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

Supporting Information

Highly efficient orange-red electroluminescence of iridium complexes with good electron mobility

Hua-Bo Han[1#], Rong-Zhen Cui[2, #], Yi-Ming Jing[1], Guang-Zhao Lu[1], You-Xuan Zheng[,1], Liang Zhou*[,2], Jing-Lin Zuo[1], Hongjie Zhang[2]*

[1] State Key Laboratory of Coordination Chemistry, Jiangsu Key Laboratory of Advanced Organic Materials, Collaborative Innovation Center of Advanced Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China, *Email - yxzheng@nju.edu.cn

[2] State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P.R. China, zhoul@ciac.jl.cn

[#] Han and Cui have the same contributions to this paper

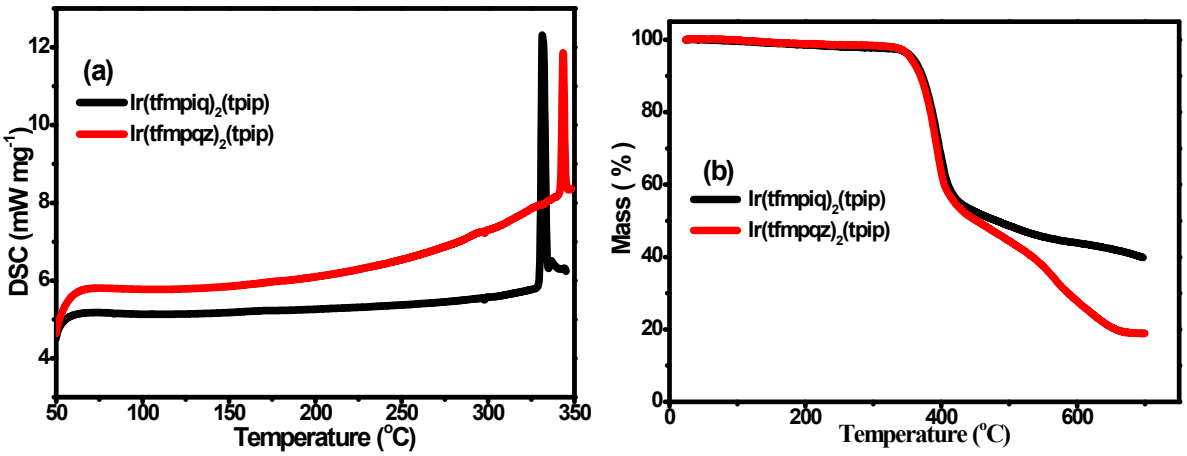

Fig. S1. The DSC (a) and TGA (b) curves of **Ir(tfmpiq)$_2$(tpip)** and **Ir(tfmpqz)$_2$(tpip)** complexes.

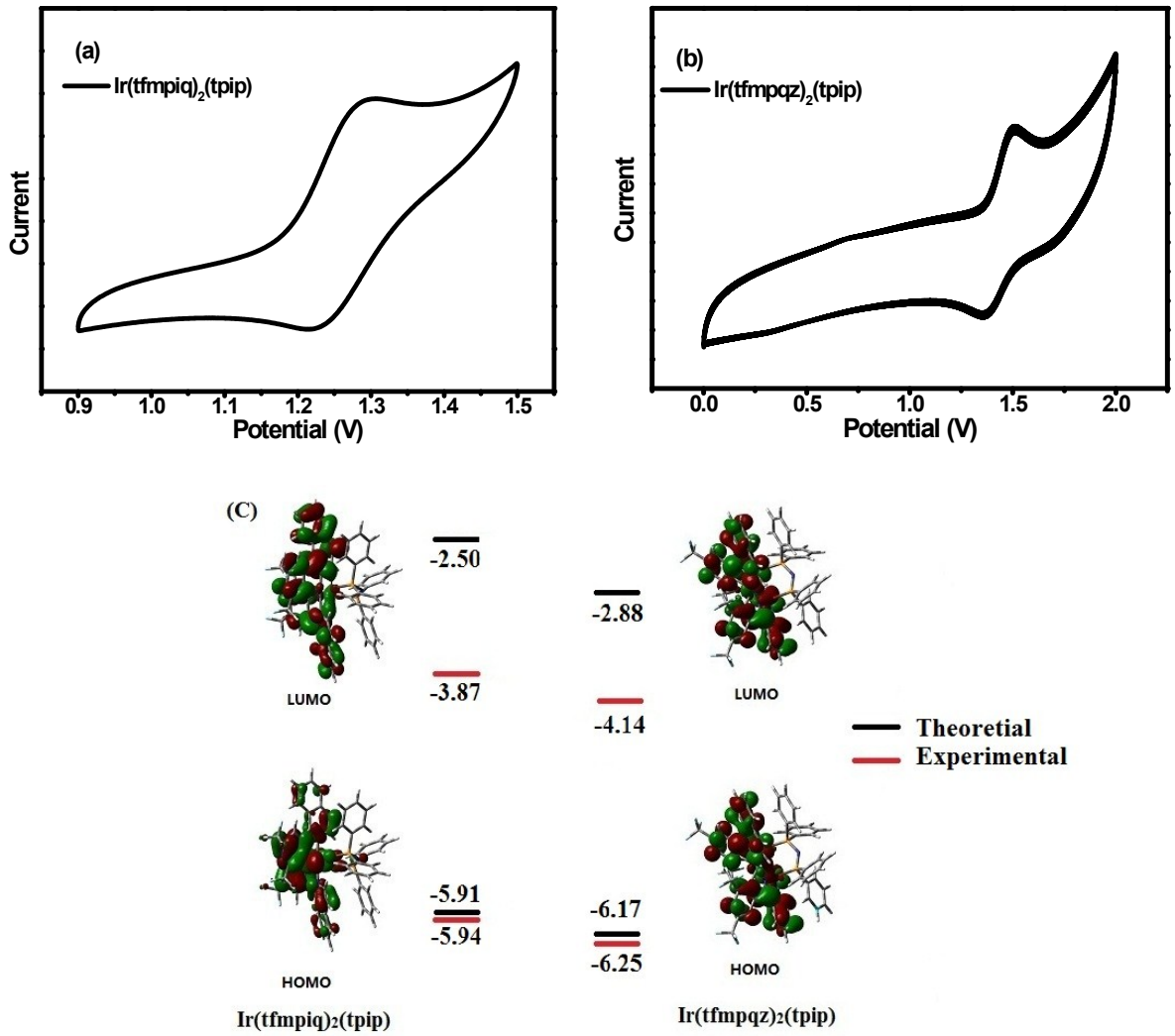

Fig. S2. (a), (b) the cyclic voltammogram curve of **Ir(tfmpiq)$_2$(tpip)** and **Ir(tfmpqz)$_2$(tpip)**; (c) Contour plots of **Ir(tfmpiq)$_2$(tpip)** and **Ir(tfmpqz)$_2$(tpip)**.

