Supporting Information

A Yellow-Emitting Homoleptic Iridium(III) Complex Constructed from Multifunctional Spiro Ligand for Highly Efficient Phosphorescent Organic Light Emitting Diodes

Bao-Yi Ren,[†,‖,§,⊥] *Run-Da Guo,*[‡,⊥] *Dao-Kun Zhong,*[†,⊥] *Chang-Jin Ou,*[§] *Gang Xiong,*[†] *Xiang-Hua Zhao,*[§] *Ya-Guang Sun,**[,†] *Matthew Jurow,*[‖] *Jun Kang,*[⌝] *Yi Zhao,*[‡] *Sheng-Biao Li,**[,┼] *Li-Xin You,*[†] *Lin-Wang Wang,*[⌝] *Yi Liu,**[,‖] *and Wei Huang*[§]

[†]Key Laboratory of Inorganic Molecule-Based Chemistry of Liaoning Province, College of Applied Chemistry, Shenyang University of Chemical Technology, Shenyang 110142, P. R. China

[‡]State Key Laboratory on Integrated Optoelectronics, College of Electronics Science and Engineering, Jilin University, Changchun 130012, P. R. China

[‖]The Molecular Foundry, [⌝]Materials Sciences Division, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley 94720, United States

[§]Key Laboratory for Organic Electronics and Information Displays & Institute of Advanced Materials (IAM), Jiangsu National Synergetic Innovation Center for Advanced Materials (SICAM), Nanjing University of Posts & Telecommunications, 9 Wenyuan Road, Nanjing 210023, China.

[┼]College of Chemistry, Central China Normal University, Wuhan 430070, P. R. China

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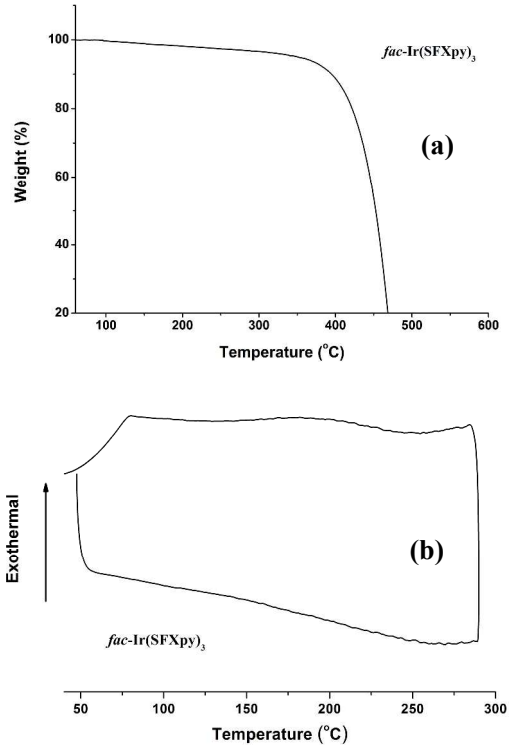

Figure S1. TGA (a) and DSC (b) curves of *fac*-Ir(SFXpy)$_3$.

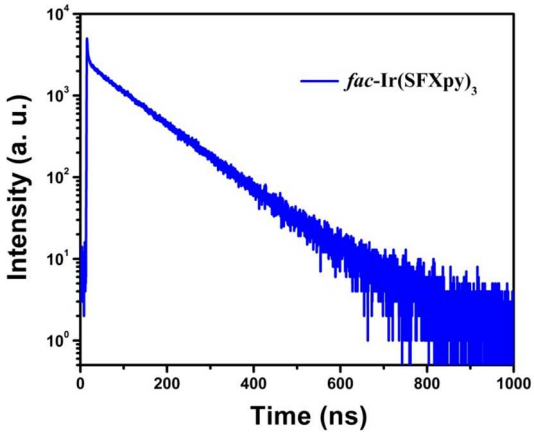

Figure S2. Transient photoluminescent decay (excited at 365 nm) curves at 298 K for *fac*-Ir(SFXpy)$_3$ in degassed CH_2Cl_2 solution.

