Electronic Supplementary Information

for

A versatile color tuning strategy for iridium(III) and platinum(II) electrophosphors by shifting the charge-transfer states with an electron-deficient core

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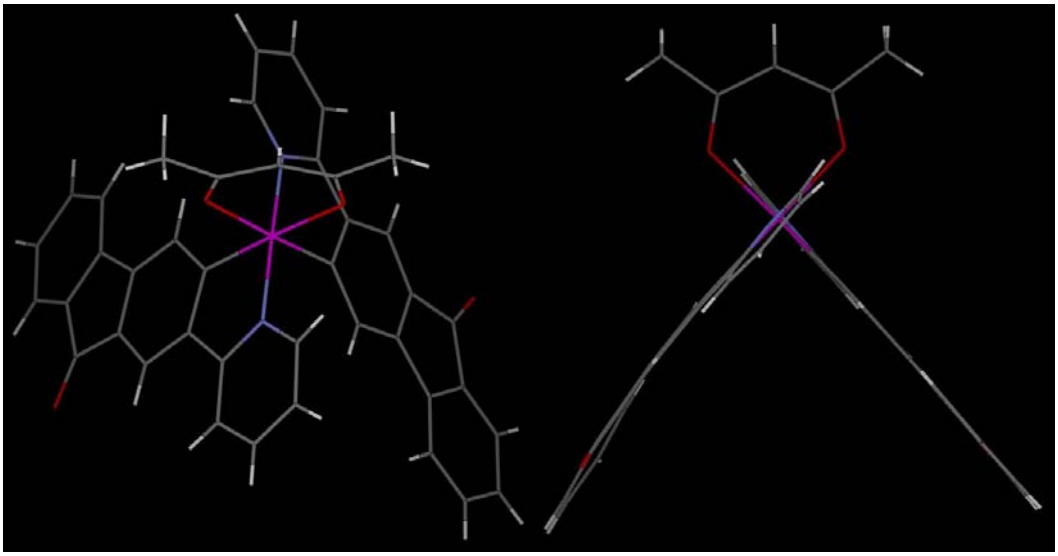
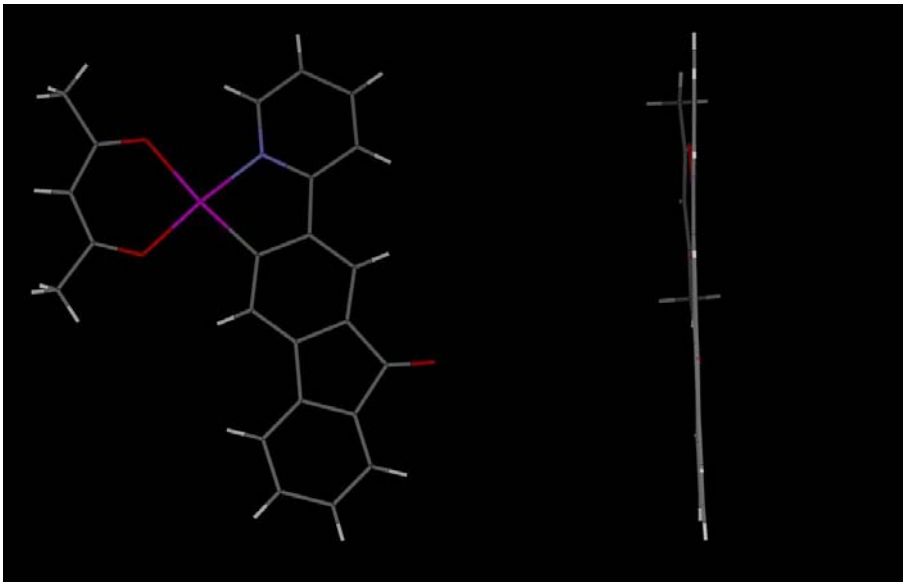


(a) Ir-1



(b) Pt-1

Fig. S1 X-ray crystal structures of **Ir-1** and **Pt-1** shown in different orientations.