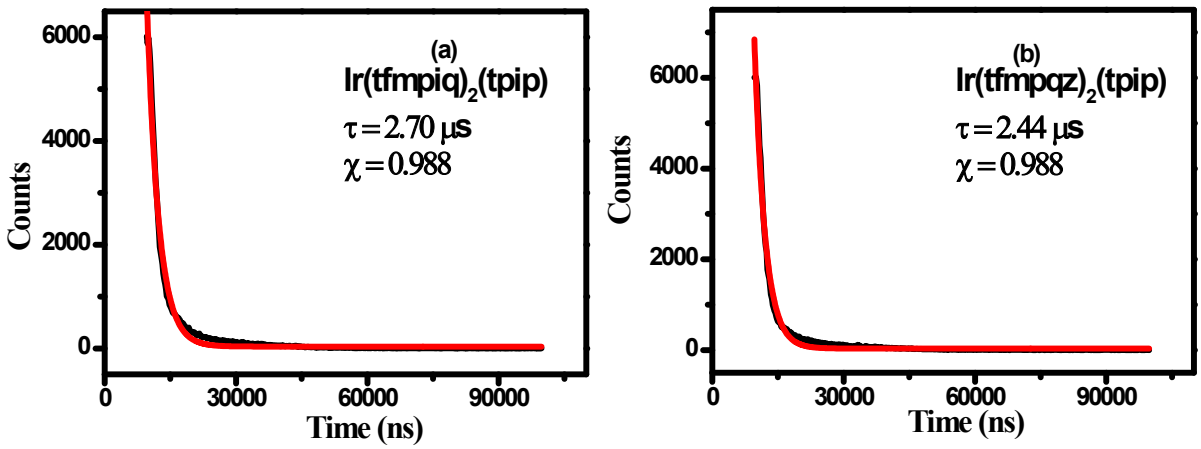

Fig. S3. The lifetime curves of **Ir(tfmpiq)$_2$(tpip)** and **Ir(tfmpqz)$_2$(tpip)** complexes.

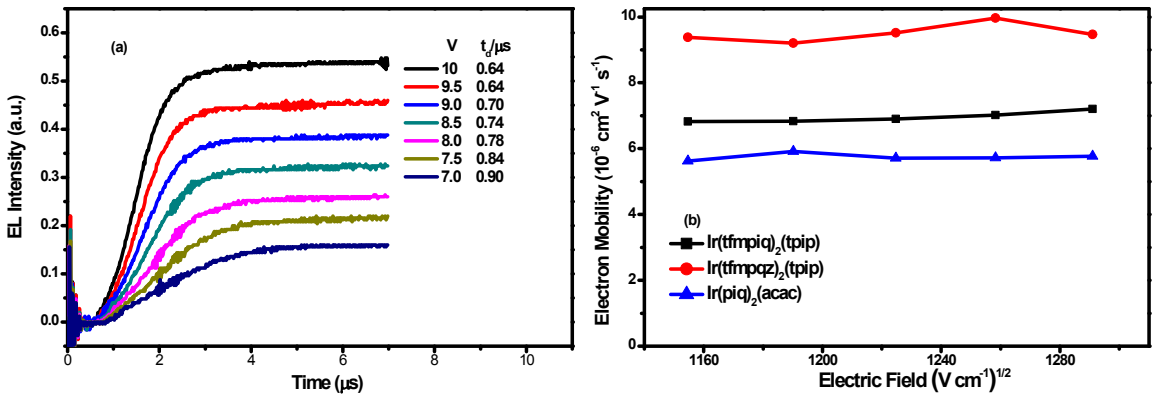

Fig. S4. (a) the transient EL signals for the device structure of ITO/ TAPC (50 nm)/ Ir complexes (60 nm) / Li (1 nm) / Al (100 nm) under different applied fields of **Ir(piq)$_2$(acac);** (b) electric field dependence of charge electron mobility in the thin films of **Ir(tfmpiq)$_2$(tpip), Ir(tfmpqz)$_2$(tpip) and Ir(piq)$_2$(acac).**

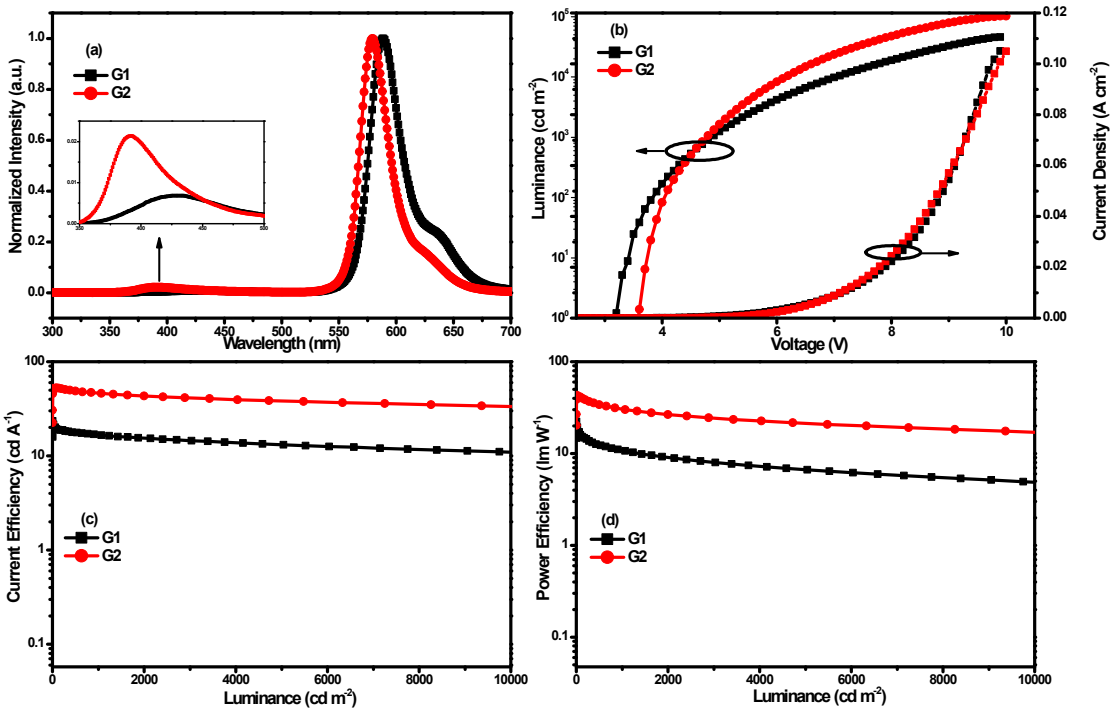

Fig. S5. Characteristics of singel-EML devices **G1** and **G2**: (a) electroluminescence spectra; (b) luminance – voltage – current density ($L - V - J$) curves; (c) current efficiency – luminance ($\eta_c - L$) curves; (d) power efficiency – luminance ($\eta_p - L$) curves.

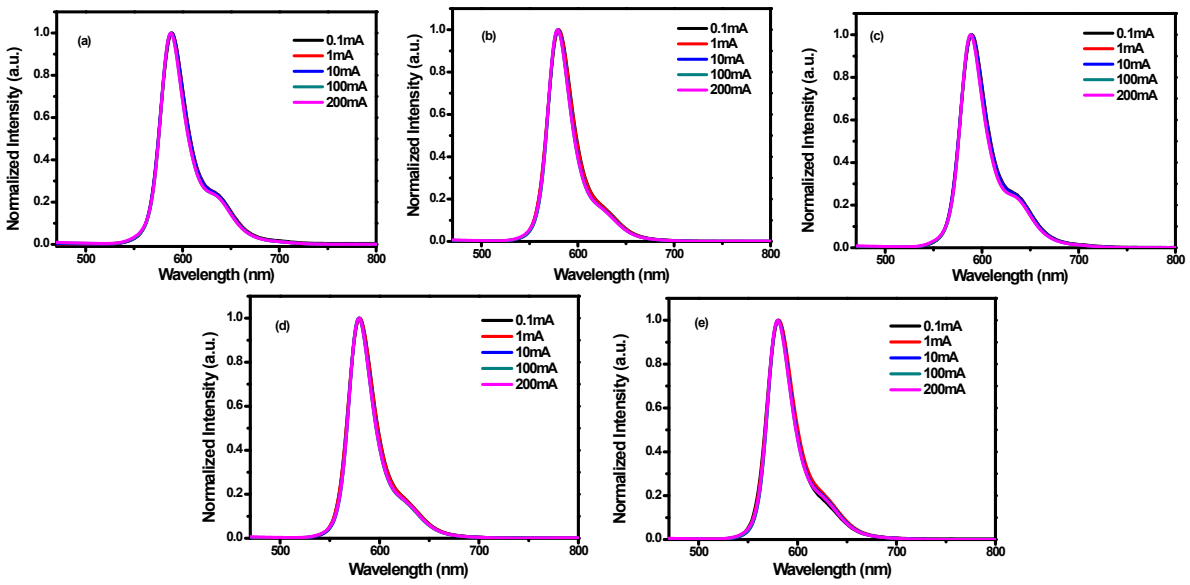

Fig. S6. Electroluminescence spectra of **G1**, **G2**, **G3**, **G4**, and **G5** at different applied current density.

