Supporting Information

Crystal structure, photoluminescence and electroluminescence of three bluish green light-emitting iridium complexes

Qiu-Lei Xu, Xiao Liang, Liang Jiang, Yue Zhao, You-Xuan Zheng*

State Key Laboratory of Coordination Chemistry, Collaborative Innovation Center of Advanced Microstructures, Collaborative Innovation Center of Chemistry for Life Sciences, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China, e-mail: yxzheng@nju.edu.cn

Table S1 Crystallographic data and structure refinement for complexes $(TPP)_2Ir(tpip)$

	$(TPP)_2Ir(tpip)$

Formula	$C_{44}H_{30}F_6IrN_7O_2P_2$
FW	1056.89
T (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	*P2(1)2(1)2(1)*
***a* (Å)**	11.2120(3)
***b* (Å)**	17.6716(5)
***c* (Å)**	20.9835(6)
***α* (deg)**	90.00
***β* (deg)**	90.00
***γ* (deg)**	90.00
***V* (Å^3)**	4157.5(2)
Z	4
ρ_{calcd} **(mg/cm^3)**	1.689
***μ* (Mo Kα) (mm^{-1})**	3.363
***F* (000)**	2080
Reflns collected	30160
Unique	10315
Data/restraints/params	10315 / 0 / 559
GOF on F^2	1.048
R_1^a, wR_2^b [$I > 2\sigma(I)$]	0.0531, 0.1514
R_1^a, wR_2^b **(all data)**	0.0549, 0.1530
CCDC NO	1436107

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

Table S2 The table of selected bond lengths of $(TPP)_2Ir(tpip)$

$(TPP)_2Ir(tpip)$					
Selected bonds Å					
Ir(1)-C(4)	1.963(9)	Ir(1)-O(1)	2.191(6)	Ir(1)-N(5)	2.041(8)

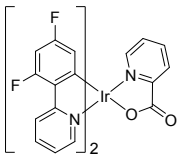
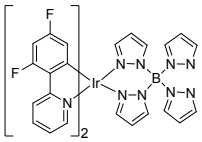
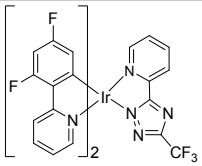
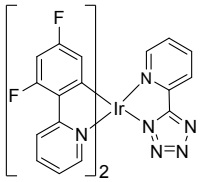
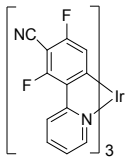
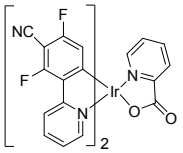
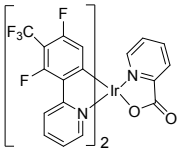
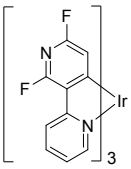
Ir(1)-C(11)	1.957(8)	Ir(1)-O(2)	2.199(6)	Ir(1)-N(6)	2.041(7)
O(1)-P(2)	1.519(7)	N(7)-P(1)	1.582(8)	C(45)-F(3)	1.326(13)
O(2)-P(1)	1.509(7)	N(7)-P(2)	1.588(8)	C(45)-F(2)	1.296(14)
C(45)-F(1)	1.287(15)	C(45)-C(10)	1.509(14)	C(11)-C(12)	1.423(11)
C(10)-N(2)	1.327(11)	C(11)-N(2)	1.347(11)	C(10)-N(1)	1.344(13)
C(12)-C(13)	1.327(11)	C(13)-N(1)	1.333(13)	C(18)-N(5)	1.353(12)
C(12)-C(14)	1.461(12)	C(14)-N(5)	1.367(11)	C(16)-C(15)	1.384(16)
C(17)-C(18)	1.375(12)	C(16)-C(17)	1.389(18)	C(15)-C(14)	1.374(14)
C(19)-C(20)	1.379(17)	C(20)-C(21)	1.40(2)	P(2)-C(19)	1.807(9)
C(22)-C(23)	1.33(3)	C(23)-C(24)	1.386(19)	C(21)-C(22)	1.37(3)
C(25)-C(26)	1.402(15)	C(24)-C(19)	1.373(16)	P(2)-C(25)	1.800(9)
C(28)-C(29)	1.33(2)	C(26)-C(27)	1.385(18)	C(27)-C(28)	1.37(2)
C(29)-C(43)	1.411(16)	C(43)-C(25)	1.372(15)		
Selected angels °					
Ir(1)-O(1)-P(2)	128.4(4)	Ir(1)-O(2)-p(1)	126.6(4)	O(1)-P(2)-N(7)	118.7(4)
P(2)-N(7)-P(1)	128.2(5)	N(7)-P(1)-O(2)	118.6(4)	P(1)-O(2)-Ir(1)	126.6(4)
N(7)-P(1)-C(31)	110.7(5)	N(7)-P(1)-C(37)	106.5(5)	O(1)-Ir(1)-O(2)	89.8(2)
N(6)-Ir(1)-C(3)	80.9(4)	C(11)-Ir(1)-N(5)	81.0(3)	Ir(1)-N(6)-C(5)	116.6(7)
N(6)-C(5)-C(3)	111.9(8)	C(5)-C(3)-C(4)	116.2(9)	C(3)-C(4)-Ir(1)	114.3(7)