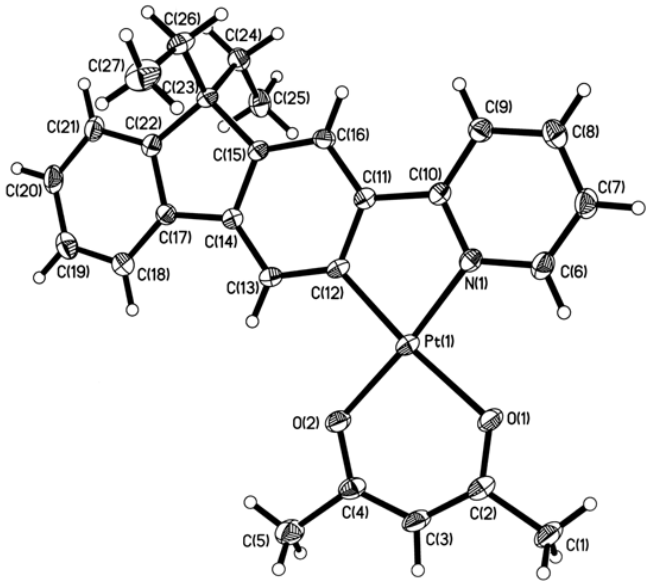


Fig. S2 ORTEP drawing of the complex **Pt-2** with thermal ellipsoids shown at 25% probability level.

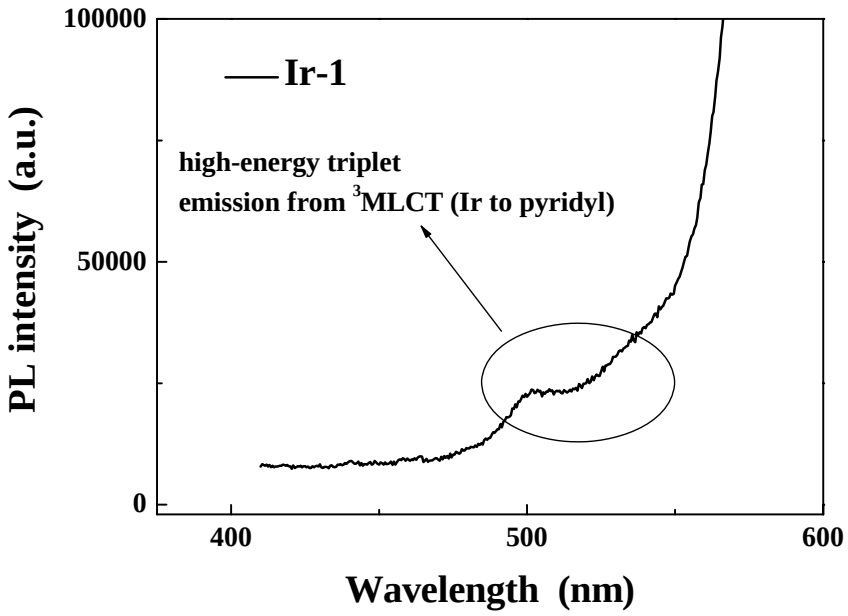


Fig. S3 An expanded view of the PL spectrum for **Ir-1** in CH_2CL_2 at 293 K.

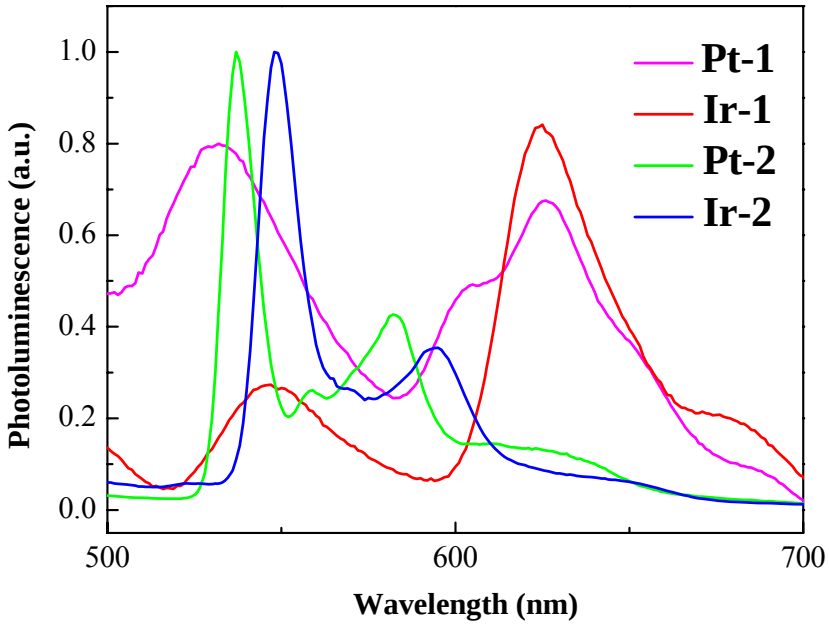


Fig. S4 PL spectra of the complexes at 77 K.