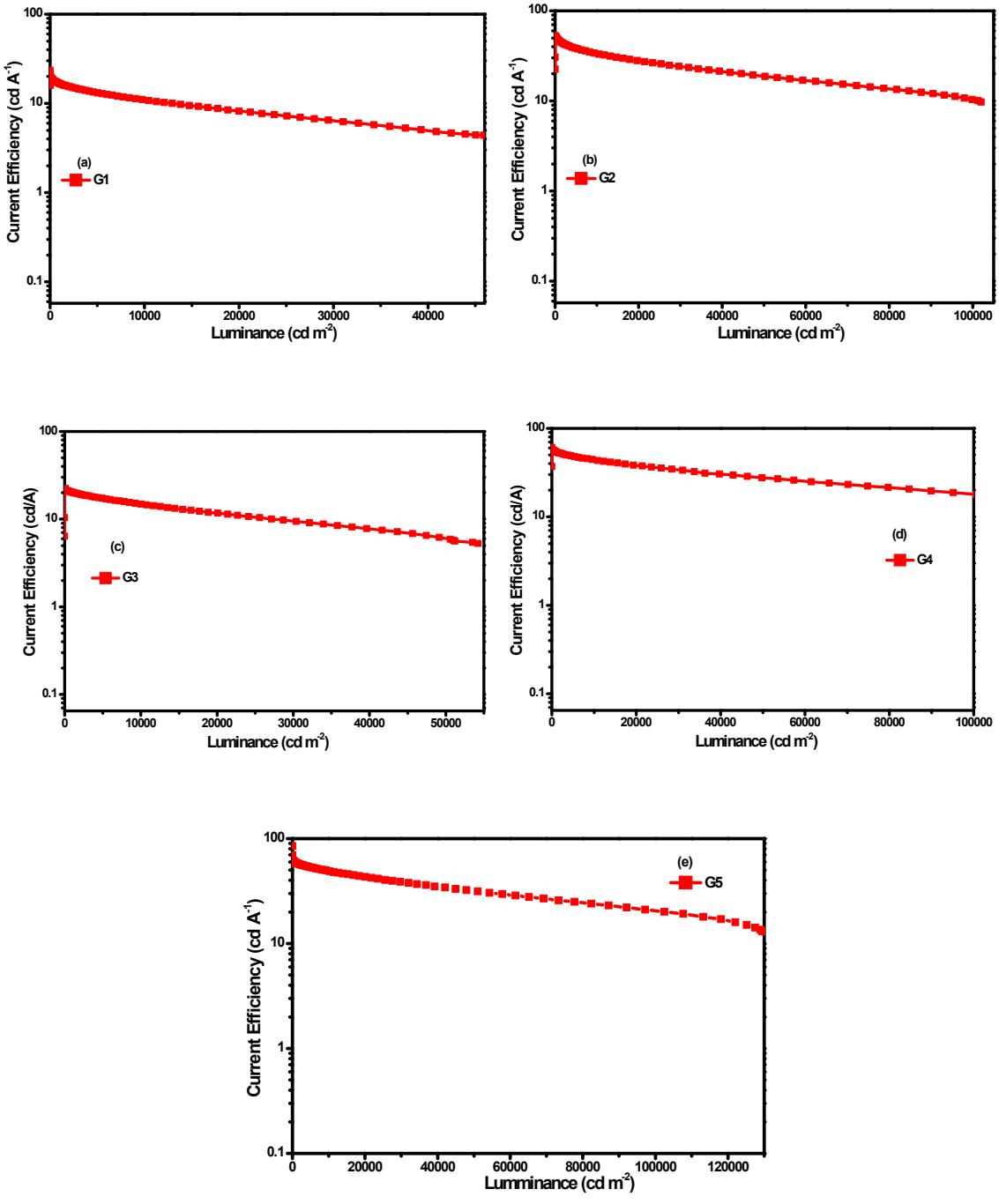

Fig. S7. Current efficiency – luminance ($\eta_c - L$) curves of **G1- G5**.

