

**Supplementary information for**

**Synthesis, characterization and electroluminescence properties of new iridium complexes based on cyclic phenylvinylpyridine derivatives: tuning of emission colour and efficiency by structural control**

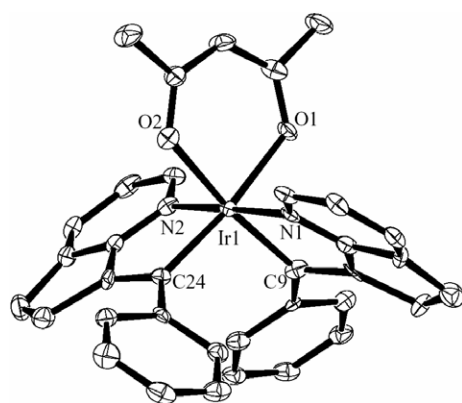
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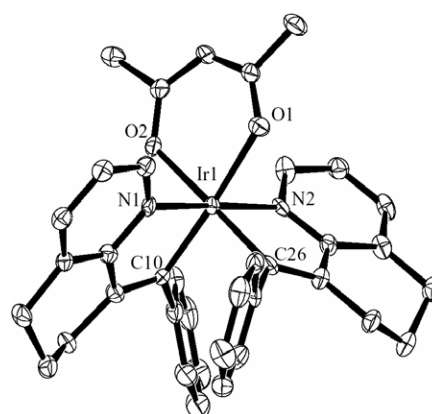
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**X-ray crystallographic data**



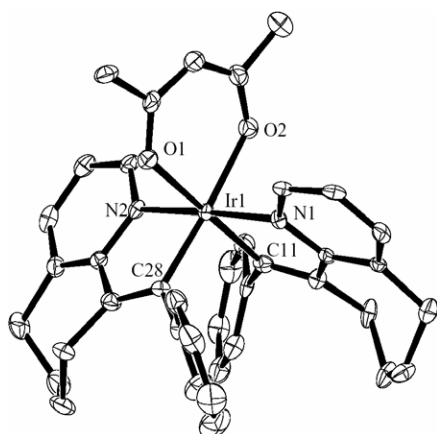
Complex 4a



Complex 4b

Complex 4a

Molecule A	Molecule B
Ir1-N1 2.038(4)	Ir2-N3 2.029(4)
Ir1-N2 2.038(4)	Ir2-N4 2.031(4)
Ir1-C9 2.021(4)	Ir2-C44 2.030(4)
Ir1-C24 2.029(5)	Ir2-C59 2.037(6)
Ir1-O1 2.119(4)	Ir2-O3 2.124(3)
Ir1-O2 2.118(3)	Ir2-O4 2.122(4)
49.5(2)°	45.5(2)°
53.5(2)°	49.8(2)°

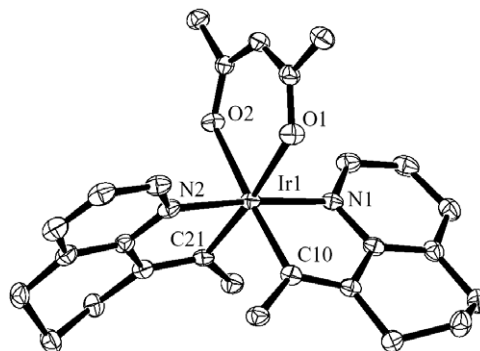


Complex 4c

Molecule A	Molecule B
Ir1-N1 2.039(3)	Ir2-N3 2.033(3)
Ir1-N2 2.024(3)	Ir2-N4 2.032(3)
Ir1-C11 1.997(3)	Ir2-C50 1.988(4)
Ir1-C28 1.994(4)	Ir2-C67 2.002(4)
Ir1-O1 2.151(2)	Ir2-O3 2.160(3)
Ir1-O2 2.140(4)	Ir2-O4 2.167(3)
68.0(1)°	63.2(2)°
57.2(2)°	69.7(2)°

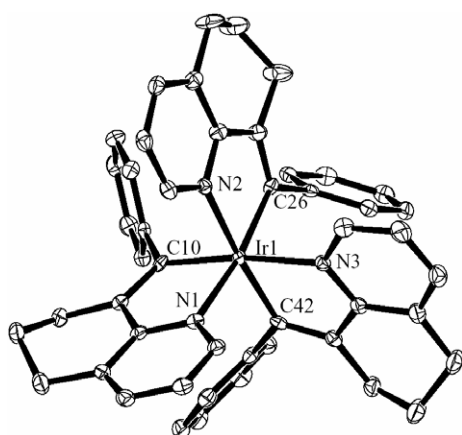
Complex 4b

Molecule A	Molecule B
Ir1-N1 2.025(5)	Ir2-N3 2.034(4)
Ir1-N2 2.045(5)	Ir2-N4 2.045(4)
Ir1-C10 1.976(5)	Ir2-C47 2.000(6)
Ir1-C26 2.004(6)	Ir2-C63 1.998(6)
Ir1-O1 2.146(4)	Ir2-O3 2.167(5)
Ir1-O2 2.145(4)	Ir2-O4 2.144(4)
54.4(2)°	78.5(2)°
74.2(2)°	62.2(2)°