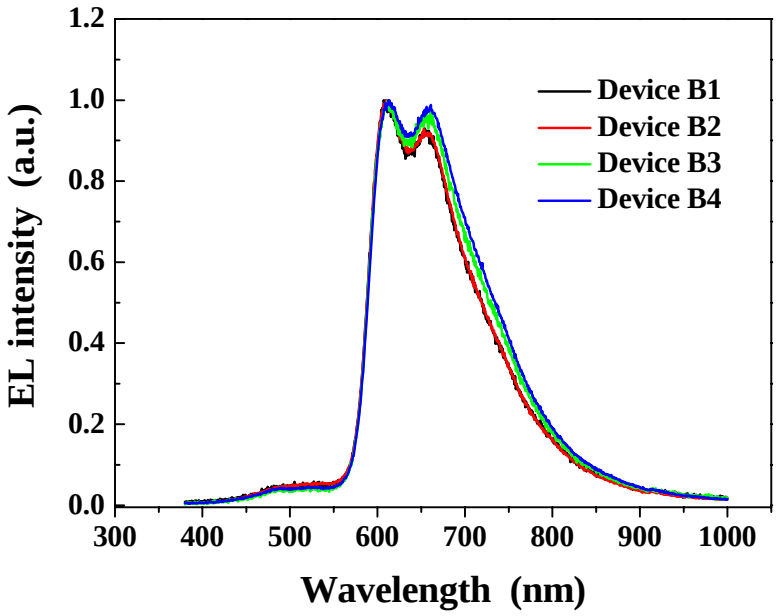


Fig. S5 EL spectra for the device **B1**–**B4** at 13 V.