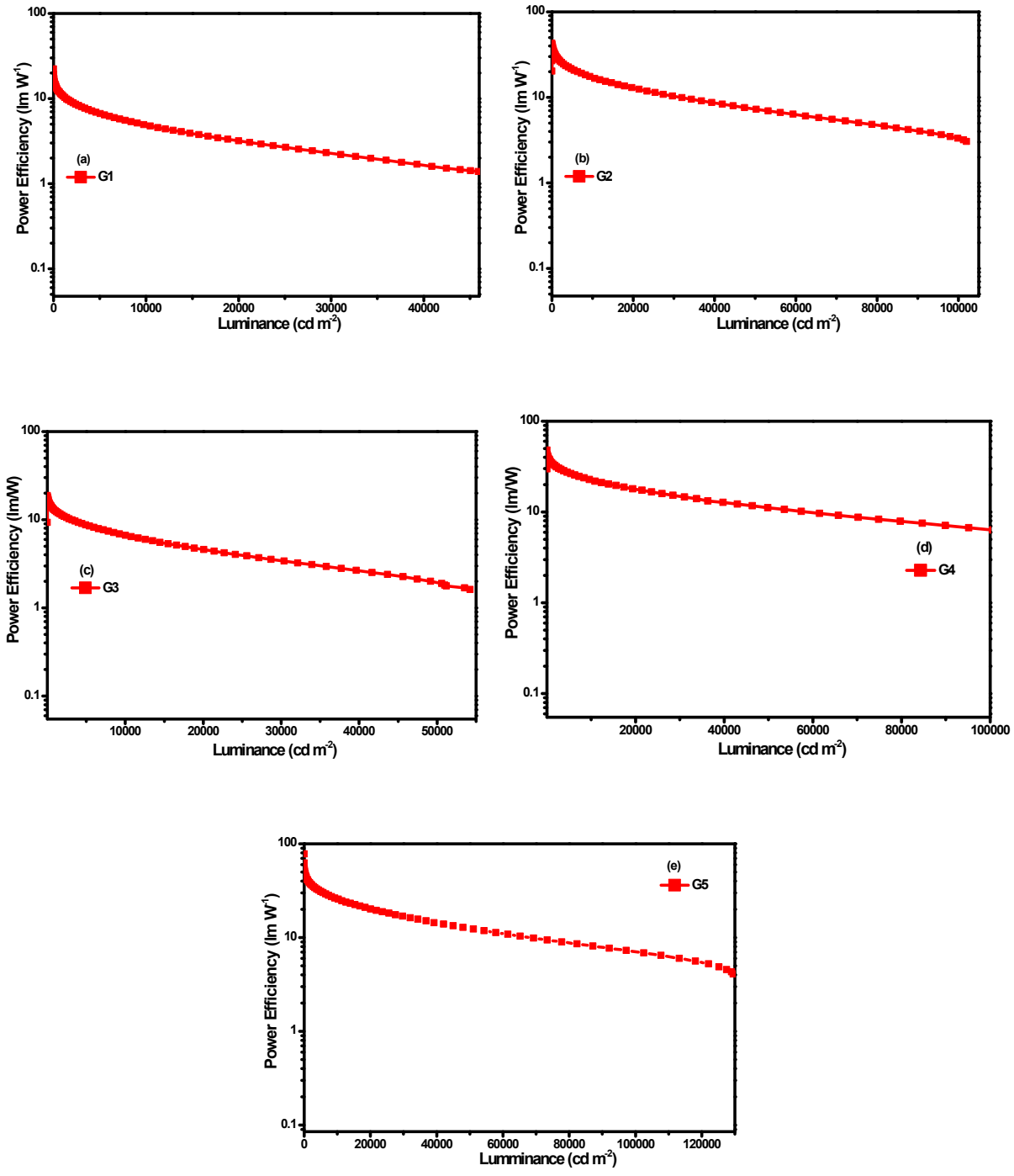

Fig. S8. Power efficiency – luminance ($\eta_p - L$) curves of **G1 - G5**.

Table S1. Crystallographic data of $Ir(tfmpiq)_2(tpip)$ and $Ir(tfmpqz)_2(tpip)$.

	$Ir(tfmpiq)_2(tpip)$	$Ir(tfmpqz)_2(tpip)$
Formula	$C_{56}H_{34}F_{12}IrN_5O_2P_2$	$C_{54}H_{32}F_{12}IrN_7O_2P_2$
FW	1291.02	1293.03
T (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	orthorhombic
Space group	*P 21/c*	*P n a 21*
a (Å)	16.5420(13)	21.9704(9)
b (Å)	13.6955(11)	16.6574(7)
c (Å)	23.0919(19)	13.7024(6)
α (deg)	90.00	90.00
β (deg)	90.00	90.00
γ (deg)	90.00	90.00
V (Å^3)	5186.7(7)	5014.7(4)
Z	4	4
ρ_{calcd} (mg/cm^3)	1.653	1.715
μ (Mo Kα) (mm^{-1})	2.727	2.822
F (000)	2544	2552
Reflns collected	34646	45075
Unique	11899	11446
Data/restraints/params	11899 / 207 / 691	11446 / 3 / 704
GOF on F^2	1.036	1.002
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0387, 0.1013	0.0328, 0.0637
$R_1{}^a$, $wR_2{}^b$ (all data)	0.0501, 0.1081	0.0460, 0.0673
CCDC NO	1536092	1536093

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)]^{1/2}$

Table S2(a) The selected bond lengths and angels of $Ir(tfmpiq)_2(tpip)$.

Selected bonds Å					
Ir(1)-C(30)	1.992(5)	C(8)-C(3)	1.418(10)	C(33)-C(34)	1.399(12)
Ir(1)-C(14)	1.999(4)	C(8)-C(7)	1.468(12)	C(39)-C(40)	1.326(11)
Ir(1)-N(3)	2.024(4)	C(11)-C(12)	1.356(9)	C(39)-C(44)	1.329(10)
Ir(1)-N(1)	2.029(4)	C(11)-H(11)	0.93	F(1)-C(32)	1.288(14)
Ir(1)-O(1)	2.157(3)	C(12)-C(16)	1.525(11)	C(38)-C(37)	1.508(13)
Ir(1)-O(2)	2.173(3)	N(3)-C(25)	1.337(6)	C(38)-H(38)	0.93
P(1)-O(1)	1.519(3)	N(3)-C(17)	1.360(6)	F(3)-C(32)	1.197(17)
P(1)-N(1AA)	1.573(5)	F(6)-C(31)	1.338(9)	C(34)-C(35)	1.377(13)
P(1)-C(51)	1.807(4)	C(18)-C(17)	1.288(7)	C(34)-H(34)	0.93
P(1)-C(45)	1.809(6)	C(18)-C(19)	1.343(8)	C(40)-C(41)	1.373(13)
P(2)-O(2)	1.517(4)	C(18)-H(18)	0.93	C(40)-H(40)	0.93
P(2)-N(1AA)	1.599(5)	C(25)-C(24)	1.430(7)	F(2)-C(32)	1.234(17)
P(2)-C(39)	1.792(5)	C(25)-C(26)	1.458(8)	F(8)-C(16)	1.203(12)
P(2)-C(33)	1.805(6)	F(5)-C(31)	1.339(9)	F(7)-C(16)	1.230(17)
C(51)-C(56)	1.39	C(24)-C(23)	1.414(8)	C(16)-F(9)	1.32(2)
C(51)-C(52)	1.39	C(24)-C(19)	1.419(9)	C(45)-C(46)	1.362(11)
C(56)-C(55)	1.39	C(19)-C(20)	1.412(8)	C(45)-C(50)	1.371(11)
C(56)-H(56)	0.93	C(17)-H(17)	0.93	C(42)-C(41)	1.311(14)
C(55)-C(54)	1.39	C(26)-C(27)	1.391(8)	C(42)-C(43)	1.359(15)
C(55)-H(55)	0.93	C(26)-C(30)	1.437(8)	C(42)-H(42)	0.93
C(54)-C(53)	1.39	N(4)-C(28)	1.305(10)	C(50)-C(49)	1.405(12)
C(54)-H(54)	0.93	N(4)-C(29)	1.307(8)	C(50)-H(50)	0.93
C(53)-C(52)	1.39	C(29)-C(30)	1.420(7)	C(36)-C(35)	1.320(17)
C(53)-H(53)	0.93	C(29)-C(31)	1.497(10)	C(36)-C(37)	1.390(16)
C(52)-H(52)	0.93	C(31)-F(4)	1.315(7)	C(36)-H(36)	0.93
F(12)-C(15)	1.331(6)	C(23)-C(22)	1.337(11)	C(46)-C(47)	1.412(15)
F(10)-C(15)	1.338(6)	C(23)-H(23)	0.93	C(46)-H(46)	0.93
F(11)-C(15)	1.346(7)	C(27)-C(28)	1.395(10)	C(37)-H(37)	0.93
N(2)-C(12)	1.318(8)	C(27)-H(27)	0.93	C(44)-C(43)	1.383(13)
N(2)-C(13)	1.331(7)	C(3)-C(4)	1.409(10)	C(44)-H(44)	0.93
C(15)-C(13)	1.500(7)	C(28)-C(32)	1.489(11)	C(35)-H(35)	0.93
C(14)-C(13)	1.416(6)	C(20)-C(21)	1.370(12)	C(41)-H(41)	0.93
C(14)-C(10)	1.428(7)	C(20)-H(20)	0.93	C(43)-H(43)	0.93
N(1)-C(9)	1.336(6)	C(22)-C(21)	1.383(13)	C(49)-C(48)	1.32(2)
N(1)-C(1)	1.363(6)	C(22)-H(22)	0.93	C(49)-H(49)	0.93
C(9)-C(8)	1.420(8)	C(21)-H(21)	0.93	C(48)-C(47)	1.37(2)
C(9)-C(10)	1.482(7)	C(4)-C(5)	1.316(16)	C(48)-H(48)	0.93
C(1)-C(2)	1.286(7)	C(4)-H(4)	0.93	C(47)-H(47)	0.93