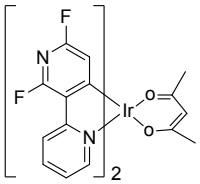
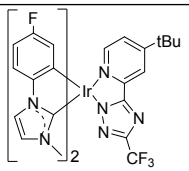
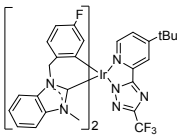
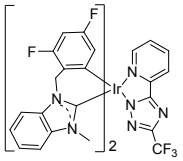
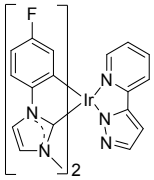
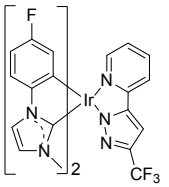
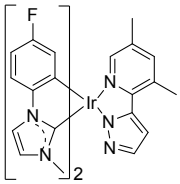
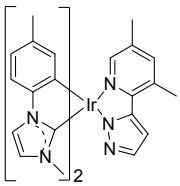
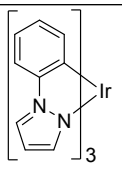
Table S3. The orbital distributions of complexes $(TPP)_2Ir(acac)$, $(TPP)_2Ir(tpip)$ and $(TPP)_2Ir(pic)$

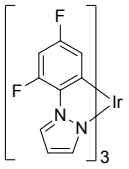
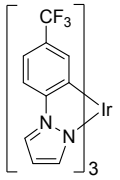
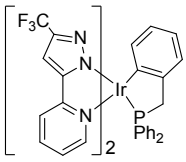
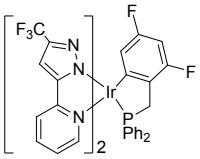
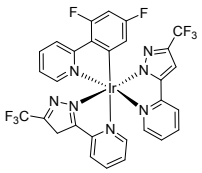
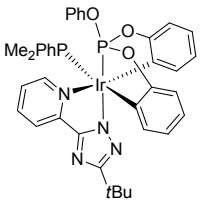
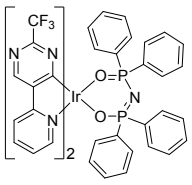
Group		$(TPP)_2Ir(acac)$	$(TPP)_2Ir(tpip)$	$(TPP)_2Ir(pic)$
Ir (%)	LUMO	2.59	2.40	2.36
	HOMO	28.79	54.00	49.36
TPP (%)	LUMO	96.19	95.84	96.08
	HOMO	8.0	35.50	41.75
Ancillary	LUMO	0.84	1.76	1.56
ligand(%)	HOMO	63.29	10.50	8.89

Table S4. The complexes and their OLEDs characteristics related this article.

Material	Structure	PL_{max}	EQE(%)	C.E.	η_p	reference

		(nm)		(cd/A)	(lm/w)	
FIrpic		470, 494	26.0[a)], 25.0[b)]	-	55.0 [a)], 46.0 [b)]	1
FIr6		457, 485	18.0[a)]	-	18.0 [a)]	2
FIrtaz		460, 489	–	–	–	3,4
FIrN4		458, 489	9.4 [a)]	-	7.2 [a)]	3
FCNIr		448, 476	19.1 [a)], 12.1 [b)]	22.5 [a)]	19.0 [a)]	5
FCNIrpic		450,	25.1 [a)], 23.1 [b)]	31.0[a)], 28.9 [b)]	21.5, [a)] 15.1 [b)]	6
FCF3Irpic		457, 485	1.2 [a)]	2.3 [a)]		7
Ir(dfpypy)$_3$		438, 463	-	-	-	8