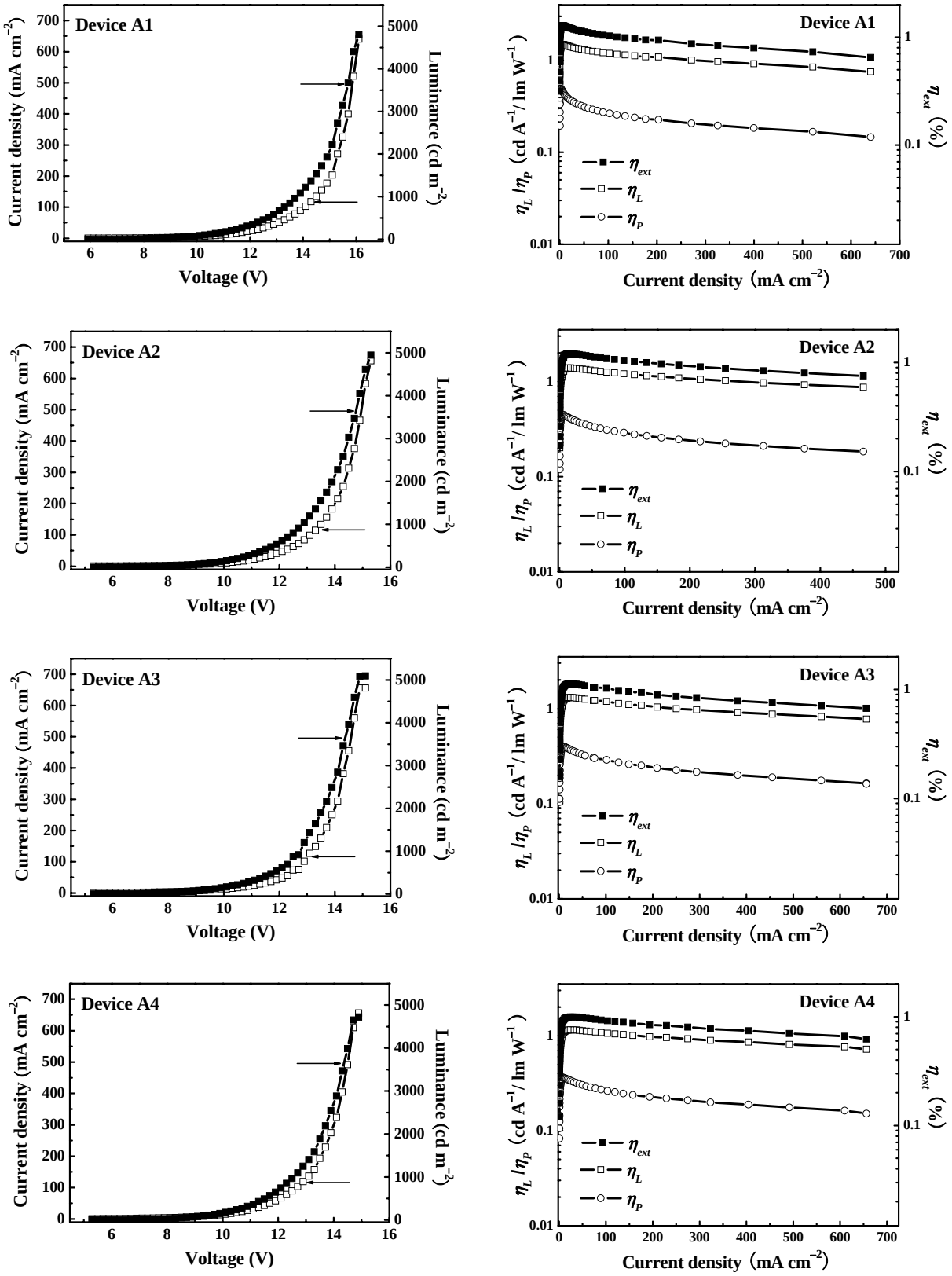


Fig. S6 The *J*–*V*–*L* curves and the efficiency versus current density relationship for devices **A1**–**A4**.