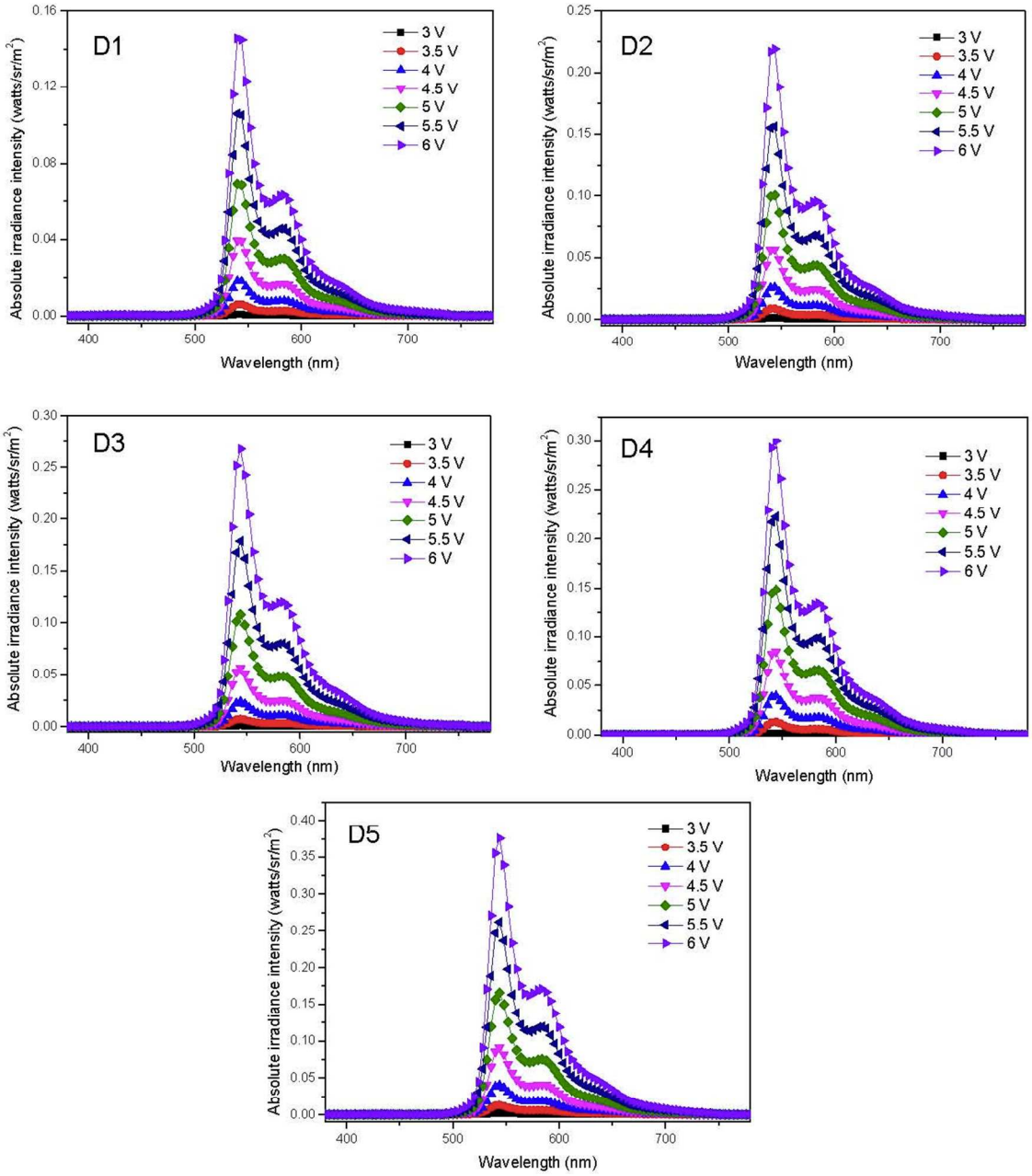

Figure S3. Non-normalized EL spetrum of devices D1–D5.

