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High-Efficiency Near-Infrared-Emitting OLEDs Based on Iridium Complex with Negligible Efficiency Roll-off

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Supporting Information

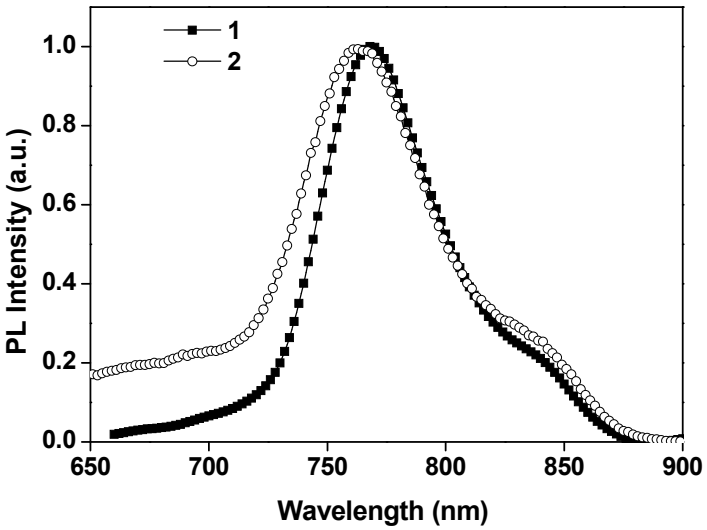

Figure S1 The uncorrected PL spectra of complex **1** and **2** in CH_2Cl_2 solutions recorded using a red PMT.

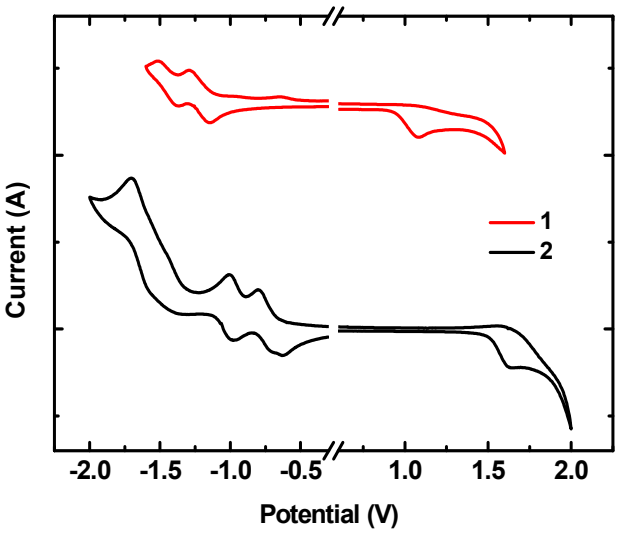

Figure S2 Cyclic Voltammetry (CV) diagram for Ir(mpbqx-*g*)$_2$(acac) **1** and Ir(mpbqx-*g*)$_2$(Bphen) **2** in CH_2Cl_2 and CH_3CN solutions, respectively.

Table S1. The first two triplet states for Ir(mpbqx-*g*)$_2$(acac) **1** calculated from TDDFT approach.

States(E[eV]) (λ[nm]) [a]	**Dominant excitations** [b]	**Character**
T_1 (1.641) (755 nm)	H → L (0.38)	π(mpbqx)/$d_π$(Ir) → π*(mpbqx)
	H-2 → L (0.27)	π(mpbqx)/$d_π$(Ir) → π*(mpbqx)
	H-1 → L+1 (0.19)	π(acac)/$d_π$(Ir) → π*(mpbqx)
T_2 (1.653) (750 nm)	H-1→ L (0.30)	π(acac)/$d_π$(Ir) → π*(mpbqx)
	H-2 → L+1 (0.28)	π(mpbqx)/$d_π$(Ir) → π*(mpbqx)
	H → L+1 (0.22)	π(mpbqx)/$d_π$(Ir) → π*(mpbqx)

[a] Data in parentheses are excitation energies and corresponding wavelengths. [b] H and L denote HOMO and LUMO, respectively; data in parentheses are the contributions of corresponding excitations.