C(1)-H(1)	0.93	C(7)-C(6)	1.331(14)	C(5)-C(6)	1.494(18)
C(2)-C(3)	1.343(9)	C(7)-H(7)	0.93	C(5)-H(5)	0.93
C(2)-H(2)	0.93	C(33)-C(38)	1.354(12)	C(6)-H(6)	0.93
C(10)-C(11)	1.380(8)				
Selected angels°					
C(30)-Ir(1)-C(14)	100.1(2)	C(11)-C(10)-C(14)	119.8(5)	C(38)-C(33)-C(34)	120.1(8)
C(30)-Ir(1)-N(3)	80.72(18)	C(11)-C(10)-C(9)	125.0(5)	C(38)-C(33)-P(2)	119.6(7)
C(14)-Ir(1)-N(3)	102.55(17)	C(14)-C(10)-C(9)	115.1(4)	C(34)-C(33)-P(2)	120.2(7)
C(30)-Ir(1)-N(1)	103.05(19)	C(3)-C(8)-C(9)	116.3(6)	C(40)-C(39)-C(44)	115.0(7)
C(14)-Ir(1)-N(1)	80.32(17)	C(3)-C(8)-C(7)	114.3(7)	C(40)-C(39)-P(2)	121.9(6)
N(3)-Ir(1)-N(1)	174.88(15)	C(9)-C(8)-C(7)	127.7(7)	C(44)-C(39)-P(2)	122.8(6)
C(30)-Ir(1)-O(1)	173.31(17)	C(12)-C(11)-C(10)	119.7(6)	C(33)-C(38)-C(37)	121.1(10)
C(14)-Ir(1)-O(1)	84.29(15)	C(12)-C(11)-H(11)	120.1	C(33)-C(38)-H(38)	119.5
N(3)-Ir(1)-O(1)	93.43(14)	C(10)-C(11)-H(11)	120.1	C(37)-C(38)-H(38)	119.5
N(1)-Ir(1)-O(1)	82.58(14)	N(2)-C(12)-C(11)	123.4(6)	C(35)-C(34)-C(33)	123.1(12)
C(30)-Ir(1)-O(2)	86.38(18)	N(2)-C(12)-C(16)	116.9(7)	C(35)-C(34)-H(34)	118.4
C(14)-Ir(1)-O(2)	170.16(16)	C(11)-C(12)-C(16)	119.6(7)	C(33)-C(34)-H(34)	118.4
N(3)-Ir(1)-O(2)	85.71(14)	C(25)-N(3)-C(17)	120.0(4)	C(39)-C(40)-C(41)	125.0(11)
N(1)-Ir(1)-O(2)	91.05(14)	C(25)-N(3)-Ir(1)	116.7(3)	C(39)-C(40)-H(40)	117.5
O(1)-Ir(1)-O(2)	89.94(13)	C(17)-N(3)-Ir(1)	123.1(3)	C(41)-C(40)-H(40)	117.5
O(1)-P(1)-N(1AA)	117.0(2)	C(17)-C(18)-C(19)	117.7(5)	F(3)-C(32)-F(2)	107.5(13)
O(1)-P(1)-C(51)	106.5(2)	C(17)-C(18)-H(18)	121.1	F(3)-C(32)-F(1)	103.9(15)
N(1AA)-P(1)-C(51)	106.8(2)	C(19)-C(18)-H(18)	121.1	F(2)-C(32)-F(1)	99.1(13)
O(1)-P(1)-C(45)	106.7(3)	N(3)-C(25)-C(24)	118.3(5)	F(3)-C(32)-C(28)	115.2(13)
N(1AA)-P(1)-C(45)	111.5(3)	N(3)-C(25)-C(26)	112.6(4)	F(2)-C(32)-C(28)	116.1(13)
C(51)-P(1)-C(45)	108.0(2)	C(24)-C(25)-C(26)	128.9(5)	F(1)-C(32)-C(28)	113.2(10)
O(2)-P(2)-N(1AA)	116.6(2)	C(23)-C(24)-C(19)	118.2(6)	F(8)-C(16)-F(7)	113.5(16)
O(2)-P(2)-C(39)	108.0(2)	C(23)-C(24)-C(25)	125.7(6)	F(8)-C(16)-F(9)	102.9(14)
N(1AA)-P(2)-C(39)	110.2(3)	C(19)-C(24)-C(25)	116.1(5)	F(7)-C(16)-F(9)	99.5(10)
O(2)-P(2)-C(33)	110.2(3)	C(18)-C(19)-C(20)	118.9(7)	F(8)-C(16)-C(12)	116.1(8)
N(1AA)-P(2)-C(33)	106.6(3)	C(18)-C(19)-C(24)	122.2(5)	F(7)-C(16)-C(12)	114.5(11)
C(39)-P(2)-C(33)	104.6(3)	C(20)-C(19)-C(24)	118.9(6)	F(9)-C(16)-C(12)	107.9(14)
P(2)-O(2)-Ir(1)	125.5(2)	C(18)-C(17)-N(3)	125.0(5)	C(46)-C(45)-C(50)	118.8(8)
P(1)-O(1)-Ir(1)	126.89(19)	C(18)-C(17)-H(17)	117.5	C(46)-C(45)-P(1)	120.9(7)
P(1)-N(1AA)-P(2)	126.0(3)	N(3)-C(17)-H(17)	117.5	C(50)-C(45)-P(1)	120.2(6)
C(56)-C(51)-C(52)	120	C(27)-C(26)-C(30)	118.9(5)	C(41)-C(42)-C(43)	118.3(9)
C(56)-C(51)-P(1)	119.2(3)	C(27)-C(26)-C(25)	125.6(6)	C(41)-C(42)-H(42)	120.8
C(52)-C(51)-P(1)	120.8(3)	C(30)-C(26)-C(25)	115.5(5)	C(43)-C(42)-H(42)	120.8
C(55)-C(56)-C(51)	120	C(28)-N(4)-C(29)	118.4(6)	C(45)-C(50)-C(49)	120.0(11)
C(55)-C(56)-H(56)	120	N(4)-C(29)-C(30)	125.7(6)	C(45)-C(50)-H(50)	120
C(51)-C(56)-H(56)	120	N(4)-C(29)-C(31)	111.1(6)	C(49)-C(50)-H(50)	120
C(56)-C(55)-C(54)	120	C(30)-C(29)-C(31)	123.2(5)	C(35)-C(36)-C(37)	134.3(12)

