triclinic | triclinic | triclinic | monoclinic | triclinic | monoclinic |
| Space group | $P2_1/n$ | $P\bar{1}$ | $P\bar{1}$ | $P\bar{1}$ | $P2_1/n$ | $P\bar{1}$ | $C2/c$ |
| Unit cell dimens | | | | | | | |
| a (Å) | 9.3240(14) | 9.524(2) | 10.378(3) | 9.130(8) | 9.311(6) | 10.335(5) | 14.992(7) |
| b (Å) | 38.685(6) | 13.963(3) | 10.421(3) | 17.026(14) | 16.719(11) | 13.420(7) | 29.691(14) |
| c (Å) | 10.3325(15) | 14.858(3) | 17.146(3) | 24.47(2) | 24.391(17) Å | 17.234(9) | 10.583(5) |
| α (°) | 90 | 73.185(3) | 85.018(3) | 88.939(13) | 90 | 80.228(7) | 90 |
| β (°) | 113.095(2) | 74.49(3) | 81.768(3) | 89.100(12) | 90.481(12) | 77.838(7) | 106.707(7) |
| γ (°) | 90 | 73.671(3) | 79.502(4) | 87.355(12) | 90 | 72.643(7) | 90 |
| V, ($Å^3$) | 3428.2(9) | 1777.5(7) | 2622(14) | 3798(5) | 3797(4) | 2216(2) | 4512(4) |
| Z | 4 | 2 | 2 | 4 | 4 | 2 | 4 |
| density(calcd), $g/cm^3$ | 1.54 | 1.62 | 1.555 | 1.53 | 1.587 | 1.498 | 1.453 |
| abs coeff, $mm^{-1}$ | 3.913 | 3.814 | 3.747 | 3.56 | 3.667 | 3.15 | 3.003 |
| F(000) | 1592 | 860 | 844 | 1752 | 1816 | 1008 | 2000 |
| θ range [°] | 2.11-25.06 | 1.56-25.07 | 1.99-25.08 | 1.47-25.34 | 1.48 to 25.08° | 1.60-25.20 | 1.58 to 25.04 |
| reflns collected | 17805 | 9323 | 9120 | 20097 | 19580 | 11639 | 11814 |
| indep reflns(Rint) | 6029(0.0603) | 6124(0.0436) | 6074(0.241) | 13267(0.0545) | 6694(0.0824) | 7659(0.0379) | 3972(0.0523) |
| data/restraints/params | 6029/0/428 | 6124/0/464 | 6074/0/464 | 13267/0/955 | 6694 / 0 / 453 | 7659/0/546 | 3972 / 0 / 264 |
| GOF on $F^2$ | 1.126 | 0.994 | 1.006 | 1.121 | 0.655 | 0.86 | 0.858 |
| Final R index [I > 2σ(I)] | 0.0488 | 0.0288 | 0.0291 | 0.0908 | 0.0422 | 0.0391 | 0.0345 |
| Rw | 0.1038 | 0.1126 | 0.0686 | 0.2107 | 0.0609 | 0.0694 | 0.0611 |