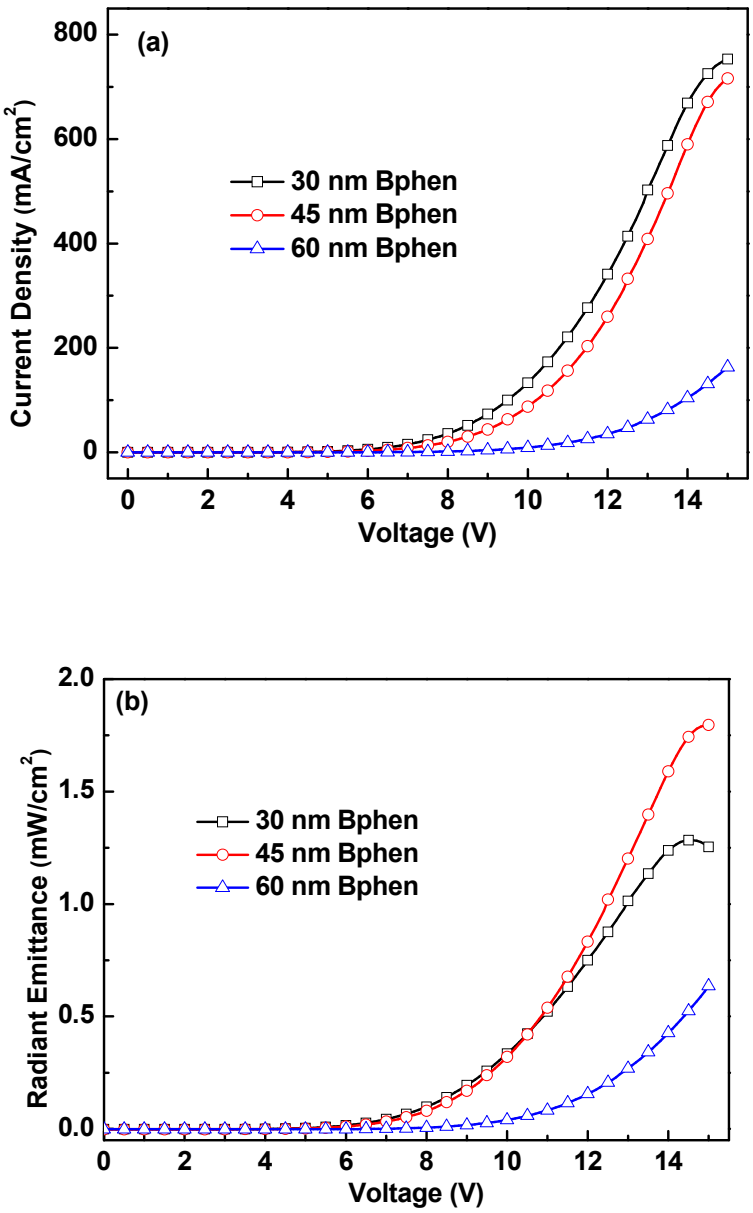

Figure S3 Current density *vs*. bias voltage characteristics and Radiant emittance *vs*. bias voltage characteristics for devices with the configurations as ITO/NPB (40 nm)/Complex **1**: $Ga_2(saph)_2q_2$ (20 wt.% 40 nm)/Bphen (30, 45, 60 nm, respectively)/Mg: Ag (150 nm).