C(56)-C(55)-H(55)	120	F(4)-C(31)-F(6)	106.2(7)	C(35)-C(36)-H(36)	112.8
C(54)-C(55)-H(55)	120	F(4)-C(31)-F(5)	106.3(6)	C(37)-C(36)-H(36)	112.8
C(55)-C(54)-C(53)	120	F(6)-C(31)-F(5)	107.4(6)	C(45)-C(46)-C(47)	120.9(12)
C(55)-C(54)-H(54)	120	F(4)-C(31)-C(29)	112.3(6)	C(45)-C(46)-H(46)	119.5
C(53)-C(54)-H(54)	120	F(6)-C(31)-C(29)	112.9(6)	C(47)-C(46)-H(46)	119.5
C(54)-C(53)-C(52)	120	F(5)-C(31)-C(29)	111.5(7)	C(36)-C(37)-C(38)	108.4(11)
C(54)-C(53)-H(53)	120	C(29)-C(30)-C(26)	113.8(5)	C(36)-C(37)-H(37)	125.8
C(52)-C(53)-H(53)	120	C(29)-C(30)-Ir(1)	134.4(4)	C(38)-C(37)-H(37)	125.8
C(53)-C(52)-C(51)	120	C(26)-C(30)-Ir(1)	111.2(4)	C(39)-C(44)-C(43)	121.6(10)
C(53)-C(52)-H(52)	120	C(22)-C(23)-C(24)	120.3(8)	C(39)-C(44)-H(44)	119.2
C(51)-C(52)-H(52)	120	C(22)-C(23)-H(23)	119.9	C(43)-C(44)-H(44)	119.2
C(12)-N(2)-C(13)	117.8(5)	C(24)-C(23)-H(23)	119.9	C(36)-C(35)-C(34)	112.7(13)
F(12)-C(15)-F(10)	106.3(4)	C(26)-C(27)-C(28)	118.5(6)	C(36)-C(35)-H(35)	123.6
F(12)-C(15)-F(11)	106.1(5)	C(26)-C(27)-H(27)	120.7	C(34)-C(35)-H(35)	123.6
F(10)-C(15)-F(11)	106.0(4)	C(28)-C(27)-H(27)	120.7	C(42)-C(41)-C(40)	118.5(10)
F(12)-C(15)-C(13)	113.6(4)	C(2)-C(3)-C(4)	117.4(7)	C(42)-C(41)-H(41)	120.7
F(10)-C(15)-C(13)	112.6(5)	C(2)-C(3)-C(8)	122.4(6)	C(40)-C(41)-H(41)	120.7
F(11)-C(15)-C(13)	111.7(4)	C(4)-C(3)-C(8)	120.1(7)	C(42)-C(43)-C(44)	120.0(11)
C(13)-C(14)-C(10)	113.7(4)	N(4)-C(28)-C(27)	123.4(6)	C(42)-C(43)-H(43)	120
C(13)-C(14)-Ir(1)	134.1(4)	N(4)-C(28)-C(32)	115.5(8)	C(44)-C(43)-H(43)	120
C(10)-C(14)-Ir(1)	111.9(3)	C(27)-C(28)-C(32)	121.0(9)	C(48)-C(49)-C(50)	120.4(14)
N(2)-C(13)-C(14)	125.2(5)	C(21)-C(20)-C(19)	120.4(8)	C(48)-C(49)-H(49)	119.8
N(2)-C(13)-C(15)	111.1(4)	C(21)-C(20)-H(20)	119.8	C(50)-C(49)-H(49)	119.8
C(14)-C(13)-C(15)	123.7(5)	C(19)-C(20)-H(20)	119.8	C(49)-C(48)-C(47)	121.5(12)
C(9)-N(1)-C(1)	120.0(4)	C(23)-C(22)-C(21)	122.4(8)	C(49)-C(48)-H(48)	119.3
C(9)-N(1)-Ir(1)	115.9(3)	C(23)-C(22)-H(22)	118.8	C(47)-C(48)-H(48)	119.3
C(1)-N(1)-Ir(1)	123.3(3)	C(21)-C(22)-H(22)	118.8	C(48)-C(47)-C(46)	118.1(13)
N(1)-C(9)-C(8)	118.5(5)	C(20)-C(21)-C(22)	119.4(7)	C(48)-C(47)-H(47)	120.9
N(1)-C(9)-C(10)	112.4(4)	C(20)-C(21)-H(21)	120.3	C(46)-C(47)-H(47)	120.9
C(8)-C(9)-C(10)	129.1(5)	C(22)-C(21)-H(21)	120.3	C(4)-C(5)-C(6)	120.8(12)
C(2)-C(1)-N(1)	125.0(5)	C(5)-C(4)-C(3)	121.3(11)	C(4)-C(5)-H(5)	119.6
C(2)-C(1)-H(1)	117.5	C(5)-C(4)-H(4)	119.3	C(6)-C(5)-H(5)	119.6
N(1)-C(1)-H(1)	117.5	C(3)-C(4)-H(4)	119.3	C(7)-C(6)-C(5)	114.7(12)
C(1)-C(2)-C(3)	117.5(5)	C(6)-C(7)-C(8)	125.2(11)	C(7)-C(6)-H(6)	122.6
C(1)-C(2)-H(2)	121.2	C(6)-C(7)-H(7)	117.4	C(5)-C(6)-H(6)	122.6
C(3)-C(2)-H(2)	121.2	C(8)-C(7)-H(7)	117.4		

Table S2(b) The selected bond lengths and angels of $Ir(tfmpqz)_2(tpip)$.

Selected bonds Å					
Ir(1)-C(8AA)	1.992(4)	C(37)-C(7BA)	1.472(6)	C(16)-C(21)	1.379(7)
Ir(1)-C(1AA)	2.010(4)	F(2AA)-C(0BA)	1.337(7)	C(16)-C(19)	1.380(7)
Ir(1)-N(6)	2.030(3)	C(8AA)-C(22)	1.427(6)	C(19)-H(19)	0.93
Ir(1)-N(5BA)	2.038(3)	C(8AA)-C(9AA)	1.427(5)	C(20)-C(33)	1.391(8)
Ir(1)-O(18)	2.167(3)	F(17)-C(0BA)	1.344(6)	C(20)-H(20)	0.93
Ir(1)-O(11)	2.167(3)	C(9AA)-C(39)	1.392(6)	C(21)-C(30)	1.406(7)
C(4BA)-N(6)	1.337(5)	C(0BA)-F(0AA)	1.320(6)	C(21)-H(21)	0.93
C(4BA)-C(6BA)	1.437(5)	C(22)-N(23)	1.326(6)	C(25)-H(25)	0.93
C(4BA)-C(9AA)	1.467(5)	C(22)-C(7AA)	1.525(6)	C(27)-C(1BA)	1.361(8)
C(17)-C(6BA)	1.402(5)	N(23)-C(32)	1.321(6)	C(27)-H(27)	0.93
C(17)-N(7)	1.420(5)	C(32)-C(39)	1.395(6)	C(30)-H(30)	0.93
C(17)-C(36)	1.425(5)	C(32)-C(6AA)	1.512(7)	C(33)-C(0CA)	1.369(10)
C(6BA)-C(3AA)	1.434(5)	N(1BA)-C(3BA)	1.370(6)	C(33)-H(33)	0.93
C(2AA)-C(36)	1.363(6)	N(1BA)-C(8BA)	1.431(7)	C(34)-C(38)	1.402(8)
C(2AA)-C(9BA)	1.407(6)	C(7BA)-C(5BA)	1.433(5)	C(34)-H(34)	0.93
C(2AA)-H(2AA)	0.93	C(8BA)-C(27)	1.403(6)	C(35)-C(8)	1.389(8)
C(3AA)-C(9BA)	1.363(5)	C(8BA)-C(5BA)	1.417(7)	C(35)-H(35)	0.93
C(3AA)-H(3AA)	0.93	C(3BA)-H(3BA)	0.93	C(38)-C(0CA)	1.343(9)
C(36)-H(36)	0.93	F(1AA)-C(7AA)	1.325(6)	C(38)-H(38)	0.93
N(6)-C(2BA)	1.364(5)	F(4)-C(6AA)	1.321(5)	F(1)-C(7)	1.328(6)
N(7)-C(2BA)	1.362(5)	F(3AA)-C(7AA)	1.328(6)	F(3)-C(7)	1.338(5)
C(2BA)-H(2BA)	0.93	F(7)-C(6AA)	1.342(7)	F(5)-C(7)	1.334(6)
P(2)-O(18)	1.529(3)	F(8)-C(7AA)	1.351(5)	C(1BA)-H(1BB)	0.93
P(2)-N(24)	1.591(4)	F(10)-C(6AA)	1.336(6)	C(1CA)-C(2CA)	1.355(7)
P(2)-C(9)	1.807(5)	C(39)-H(39)	0.93	C(1CA)-H(1CA)	0.93
P(2)-C(16)	1.819(5)	C(9BA)-H(9BA)	0.93	C(2CA)-C(8)	1.383(9)
P(4)-O(11)	1.521(3)	C(5BA)-C(25)	1.427(6)	C(2CA)-H(2CA)	0.93
P(4)-N(24)	1.576(4)	C(9)-C(10)	1.379(6)	C(8)-H(8)	0.93
P(4)-C(11)	1.805(5)	C(9)-C(35)	1.383(7)	C(0CA)-H(0CA)	0.93
P(4)-C(3CA)	1.816(6)	C(10)-C(1CA)	1.397(8)	C(1)-C(3CA)	1.336(9)
N(5BA)-C(7BA)	1.345(5)	C(10)-H(10)	0.93	C(1)-C(4)	1.407(8)
N(5BA)-C(3BA)	1.354(6)	C(11)-C(20)	1.392(7)	C(1)-H(1)	0.93
C(0AA)-N(28)	1.333(5)	C(11)-C(34)	1.392(8)	C(3CA)-C(4CA)	1.389(8)
C(0AA)-C(5AA)	1.372(6)	C(13)-C(30)	1.351(8)	C(4CA)-C(2)	1.399(8)
C(0AA)-C(7)	1.481(7)	C(13)-C(14)	1.380(8)	C(4CA)-H(4CA)	0.93
C(1AA)-C(37)	1.415(5)	C(13)-H(13)	0.93	C(2)-C(5)	1.435(10)
C(1AA)-C(4AA)	1.434(6)	C(14)-C(19)	1.381(7)	C(2)-H(2)	0.93
N(28)-C(4AA)	1.325(5)	C(14)-H(14)	0.93	C(4)-C(5)	1.316(10)
C(4AA)-C(0BA)	1.511(6)	C(15)-C(25)	1.361(6)	C(4)-H(4)	0.93