$Ir(dfpypy)_2(acac)$		457, 459	16.2 [c], 11.2 [b]	-	15.3 [a]	9
$(fpmb)_2Ir(bptz)$		392, 461	-	-	-	10
$(fbmb)_2Ir(bptz)$		460	-	-	-	10
$(dfbmb)_2Ir(fbptz)$		458	6.0 [a]	6.3 [a]	4.0 [a]	10
$(fpmi)_2Ir(pypz)$		468	14.1 [a]	19.7 [a]	13.8 [a]	11
$(fpmi)_2Ir(tfpypz)$		456	7.6 [a]	6.5 [a]	4.1 [a]	11
$(fpmi)_2Ir(dmpypz)$		455	17.1 [a], 15.1 [b]	22.3 [a], 19.6 [b]	19.8 [a], 11.2 [b]	12
$(mpmi)_2Ir(dmpypz)$		466	15.4 [a], 13.6 [b]	21.9 [a], 19.3 [b]	19.1 [a], 11.0 [b]	12
$Ir(ppz)_3$		437	-	-	-	13

$Ir(dfppz)_3$		-	-	-	-	13
$Ir(tfmppz)_3$		428	-	-	-	13
$Ir(fppz)_2(bdp)$		461	-	-	-	14
$Ir(fppz)_2(dfbdp)$		430, 458	11.9 [a]	11.4 [a]	7.9 [a]	14
$Ir(dfppy)_2Ir(fppz)$		450, 479	8.5 [a]	-	8.5 [a]	15
[Ir(P^C2)(PPhMe$_2$)-(bptz)]		451, 473, 498	11.0 [a]	22.3 [a], 16.9 [c]	16.7 [a], 8.1 [c]	16
$(TPP)_2Ir(tpip)$		483, 518	13.7 [a]	37.61 [a]	19.05 [a]	This article

a) Maximum efficiency; b) Efficiency at 1000 cd m^{-2}; c) Efficiency at 100 cd m^{-2}.

Reference

1. J. S. Swensen, E. Polikarpov, A. V. Ruden, L. Wang, L. S. Sapochak and A. B. Padmaperuma,

Adv. Func. Mater., 2011, **21**, 3250.

2. Y. Zheng, S.-H. Eom, N. Chopra and J. Lee, F. So, *Appl. Phys. Lett.*, 2008, **92**, 223301.
3. S.-J. Ye, M.-F. Wu, C.-T. Chen, Y.-H. Song, Y. Chi, M.-H. Ho, S.-F. Chen and C. H. Chen, *Adv. Mater.*, 2005, **17**, 285.
4. C.-H. Yang, Y.-M. Cheng, Y. Chi, C.-J. Hsu, F.-C. Fang, K.-T. Wong, P.-T. Chou, C.-H. Chang, M.-H. Tsai and C.-C. Wu, *Angew. Cheme. Int. Ed.*, 2007, **46**, 2418.
5. K. S. Yook, S. E. Jang, S. O. Jeon and J. Y. Lee, *Adv. Mater.*, 2010, **22**, 4479.
6. S. O. Jeon, S. E. Jang, H. S. Son and J. Y. Lee, *Adv. Mater.*, 2011, **23**, 1436
7. S.-Y. Takizawa, H. Echizen, J. Nishida, T. Tsuzuki, S. Tokito and Y. Yamashita, *Chem. Lett*., 2006, **35**, 748.
8. S. J. Lee, K.-M. Park, K. Yang and Y. Kang, *Inorg. Chem.*, 2009, **48**, 1030.
9. J. Wang, J. Liu, S. Huang, X. Wu, X. Shi, G. He and Y. Zheng, **Org. Electron.**, 2013, **14**, 26.
10. C.-F. Chang, Y.-M. Cheng, Y. Chi, Y.-C. Chiu, C.-C. Lin, G.-H. Lee, P.-T. Chou, C.-C. Chen, C.-H. Chang and C.-C. Wu, *Angew. Chem. Int. Ed.*, 2008, **47**, 4542.
11. C.-H. Hsieh, F.-I. Wu, C.-H. Fan, M.-J. Huang, K.-Y. Lu, P.-Y. Chou, Y.-H. O. Yang, S.-H. Wu, I.-C. Chen, S.-H. Chou, K.-T. Wong and C.-H. Cheng, *Chem. Eur. J.*, 2011, **17**, 9180.
12. K.-Y. Lu, H.-H. Chou, C.-H. Hsieh, Y.-H. O. Yang, H.-R. Tsai, H.-Y. Tsai, L.-C. Hsu, C.-Y. Chen, I.-C. Chen and C.-H. Cheng, *Adv. Mater.*, 2011, **23**, 4933.
13. A. B. Tamayo, B. D. Alleyne, P. I. Djurovich, S. Lamansky, I. Tsyba, N. N. Ho, R. Bau and M. E. Thompson, *J. Am. Chem. Soc.*, 2003, **125**, 7377.
14. Y.-C. Chiu, J.-Y. Hung, T. Chi, C.-C. Chen, C.-H. Chang, C.-C. Wu, Y.-M. Cheng, Y.-C. Yu, G.-H. Lee and P.-T. Chou, *Adv. Mater.*, 2009, **21**, 2221.
15. C.-H. Yang, Y.-M. Cheng, Y. Chi, C.-J. Hsu, F.-C. Fang, K.-T. Wong, P.-T. Chou, C.-H. Chang, M.-H. Tsai and C.-C. Wu, *Angew. Chem. Int. Ed.*, 2007, **46**, 2418.
16. C.-H. Lin, Y.-Y. Chang, J.-Y. Hung, C.-Y. Lin, Y. Chi, M.-W. Chung, C.-L. Lin, P.-T. Chou, G.-H. Lee, C.-H. Chang and W.-C. Lin, *Angew. Chem. Int. Ed.*, 2011, **50**, 3182.