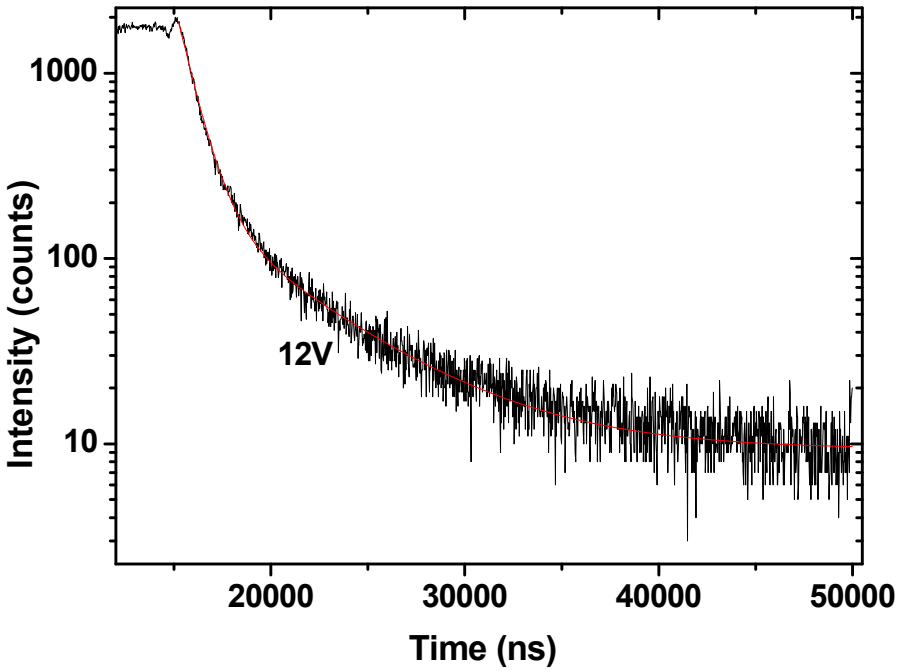

Figure S4 Electroluminescence transients of the OLEDs (ITO/NPB (40 nm)/Complex **1**: $Ga_2(saph)_2q_2$ (20 wt.% 40 nm)/Bphen (45 nm)/Mg: Ag (150 nm)) at 12V (gray lines) and the fit (red lines).

Table S2. Atomic coordinates and equivalent isotropic temperature factors* (Å^2)

Atoms	*x*	*y*	*z*	$U_{eq.}$
Ir(1)	0.5000	0.43179(2)	0.2500	0.01941(12)
Cl(1)	0.64865(17)	1.0059(4)	0.4835(3)	0.1328(13)
Cl(2)	0.6679(4)	0.8120(8)	0.3675(3)	0.313(6)
O(1)	0.51517(14)	0.2683(3)	0.1692(2)	0.0266(7)
N(1)	0.43073(17)	0.4450(4)	0.1616(2)	0.0222(8)
N(2)	0.34291(19)	0.4666(6)	0.0303(3)	0.0377(10)
C(1)	0.5000	0.0759(7)	0.2500	0.041(2)
C(2)	0.5107(2)	0.1415(5)	0.1810(3)	0.0359(12)
C(3)	0.5191(4)	0.0509(6)	0.1117(4)	0.055(2)
C(4)	0.38206(19)	0.3793(5)	0.1638(3)	0.0267(9)
C(5)	0.3750(2)	0.3039(5)	0.2306(3)	0.0318(10)
C(6)	0.3264(2)	0.2309(6)	0.2298(3)	0.0380(12)
C(7)	0.3193(3)	0.1481(8)	0.2961(4)	0.0530(16)
C(8)	0.2723(3)	0.0759(7)	0.2939(6)	0.062(2)
C(9)	0.2303(3)	0.0819(8)	0.2253(6)	0.065(2)
C(10)	0.2353(2)	0.1586(8)	0.1609(4)	0.0537(17)
C(11)	0.2835(2)	0.2361(6)	0.1612(4)	0.0404(13)
C(12)	0.2904(2)	0.3182(7)	0.0970(4)	0.0426(14)
C(13)	0.3391(2)	0.3879(6)	0.0965(3)	0.0332(11)
C(14)	0.3886(2)	0.5308(6)	0.0299(3)	0.0324(11)
C(15)	0.43527(19)	0.5188(5)	0.0964(3)	0.0250(9)
C(16)	0.3887(3)	0.6174(7)	-0.0434(3)	0.0467(14)
C(17)	0.4882(2)	0.5872(5)	0.1026(3)	0.0238(9)
C(18)	0.5225(2)	0.5706(4)	0.1783(3)	0.0219(10)
C(19)	0.5718(2)	0.6412(5)	0.1928(3)	0.0289(10)
C(20)	0.5885(2)	0.7195(5)	0.1339(3)	0.0349(11)
C(21)	0.5558(2)	0.7249(5)	0.0568(3)	0.0340(11)
C(22)	0.5060(2)	0.6622(5)	0.0414(3)	0.0309(10)
C(23)	0.6932(6)	0.895(2)	0.4525(10)	0.41(3)