C(5AA)-C(37)	1.392(6)	C(15)-C(1BA)	1.401(8)	C(5)-H(5)	0.93
C(5AA)-H(5AA)	0.93	C(15)-H(15)	0.93		
Selected angels˚					
C(8AA)-Ir(1)-C(1AA)	96.33(17)	C(5AA)-C(37)-C(7BA)	122.6(4)	C(21)-C(16)-P(2)	119.9(4)
C(8AA)-Ir(1)-N(6)	80.06(14)	C(1AA)-C(37)-C(7BA)	115.4(4)	C(19)-C(16)-P(2)	120.6(4)
C(1AA)-Ir(1)-N(6)	102.53(18)	C(22)-C(8AA)-C(9AA)	113.4(4)	C(16)-C(19)-C(14)	120.6(5)
C(8AA)-Ir(1)-N(5BA)	106.72(15)	C(22)-C(8AA)-Ir(1)	134.1(3)	C(16)-C(19)-H(19)	119.7
C(1AA)-Ir(1)-N(5BA)	80.47(15)	C(9AA)-C(8AA)-Ir(1)	112.4(3)	C(14)-C(19)-H(19)	119.7
N(6)-Ir(1)-N(5BA)	172.38(15)	C(39)-C(9AA)-C(8AA)	120.5(4)	C(33)-C(20)-C(11)	121.6(6)
C(8AA)-Ir(1)-O(18)	86.59(14)	C(39)-C(9AA)-C(4BA)	122.8(4)	C(33)-C(20)-H(20)	119.2
C(1AA)-Ir(1)-O(18)	172.17(14)	C(8AA)-C(9AA)-C(4BA)	115.8(4)	C(11)-C(20)-H(20)	119.2
N(6)-Ir(1)-O(18)	85.11(17)	F(0AA)-C(0BA)-F(2AA)	105.6(4)	C(16)-C(21)-C(30)	119.4(5)
N(5BA)-Ir(1)-O(18)	91.73(12)	F(0AA)-C(0BA)-F(17)	105.9(4)	C(16)-C(21)-H(21)	120.3
C(8AA)-Ir(1)-O(11)	171.83(13)	F(2AA)-C(0BA)-F(17)	105.6(4)	C(30)-C(21)-H(21)	120.3
C(1AA)-Ir(1)-O(11)	87.41(15)	F(0AA)-C(0BA)-C(4AA)	115.6(5)	C(15)-C(25)-C(5BA)	121.5(5)
N(6)-Ir(1)-O(11)	92.06(12)	F(2AA)-C(0BA)-C(4AA)	112.4(4)	C(15)-C(25)-H(25)	119.3
N(5BA)-Ir(1)-O(11)	81.02(12)	F(17)-C(0BA)-C(4AA)	111.1(4)	C(5BA)-C(25)-H(25)	119.3
O(18)-Ir(1)-O(11)	90.64(12)	N(23)-C(22)-C(8AA)	126.6(4)	C(1BA)-C(27)-C(8BA)	121.3(5)
N(6)-C(4BA)-C(6BA)	119.2(3)	N(23)-C(22)-C(7AA)	111.9(4)	C(1BA)-C(27)-H(27)	119.4
N(6)-C(4BA)-C(9AA)	111.6(3)	C(8AA)-C(22)-C(7AA)	121.4(4)	C(8BA)-C(27)-H(27)	119.4
C(6BA)-C(4BA)-C(9AA)	128.6(4)	C(32)-N(23)-C(22)	117.1(4)	C(13)-C(30)-C(21)	120.4(5)
C(6BA)-C(17)-N(7)	119.8(3)	N(23)-C(32)-C(39)	123.8(4)	C(13)-C(30)-H(30)	119.8
C(6BA)-C(17)-C(36)	120.3(4)	N(23)-C(32)-C(6AA)	116.8(4)	C(21)-C(30)-H(30)	119.8
N(7)-C(17)-C(36)	119.8(4)	C(39)-C(32)-C(6AA)	119.4(4)	C(0CA)-C(33)-C(20)	118.1(6)
C(17)-C(6BA)-C(3AA)	117.8(3)	C(3BA)-N(1BA)-C(8BA)	118.5(5)	C(0CA)-C(33)-H(33)	120.9
C(17)-C(6BA)-C(4BA)	118.0(3)	N(5BA)-C(7BA)-C(5BA)	120.4(4)	C(20)-C(33)-H(33)	120.9
C(3AA)-C(6BA)-C(4BA)	124.2(3)	N(5BA)-C(7BA)-C(37)	112.9(4)	C(11)-C(34)-C(38)	121.0(6)
C(36)-C(2AA)-C(9BA)	119.9(4)	C(5BA)-C(7BA)-C(37)	126.5(4)	C(11)-C(34)-H(34)	119.5
C(36)-C(2AA)-H(2AA)	120.1	C(27)-C(8BA)-C(5BA)	119.7(5)	C(38)-C(34)-H(34)	119.5
C(9BA)-C(2AA)-H(2AA)	120.1	C(27)-C(8BA)-N(1BA)	121.8(5)	C(9)-C(35)-C(8)	120.2(5)
C(9BA)-C(3AA)-C(6BA)	120.4(4)	C(5BA)-C(8BA)-N(1BA)	118.5(4)	C(9)-C(35)-H(35)	119.9
C(9BA)-C(3AA)-H(3AA)	119.8	N(5BA)-C(3BA)-N(1BA)	123.0(5)	C(8)-C(35)-H(35)	119.9
C(6BA)-C(3AA)-H(3AA)	119.8	N(5BA)-C(3BA)-H(3BA)	118.5	C(0CA)-C(38)-C(34)	118.9(7)
C(2AA)-C(36)-C(17)	120.2(4)	N(1BA)-C(3BA)-H(3BA)	118.5	C(0CA)-C(38)-H(38)	120.6
C(2AA)-C(36)-H(36)	119.9	F(1AA)-C(7AA)-F(3AA)	107.7(4)	C(34)-C(38)-H(38)	120.6
C(17)-C(36)-H(36)	119.9	F(1AA)-C(7AA)-F(8)	106.0(4)	F(1)-C(7)-F(5)	105.9(4)
C(4BA)-N(6)-C(2BA)	122.0(3)	F(3AA)-C(7AA)-F(8)	106.2(4)	F(1)-C(7)-F(3)	105.4(4)
C(4BA)-N(6)-Ir(1)	116.1(3)	F(1AA)-C(7AA)-C(22)	111.2(4)	F(5)-C(7)-F(3)	105.9(4)
C(2BA)-N(6)-Ir(1)	121.6(3)	F(3AA)-C(7AA)-C(22)	113.9(4)	F(1)-C(7)-C(0AA)	113.2(4)
C(2BA)-N(7)-C(17)	118.4(4)	F(8)-C(7AA)-C(22)	111.4(4)	F(5)-C(7)-C(0AA)	113.0(4)