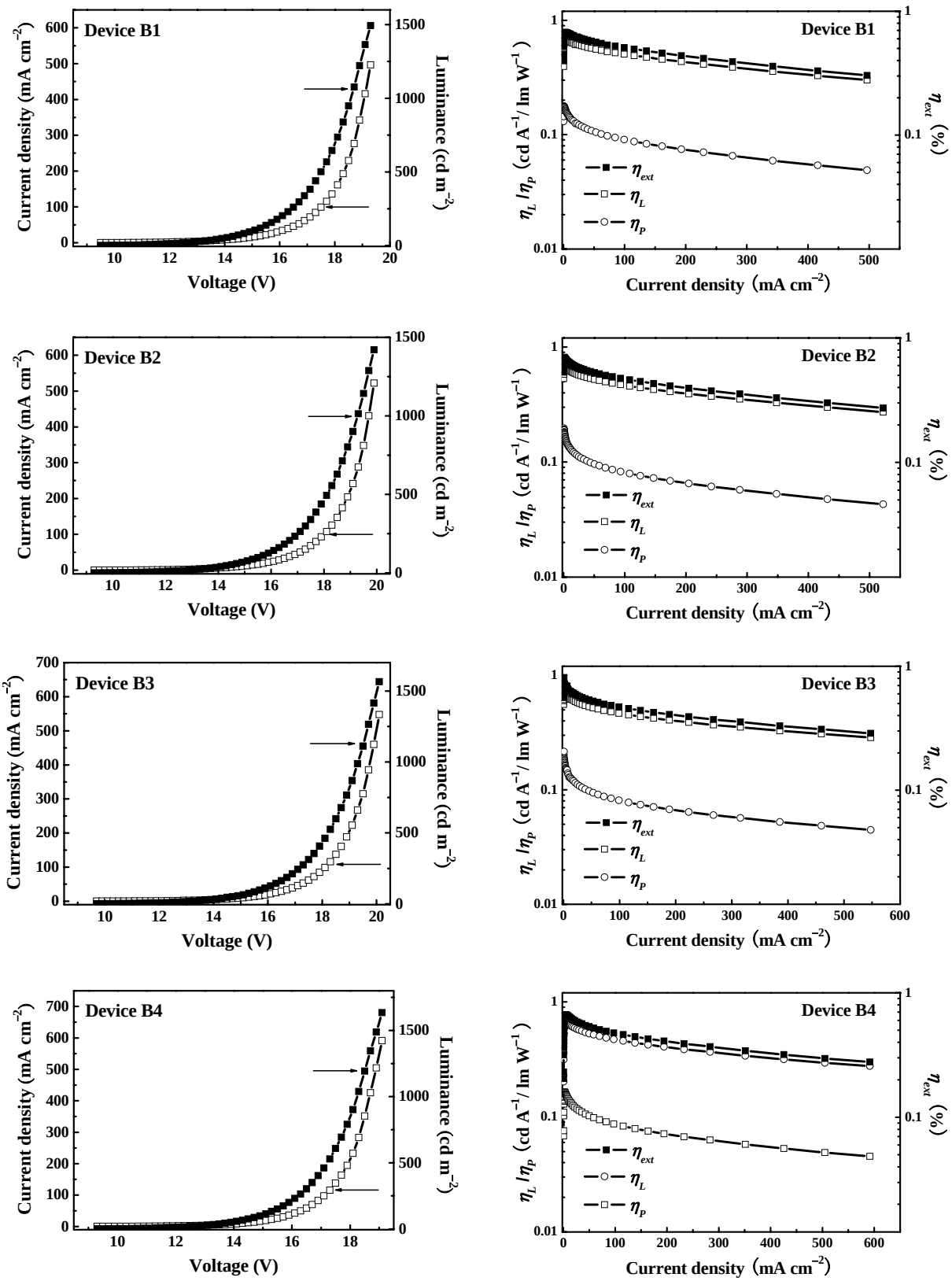


Fig. S7 The *J*–*V*–*L* curves and the efficiency versus current density relationship for devices **B1**–**B4**.

Table S1 Selected bond lengths [Å] and angles [°] for **Ir-1** and **Pt-1**.

Ir-1				**Pt-1**			
bond lengths [Å]		bond angles [°]		bond lengths [Å]		bond angles [°]	
Ir(1)–C(1)	1.982(5)	C(1)–Ir(1)–N(1)	80.0(2)	Pt(1)–C(1)	1.968(5)	C(1)–Pt(1)–N(1)	81.5(2)
Ir(1)–C(19)	1.985(5)	C(19)–Ir(1)–N(2)	80.5(2)	Pt(1)–O(2)	2.000(3)	O(2)–Pt(1)–O(3)	92.0(1)
Ir(1)–O(3)	2.144(4)	N(1)–Ir(1)–N(2)	172.9(2)	Pt(1)–O(3)	2.080(3)	N(1)–Pt(1)–O(2)	175.1(1)
Ir(1)–O(4)	2.145(4)	O(3)–Ir(1)–O(4)	88.7(2)	Pt(1)–N(1)	1.982(4)	C(1)–Pt(1)–O(3)	173.9(2)
Ir(1)–N(1)	2.033(4)	C(19)–Ir(1)–O(3)	176.8(2)				
Ir(1)–N(2)	2.037(4)	C(1)–Ir(1)–O(4)	176.0(2)	C(3)–C(4)	1.486(6)	O(1)–C(10)–C(11)	128.3(5)
				C(3)–C(11)	1.398(7)	O(1)–C(10)–C(9)	126.4(5)
C(3)–C(4)	1.491(8)	O(1)–C(10)–C(9)	127.6(5)	C(4)–C(9)	1.396(7)	C(11)–C(10)–C(9)	105.3(4)
C(3)–C(11)	1.398(8)	O(1)–C(10)-C(11)	127.3(6)	C(10)–O(1)	1.216(6)		
C(4)–C(9)	1.416(8)	C(9)–C(10)–C(11)	105.1(5)	C(10)–C(11)	1.484(7)		
C(10)–O(1)	1.217(7)	O(2)–C(28)–C(29)	128.8(6)	C(9)–C(10)	1.502(7)		
C(10)–C(11)	1.502(7)	O(2)–C(28)–C(27)	126.3(6)				
C(9)–C(10)	1.491(9)	C(29)–C(28)–C(27)	104.8(5)				
C(21)–C(22)	1.489(7)						
C(21)–C(29)	1.395(7)						
C(22)–C(27)	1.396(8)						
C(28)–O(2)	1.208(7)						
C(28)–C(29)	1.493(8)						
C(27)–C(28)	1.496(9)						

Table S2 Selected bond lengths [Å] for the phenyl and pyridyl rings in the ligand groups of the complexes **Ir-1** and **Pt-1**.