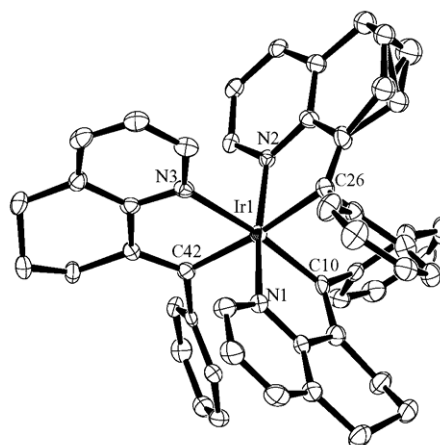
Complex 5

Ir-N1 2.032(2)
Ir-N2 2.037(2)
Ir-C10 1.995(3)
Ir-C21 1.988(3)
Ir-O1 2.161(2)
Ir-O2 2.159(2)



Complex **6a**

Ir-N1	2.109(2)	77.1(1)°
Ir-N2	2.122(3)	67.5(1)°
Ir-N3	2.123(2)	74.1(1)°
Ir-C10	2.022(3)	
Ir-C26	2.023(3)	
Ir-C42	2.029(3)	



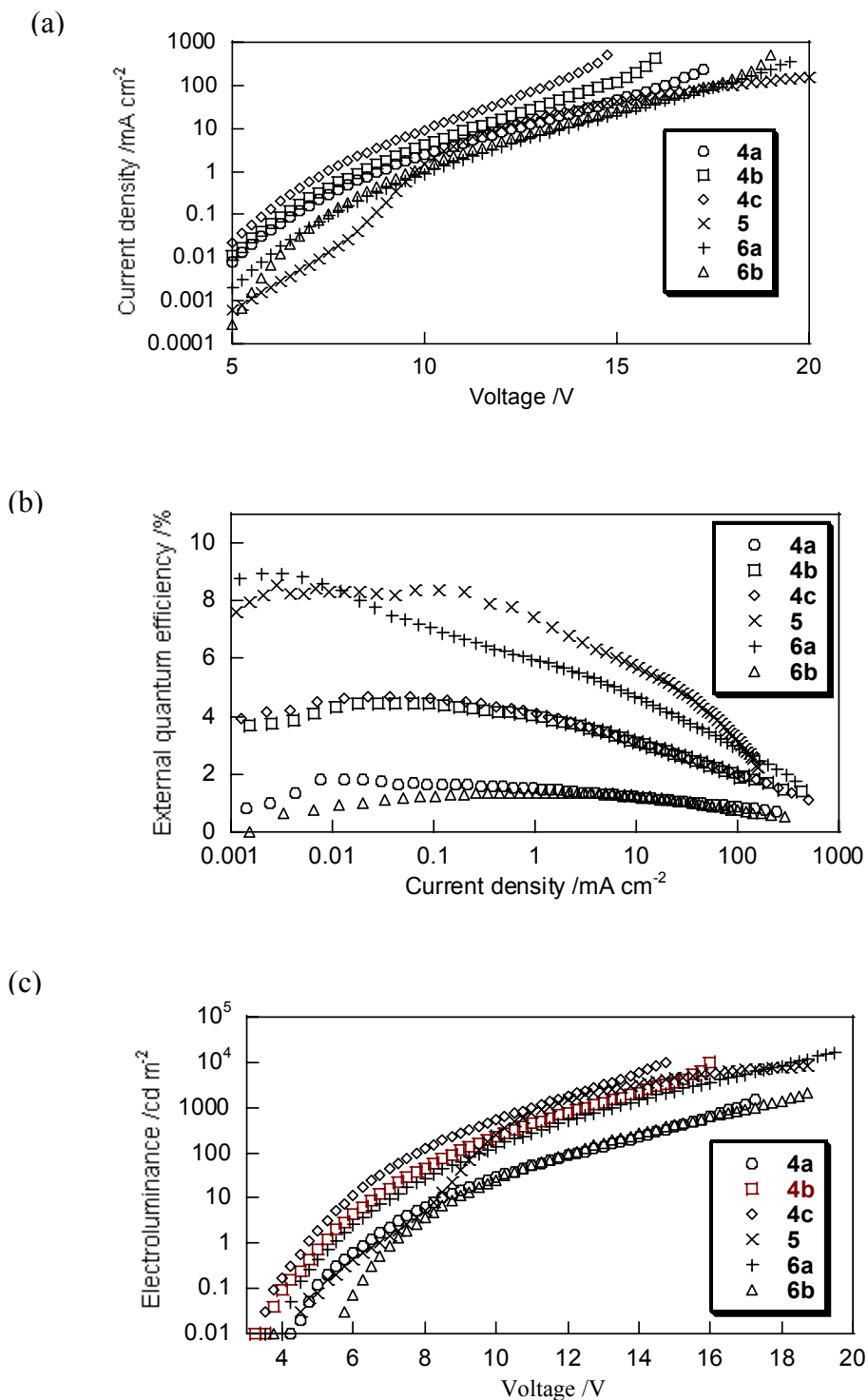
Complex **6b**

Ir-N1	2.033(3)	91.1(1)°
Ir-N2	2.053(3)	85.8(1)°
Ir-N3	2.141(3)	65.9(1)°
Ir-C10	2.026(3)	
Ir-C26	2.086(4)	
Ir-C42	2.097(4)	