N(7)-C(2BA)-N(6)	121.6(4)	F(4)-C(6AA)-F(10)	108.0(4)	F(3)-C(7)-C(0AA)	112.8(4)
N(7)-C(2BA)-H(2BA)	119.2	F(4)-C(6AA)-F(7)	106.4(4)	C(27)-C(1BA)-C(15)	119.8(5)
N(6)-C(2BA)-H(2BA)	119.2	F(10)-C(6AA)-F(7)	107.1(4)	C(27)-C(1BA)-H(1BB)	120.1
O(18)-P(2)-N(24)	117.8(2)	F(4)-C(6AA)-C(32)	113.5(4)	C(15)-C(1BA)-H(1BB)	120.1
O(18)-P(2)-C(9)	107.4(2)	F(10)-C(6AA)-C(32)	111.3(4)	C(2CA)-C(1CA)-C(10)	120.2(6)
N(24)-P(2)-C(9)	108.6(2)	F(7)-C(6AA)-C(32)	110.3(4)	C(2CA)-C(1CA)-H(1CA)	119.9
O(18)-P(2)-C(16)	109.9(2)	C(9AA)-C(39)-C(32)	118.4(4)	C(10)-C(1CA)-H(1CA)	119.9
N(24)-P(2)-C(16)	107.4(2)	C(9AA)-C(39)-H(39)	120.8	C(1CA)-C(2CA)-C(8)	120.2(6)
C(9)-P(2)-C(16)	105.0(2)	C(32)-C(39)-H(39)	120.8	C(1CA)-C(2CA)-H(2CA)	119.9
O(11)-P(4)-N(24)	118.0(2)	C(3AA)-C(9BA)-C(2AA)	121.2(4)	C(8)-C(2CA)-H(2CA)	119.9
O(11)-P(4)-C(11)	109.52(19)	C(3AA)-C(9BA)-H(9BA)	119.4	C(2CA)-C(8)-C(35)	120.0(5)
N(24)-P(4)-C(11)	108.6(2)	C(2AA)-C(9BA)-H(9BA)	119.4	C(2CA)-C(8)-H(8)	120
O(11)-P(4)-C(3CA)	107.0(2)	C(8BA)-C(5BA)-C(25)	117.0(4)	C(35)-C(8)-H(8)	120
N(24)-P(4)-C(3CA)	107.9(2)	C(8BA)-C(5BA)-C(7BA)	118.2(4)	C(38)-C(0CA)-C(33)	122.9(6)
C(11)-P(4)-C(3CA)	105.1(3)	C(25)-C(5BA)-C(7BA)	124.7(5)	C(38)-C(0CA)-H(0CA)	118.6
P(4)-O(11)-Ir(1)	129.09(19)	C(10)-C(9)-C(35)	119.2(5)	C(33)-C(0CA)-H(0CA)	118.6
P(2)-O(18)-Ir(1)	127.52(19)	C(10)-C(9)-P(2)	119.9(4)	C(3CA)-C(1)-C(4)	120.7(6)
P(4)-N(24)-P(2)	129.1(3)	C(35)-C(9)-P(2)	120.9(4)	C(3CA)-C(1)-H(1)	119.7
C(7BA)-N(5BA)-C(3BA)	120.4(4)	C(9)-C(10)-C(1CA)	120.3(5)	C(4)-C(1)-H(1)	119.7
C(7BA)-N(5BA)-Ir(1)	113.2(3)	C(9)-C(10)-H(10)	119.8	C(1)-C(3CA)-C(4CA)	120.1(6)
C(3BA)-N(5BA)-Ir(1)	124.6(3)	C(1CA)-C(10)-H(10)	119.8	C(1)-C(3CA)-P(4)	121.2(5)
N(28)-C(0AA)-C(5AA)	122.7(4)	C(20)-C(11)-C(34)	117.4(5)	C(4CA)-C(3CA)-P(4)	118.6(5)
N(28)-C(0AA)-C(7)	115.6(4)	C(20)-C(11)-P(4)	121.7(5)	C(3CA)-C(4CA)-C(2)	119.2(6)
C(5AA)-C(0AA)-C(7)	121.6(4)	C(34)-C(11)-P(4)	120.7(4)	C(3CA)-C(4CA)-H(4CA)	120.4
C(37)-C(1AA)-C(4AA)	113.5(4)	C(30)-C(13)-C(14)	120.4(5)	C(2)-C(4CA)-H(4CA)	120.4
C(37)-C(1AA)-Ir(1)	111.7(3)	C(30)-C(13)-H(13)	119.8	C(4CA)-C(2)-C(5)	119.7(6)
C(4AA)-C(1AA)-Ir(1)	134.7(3)	C(14)-C(13)-H(13)	119.8	C(4CA)-C(2)-H(2)	120.2
C(4AA)-N(28)-C(0AA)	118.7(4)	C(13)-C(14)-C(19)	119.7(6)	C(5)-C(2)-H(2)	120.2
N(28)-C(4AA)-C(1AA)	124.9(4)	C(13)-C(14)-H(14)	120.2	C(5)-C(4)-C(1)	122.0(7)
N(28)-C(4AA)-C(0BA)	110.5(4)	C(19)-C(14)-H(14)	120.2	C(5)-C(4)-H(4)	119
C(1AA)-C(4AA)-C(0BA)	124.3(4)	C(25)-C(15)-C(1BA)	120.3(5)	C(1)-C(4)-H(4)	119
C(0AA)-C(5AA)-C(37)	118.9(4)	C(25)-C(15)-H(15)	119.8	C(4)-C(5)-C(2)	118.3(7)
C(0AA)-C(5AA)-H(5AA)	120.6	C(1BA)-C(15)-H(15)	119.8	C(4)-C(5)-H(5)	120.9
C(37)-C(5AA)-H(5AA)	120.6	C(21)-C(16)-C(19)	119.5(5)	C(2)-C(5)-H(5)	120.9
C(5AA)-C(37)-C(1AA)	121.1(4)				