Ir-1		**Pt-1**
C(1)-C(13) 1.415(7)	C(19)-C(20) 1.397(7)	C(1)-C(2) 1.400(7)
C(1)-C(2) 1.419(7)	C(19)-C(31) 1.423(7)	C(1)-C(13) 1.409(7)
C(2)-C(3) 1.375(7)	C(20)-C(21) 1.369(7)	C(2)-C(3) 1.379(6)
C(3)-C(11) 1.398(8)	C(21)-C(29) 1.395(7)	C(3)-C(11) 1.398(7)
C(4)-C(5) 1.363(9)	C(22)-C(23) 1.376(8)	C(4)-C(5) 1.370(7)
C(4)-C(9) 1.416(8)	C(22)-C(27) 1.396(8)	C(4)-C(9) 1.396(7)
C(5)-C(6) 1.396(9)	C(23)-C(24) 1.375(8)	C(5)-C(6) 1.389(7)
C(6)-C(7) 1.36(1)	C(24)-C(25) 1.40(1)	C(6)-C(7) 1.377(8)
C(7)-C(8) 1.40(1)	C(25)-C(26) 1.386(9)	C(7)-C(8) 1.380(9)
C(8)-C(9) 1.385(9)	C(26)-C(27) 1.377(8)	C(8)-C(9) 1.372(7)
C(11)-C(12) 1.381(8)	C(29)-C(30) 1.389(8)	C(11)-C(12) 1.380(7)
C(12)-C(13) 1.403(7)	C(30)-C(31) 1.390(7)	C(12)-C(13) 1.395(6)
C(14)-N(1) 1.358(6)	C(32)-N(2) 1.366(7)	C(14)-N(1) 1.363(6)
C(14)-C(15) 1.392(7)	C(32)-C(33) 1.397(7)	C(14)-C(15) 1.401(7)
C(15)-C(16) 1.374(8)	C(33)-C(34) 1.361(9)	C(15)-C(16) 1.350(8)
C(16)-C(17) 1.386(9)	C(34)-C(35) 1.37(1)	C(16)-C(17) 1.390(8)
C(17)-C(18) 1.378(8)	C(35)-C(36) 1.399(8)	C(17)-C(18) 1.355(8)
C(18)-N(1) 1.347(7)	C(36)-N(2) 1.340(7)	C(18)-N(1) 1.346(6)

Table S3 Selected bond lengths [Å] and angles [°] for the complex **Pt-2**.

Pt-2	
bond lengths [Å]	bond angles [°]
Pt(1)-C(12) 1.973(3)	C(12)-Pt(1)-N(1) 81.5 (1)
Pt(1)-O(1) 2.080(2)	C(12)-Pt(1)-O(2) 93.2(1)
Pt(1)-O(2) 1.995(3)	N(1)-Pt(1)-O(1) 93.5(1)
Pt(1)-N(1) 1.985(3)	O(1)-Pt(1)-O(2) 91.9(1)
	N(1)-Pt(1)-O(2) 174.4(1)
C(14)-C(15) 1.395(5)	C(12)-Pt(1)-O(1) 174.3(1)
C(14)-C(17) 1.4705)	
C(15)-C(23) 1.525(5)	C(15)-C(23)-C(22) 101.0(3)
C(17)-C(22) 1.395(5)	
C(22)-O(23) 1.517(5)	

Table S4 X-ray crystal data for the complexes.