### Performance of the EL devices

**Table S1.** EL characteristics of iridium complexes at 100 cd m<sup>-2</sup>.

complex	EL <sub>max</sub> (nm)	CIE <sub>x</sub>	CIE <sub>y</sub>	EQE(%)	lm/w	cd/A	v
<b>4a</b>	635	0.667	0.327	1.2	0.3	1.0	12.41
<b>4b</b>	605	0.619	0.377	3.8	2.2	6.1	8.82
<b>4c</b>	599	0.596	0.491	4.0	2.9	7.3	7.78
<b>5</b>	588	0.542	0.457	8.1	6.8	19.8	9.16
<b>6a</b>	571	0.534	0.465	6.1	5.2	15.6	9.48
<b>6b</b>	624	0.596	0.402	1.3	0.5	1.9	11.92



**Fig. S1** (a) Voltage dependency of current density, (b) current-density dependency of external quantum efficiency, (c) voltage dependency of electroluminescence of OLED devices.

**PL spectra of the Ir complexes**

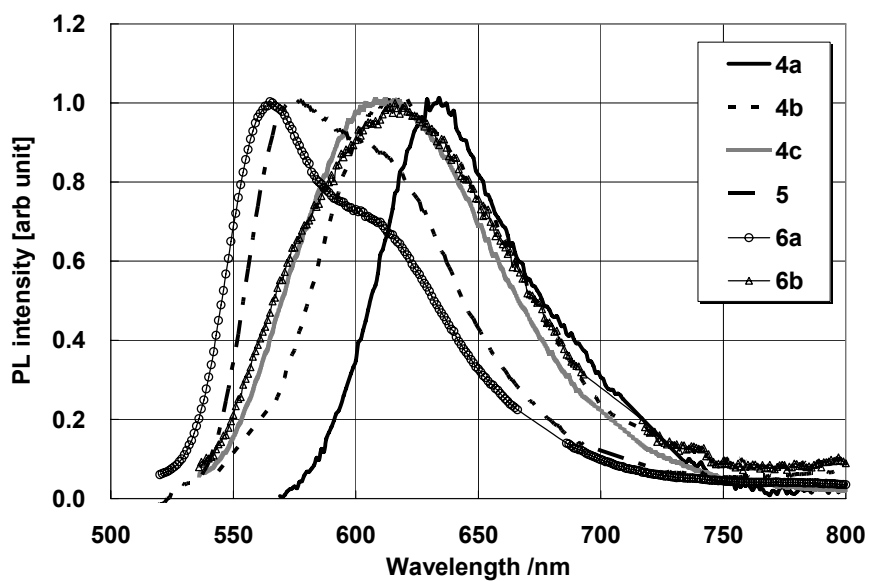


Fig. S2 PL spectra of the Ir complexes in PC film at room temperature.

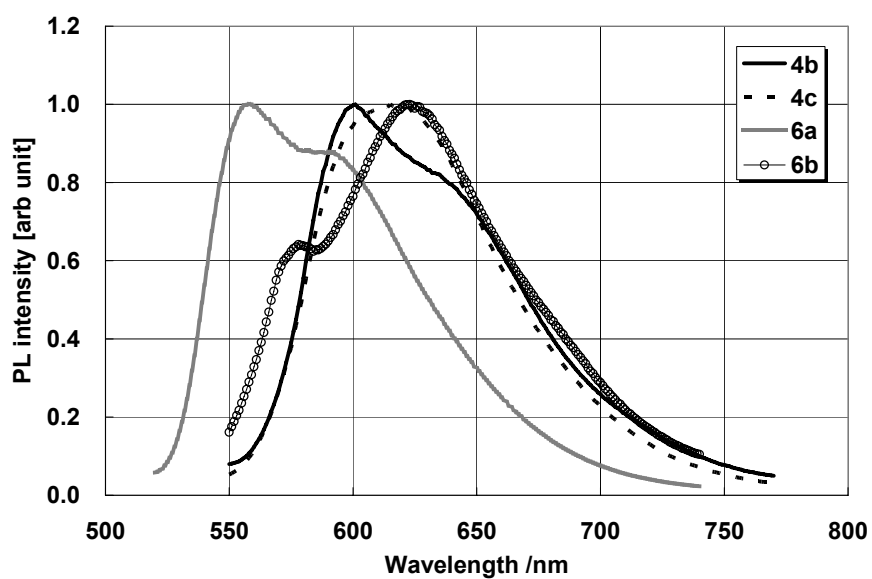


Fig. S3 PL spectra of the Ir complexes in the solid state.