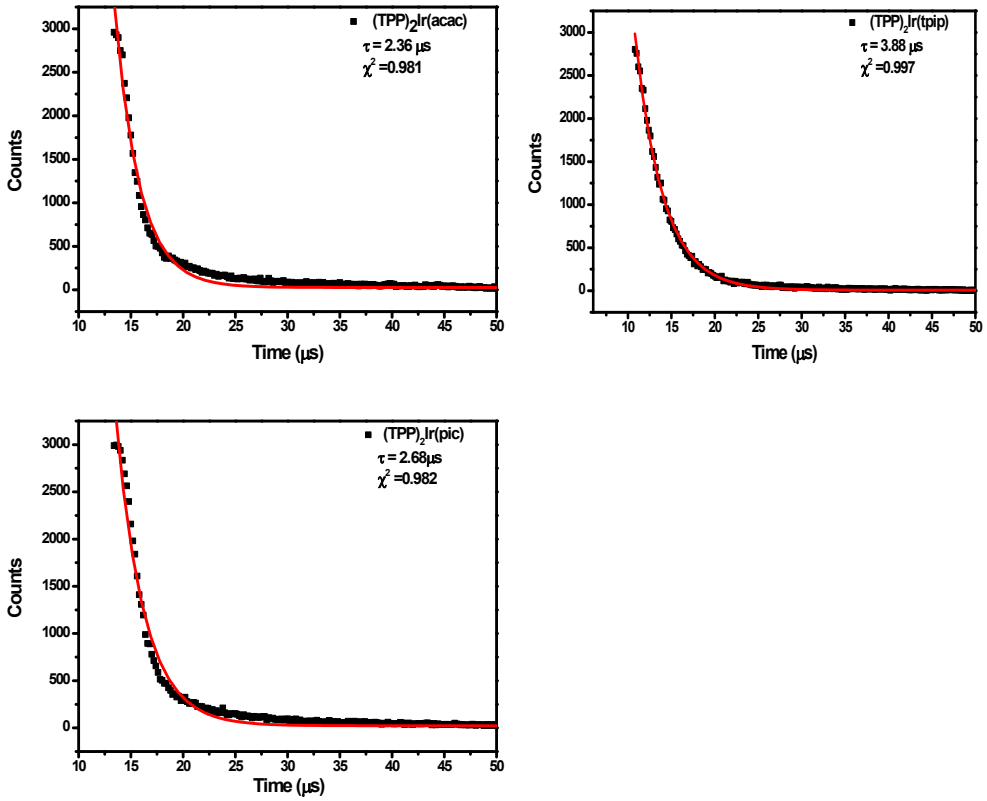


Figure S1. The lifetime curves of $(TPP)_2Ir(acac)$, $(TPP)_2Ir(tpip)$ and $(TPP)_2Ir(pic)$ in degassed CH_2Cl_2 solution at room temperature.