Compound	**Ir-1**	**Pt-1**	**Pt-2**
CCDC no.	698299	698300	639792
formula	$C_{41}H_{27}IrN_2O_4{\cdot}2CH_2Cl_2$	$C_{23}H_{17}NO_3Pt$	$C_{27}H_{27}NO_2Pt$
formula weight	973.70	550.47	592.59
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2_1/c$	$P2_1/c$
a (Å)	12.2247(18)	9.6884(7)	8.1679(5)
b (Å)	13.728(2)	7.8986(6)	26.7111(15)
c (Å)	13.838(2)	23.7456(18)	10.9458(6)
α (deg)	63.248(2)	90	90
β (deg)	74.128(2)	95.0830(10)	107.2510(10)
γ (deg)	74.473(3)	90	90
V (Å^3)	1966.2(5)	1810.0(2)	2280.7(2)
Z	2	4	4
D_{calcd} (g cm^{-3})	1.645	2.020	1.726
μ (mm^{-1})	3.712	7.777	6,176
F(000)	960	1056	1160
θ range (deg)	1.69–28.31	2.11–25.00	2.47–28.30
reflections collected	11580	8447	13355
unique reflections	8501	3170	5267
R_{int}	0.0301	0.0277	0.0232
observed reflections	7481	2909	4382
no. of parameters	487	253	280
*R1, wR2 [*I > 2.0σ(I)*]* [a]	0.0430, 0.1124	0.0275, 0.0681	0.0272, 0.0616
R1, wR2 (all data)	0.0498, 0.1176	0.0304, 0.0694	0.0309, 0.0628
GoF on F^2 [b]	1.024	1.082	1.176

[a] $R1 = \Sigma \, ||F_o| - |F_c|| \, / \, \Sigma \, |F_o|$. $wR2 = \{\Sigma \, [w(F_o^2 - F_c^2)^2] \, / \, \Sigma \, [w(F_o^2)^2]\}^{1/2}$.

[b] $GoF = [(\Sigma w|F_o| - |F_c|)^2 \, / \, (N_{obs} - N_{param})]^{1/2}$.

Table S5 Performance of the electrophosphorescent red OLEDs made from **Ir-1** and **Pt-1**.

Device	Phosphor dopant	$V_{turn\text{-}on}$ /V	Luminance L /cd m^{-2}	η_{ext} /%	η_L /cd A^{-1}	η_p /lm W^{-1}	λ_{max} /nm[d]
A1	**Ir-1** (4wt.-%)	5.9	4803 (16.1)[a]	1.29 (10.5)	1.48 (10.5)	0.49 (7.9)	609
			282[b]	1.22	1.41	0.38	(0.63, 0.38)
			1193[c]	1.03	1.19	0.27	
A2	**Ir-1** (6 wt.-%)	5.3	4944 (15.3)	1.20 (10.7)	1.39 (10.7)	0.45 (9.5)	609
			277	1.19	1.38	0.40	(0.63, 0.38)
			1205	1.04	1.21	0.29	
A3	**Ir-1** (8 wt.-%)	5.3	5096 (15.1)	1.13 (11.1)	1.30 (11.1)	0.40 (9.1)	609
			260	1.12	1.29	0.39	(0.63, 0.38)
			1185	1.03	1.18	0.29	
A4	**Ir-1** (10 wt.-%)	5.3	4722 (14.9)	1.00 (10.7)	1.15 (10.7)	0.36 (8.9)	609
			229	0.99	1.14	0.34	(0.63, 0.38)
			1064	0.92	1.06	0.26	
B1	**Pt-1** (4 wt.-%)	9.5	1494 (19.3)	0.68 (12.7)	0.67 (12.7)	0.18 (11.1)	611
			123	0.62	0.61	0.13	(0.61, 0.36)
			504	0.51	0.50	0.09	
B2	**Pt-1** (6 wt.-%)	9.3	1420 (19.9)	0.70 (11.5)	0.69 (11.5)	0.20 (9.9)	611
			117	0.59	0.59	0.12	(0.61, 0.36)
			464	0.47	0.46	0.08	
B3	**Pt-1** (8 wt.-%)	9.7	1566 (20.1)	0.81 (11.7)	0.80 (11.7)	0.22 (11.7)	611
			119	0.60	0.60	0.12	(0.62, 0.35)
			466	0.47	0.47	0.08	
B4	**Pt-1** (10 wt.-%)	9.3	1635 (19.1)	0.67 (13.5)	0.66 (13.5)	0.16 (11.5)	611
			120	0.60	0.60	0.12	(0.62, 0.35)
			471	0.47	0.47	0.09	

[a] Maximum values of the devices. Values in parentheses are the voltages at which they were obtained. [b] Values collected at 20 mA cm^{-2}. [c] Values collected at 100 mA cm^{-2}. [d] CIE coordinates [x, y] in parentheses.