*$U_{eq.}$ defined as one third of the trace of the orthogonalized **U** tensor.

Table S3. Bond lengths (Å) and bond angles (°)

Ir(1)-C(18)	1.971(5)	C(5)-C(6)	1.409(7)
Ir(1)-C(18)$^{\#1}$	1.971(5)	C(6)-C(7)	1.420(9)
Ir(1)-N(1)$^{\#1}$	2.065(4)	C(6)-C(11)	1.423(8)
Ir(1)-N(1)	2.066(4)	C(7)-C(8)	1.367(9)
Ir(1)-O(1)	2.182(3)	C(8)-C(9)	1.409(13)
Ir(1)-O(1)$^{\#1}$	2.182(3)	C(9)-C(10)	1.346(11)
Cl(1)-C(23)	1.713(10)	C(10)-C(11)	1.426(8)
Cl(2)-C(23)	1.665(10)	C(11)-C(12)	1.386(9)
O(1)-C(2)	1.262(6)	C(12)-C(13)	1.401(7)
N(1)-C(15)	1.339(6)	C(14)-C(15)	1.463(7)
N(1)-C(4)	1.386(6)	C(14)-C(16)	1.499(8)
N(2)-C(14)	1.308(8)	C(15)-C(17)	1.471(7)
N(2)-C(13)	1.376(8)	C(17)-C(18)	1.408(7)
C(1)-C(2)	1.402(6)	C(17)-C(22)	1.409(7)
C(1)-C(2)$^{\#1}$	1.402(6)	C(18)-C(19)	1.396(7)
C(2)-C(3)	1.515(8)	C(19)-C(20)	1.383(7)
C(4)-C(5)	1.388(7)	C(20)-C(21)	1.400(8)
C(4)-C(13)	1.410(7)	C(21)-C(22)	1.370(8)