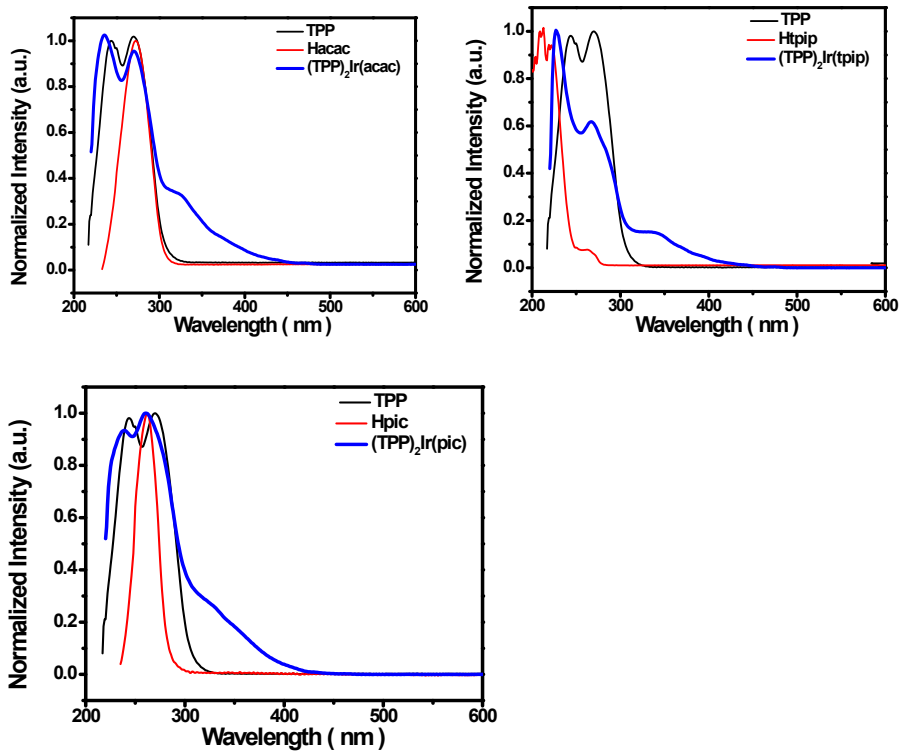


Figure S2. The UV-vis absorption of free ligands and complexes $(TPP)_2Ir(acac)$, $(TPP)_2Ir(tpip)$ and $(TPP)_2Ir(pic)$ in CH_2Cl_2 solution at room temperature.

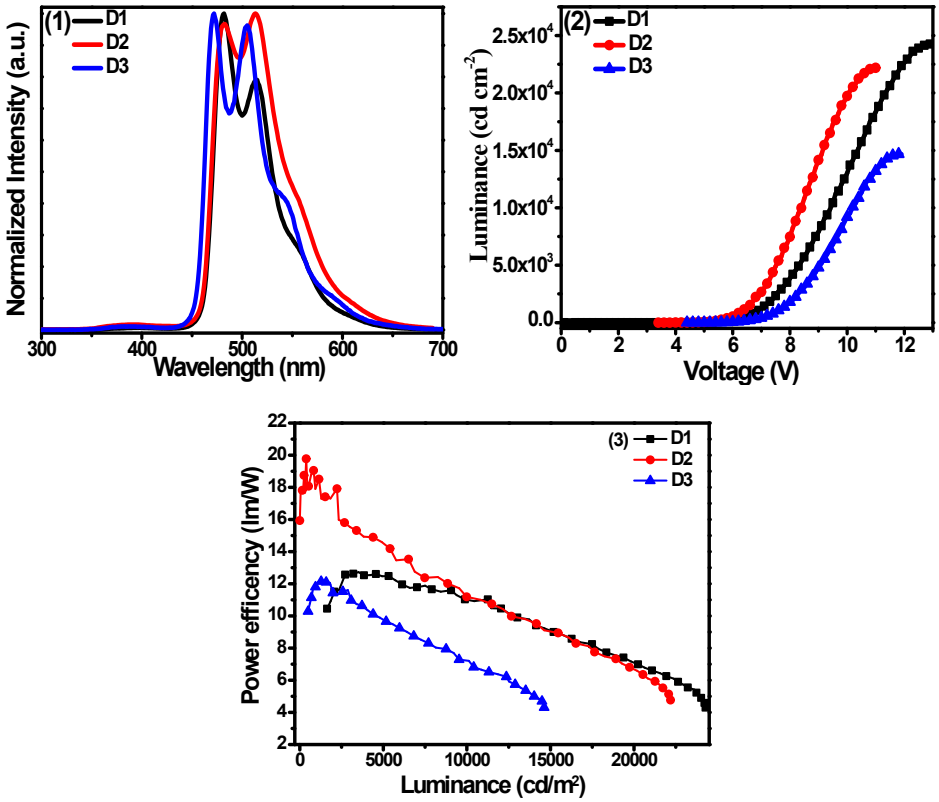


Figure S3. (1) electroluminescence spectra; (2) luminance – voltage (L – V) curves; (3) power efficiency–luminance (η_p–L) curves of device **D1**, **D2** and **D3**.