C(18)-Ir(1)-C(18)$^{\#1}$	93.1(3)	C(1)-C(2)-C(3)	117.0(5)
C(18)-Ir(1)-N(1)$^{\#1}$	95.80(19)	N(1)-C(4)-C(5)	121.3(4)
C(18)$^{\#1}$-Ir(1)-N(1)$^{\#1}$	79.23(19)	N(1)-C(4)-C(13)	119.4(5)
C(18)-Ir(1)-N(1)	79.23(19)	C(5)-C(4)-C(13)	119.3(5)
C(18)$^{\#1}$-Ir(1)-N(1)	95.80(19)	C(4)-C(5)-C(6)	120.5(5)
N(1)$^{\#1}$-Ir(1)-N(1)	172.8(2)	C(5)-C(6)-C(7)	121.4(5)
C(18)-Ir(1)-O(1)	90.74(17)	C(5)-C(6)-C(11)	120.4(5)
C(18)$^{\#1}$-Ir(1)-O(1)	173.20(16)	C(7)-C(6)-C(11)	118.2(5)
N(1)$^{\#1}$-Ir(1)-O(1)	105.94(14)	C(8)-C(7)-C(6)	120.7(7)
N(1)-Ir(1)-O(1)	79.43(14)	C(7)-C(8)-C(9)	120.2(8)
C(18)-Ir(1)-O(1)$^{\#1}$	173.20(16)	C(10)-C(9)-C(8)	121.2(6)
C(18)$^{\#1}$-Ir(1)-O(1)$^{\#1}$	90.74(17)	C(9)-C(10)-C(11)	120.2(6)
N(1)$^{\#1}$-Ir(1)-O(1)$^{\#1}$	79.43(14)	C(12)-C(11)-C(6)	118.1(5)
N(1)-Ir(1)-O(1)$^{\#1}$	105.95(14)	C(12)-C(11)-C(10)	122.5(6)
O(1)-Ir(1)-O(1)$^{\#1}$	85.98(18)	C(6)-C(11)-C(10)	119.4(6)
C(2)-O(1)-Ir(1)	125.9(3)	C(11)-C(12)-C(13)	121.8(5)
C(15)-N(1)-C(4)	119.1(4)	N(2)-C(13)-C(12)	118.3(5)
C(15)-N(1)-Ir(1)	115.8(3)	N(2)-C(13)-C(4)	121.8(5)
C(4)-N(1)-Ir(1)	125.0(3)	C(12)-C(13)-C(4)	119.8(5)
C(14)-N(2)-C(13)	118.1(5)	N(2)-C(14)-C(15)	122.0(5)
C(2)-C(1)-C(2)$^{\#1}$	125.6(7)	N(2)-C(14)-C(16)	114.5(5)
O(1)-C(2)-C(1)	128.1(5)	C(15)-C(14)-C(16)	123.5(5)
O(1)-C(2)-C(3)	114.9(5)	N(1)-C(15)-C(14)	119.5(5)

(Table S3. continued)

N(1)-C(15)-C(17)	113.9(4)	C(17)-C(18)-Ir(1)	116.1(4)
C(14)-C(15)-C(17)	126.5(5)	C(20)-C(19)-C(18)	121.9(5)
C(18)-C(17)-C(22)	120.2(5)	C(19)-C(20)-C(21)	119.0(5)
C(18)-C(17)-C(15)	113.4(4)	C(22)-C(21)-C(20)	120.7(5)
C(22)-C(17)-C(15)	126.5(5)	C(21)-C(22)-C(17)	119.9(5)
C(19)-C(18)-C(17)	117.9(4)	Cl(2)-C(23)-Cl(1)	114.1(9)
C(19)-C(18)-Ir(1)	125.5(4)		

Symmetry transformation code: #1 (1-*x*, *y*, 0.5-*z*).

Table S4. Anisotropic thermal parameters* (Å^2)

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir(1)	0.01792(15)	0.02331(16)	0.01712(16)	0.000	0.00373(10)	0.000
Cl(1)	0.149(3)	0.104(2)	0.171(3)	0.020(2)	0.094(3)	0.010(2)
Cl(2)	0.581(16)	0.231(7)	0.156(4)	-0.101(5)	0.144(7)	-0.228(9)
O(1)	0.0321(18)	0.0264(17)	0.0206(16)	-0.0018(13)	0.0034(14)	0.0037(13)
N(1)	0.0196(19)	0.031(2)	0.0157(19)	-0.0026(13)	0.0021(15)	0.0024(13)
N(2)	0.027(2)	0.057(3)	0.028(2)	-0.005(2)	0.0002(18)	0.012(2)
C(1)	0.058(6)	0.031(4)	0.033(5)	0.000	0.003(4)	0.000
C(2)	0.046(3)	0.033(3)	0.027(2)	-0.006(2)	0.002(2)	0.010(2)
C(3)	0.092(6)	0.034(3)	0.038(4)	-0.008(2)	0.014(4)	0.016(3)
C(4)	0.020(2)	0.032(2)	0.028(2)	-0.0080(19)	0.0044(18)	0.0025(17)
C(5)	0.024(2)	0.042(3)	0.028(2)	-0.006(2)	0.0002(19)	-0.007(2)
C(6)	0.029(3)	0.047(3)	0.038(3)	-0.006(2)	0.007(2)	-0.008(2)
C(7)	0.036(3)	0.073(4)	0.051(4)	0.001(3)	0.009(3)	-0.024(3)
C(8)	0.048(4)	0.073(5)	0.068(5)	0.001(3)	0.019(4)	-0.031(3)
C(9)	0.035(4)	0.088(6)	0.076(6)	-0.015(4)	0.019(4)	-0.036(3)
C(10)	0.026(3)	0.073(4)	0.061(4)	-0.019(4)	0.004(3)	-0.012(3)
C(11)	0.027(3)	0.055(3)	0.039(3)	-0.020(3)	0.005(2)	-0.006(2)
C(12)	0.018(2)	0.067(4)	0.040(3)	-0.012(3)	-0.002(2)	-0.003(2)
C(13)	0.019(2)	0.051(3)	0.029(3)	-0.014(2)	0.0031(19)	0.001(2)
C(14)	0.031(3)	0.042(3)	0.023(2)	-0.004(2)	0.001(2)	0.012(2)
C(15)	0.026(2)	0.028(2)	0.021(2)	-0.0008(18)	0.0026(17)	0.0073(18)
C(16)	0.045(3)	0.065(4)	0.026(3)	0.009(3)	-0.004(2)	0.013(3)
C(17)	0.029(2)	0.026(2)	0.017(2)	0.0008(16)	0.0065(19)	0.0052(17)
C(18)	0.023(2)	0.024(2)	0.021(2)	0.0000(15)	0.0088(19)	0.0029(15)
C(19)	0.029(2)	0.029(2)	0.030(2)	0.0043(19)	0.008(2)	-0.0003(18)
C(20)	0.034(3)	0.034(3)	0.040(3)	0.007(2)	0.014(2)	-0.002(2)
C(21)	0.043(3)	0.029(2)	0.035(3)	0.008(2)	0.020(2)	0.005(2)
C(22)	0.041(3)	0.028(2)	0.025(2)	0.0048(19)	0.011(2)	0.008(2)
C(23)	0.66(7)	0.25(3)	0.47(5)	-0.23(3)	0.46(5)	-0.27(4)

*The exponent takes the form: $-2\pi^2\Sigma\Sigma U_{ij}h_ih_j\mathbf{a}_i^*\mathbf{a}_j^*$

Table S5. Coordinates and isotropic temperature factors* ($Å^2$) for H atoms

Atoms	*x*	*y*	*z*	$U_{eq.}$
H(1)	0.5000	-0.0194	0.2500	0.050
H(3A)	0.5120	0.1026	0.0624	0.082
H(3B)	0.4947	-0.0257	0.1072	0.082
H(3C)	0.5559	0.0184	0.1214	0.082
H(5)	0.4025	0.3014	0.2762	0.038
H(7)	0.3469	0.1430	0.3415	0.064
H(8)	0.2681	0.0225	0.3378	0.074
H(9)	0.1987	0.0321	0.2244	0.079
H(10)	0.2072	0.1610	0.1161	0.064
H(12)	0.2618	0.3273	0.0531	0.051
H(16A)	0.4148	0.5819	-0.0728	0.070
H(16B)	0.3981	0.7099	-0.0271	0.070
H(16C)	0.3532	0.6159	-0.0771	0.070
H(19)	0.5941	0.6354	0.2435	0.035
H(20)	0.6211	0.7679	0.1453	0.042
H(21)	0.5680	0.7715	0.0157	0.041
H(22)	0.4840	0.6691	-0.0095	0.037
H(23A)	0.7252	0.9453	0.4450	0.494
H(23B)	0.7048	0.8278	0.4949	0.494

*The exponent takes the form: $-8\pi^2 U\sin^2\theta/\lambda^2$

The complete author list of reference 30:

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