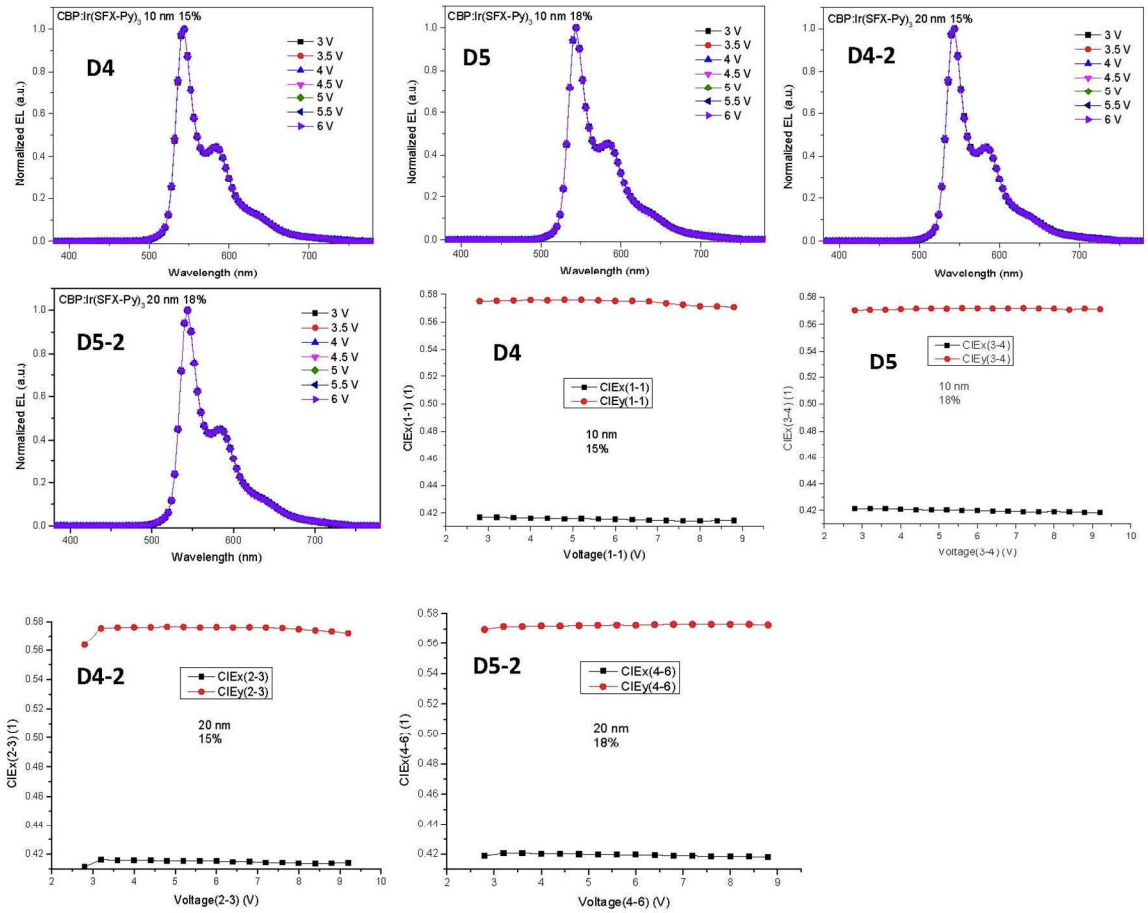

Figure S4. Normalized EL and CIE coordinates curves of devices D4, D5, D4-2, and D5-2.

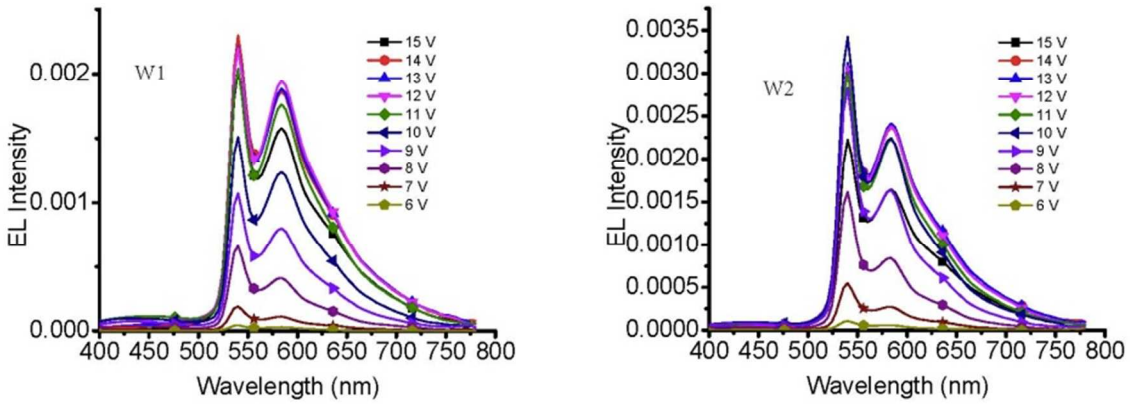

Figure S5. Non-normalized EL spectrum of devices W1 and W2**.**

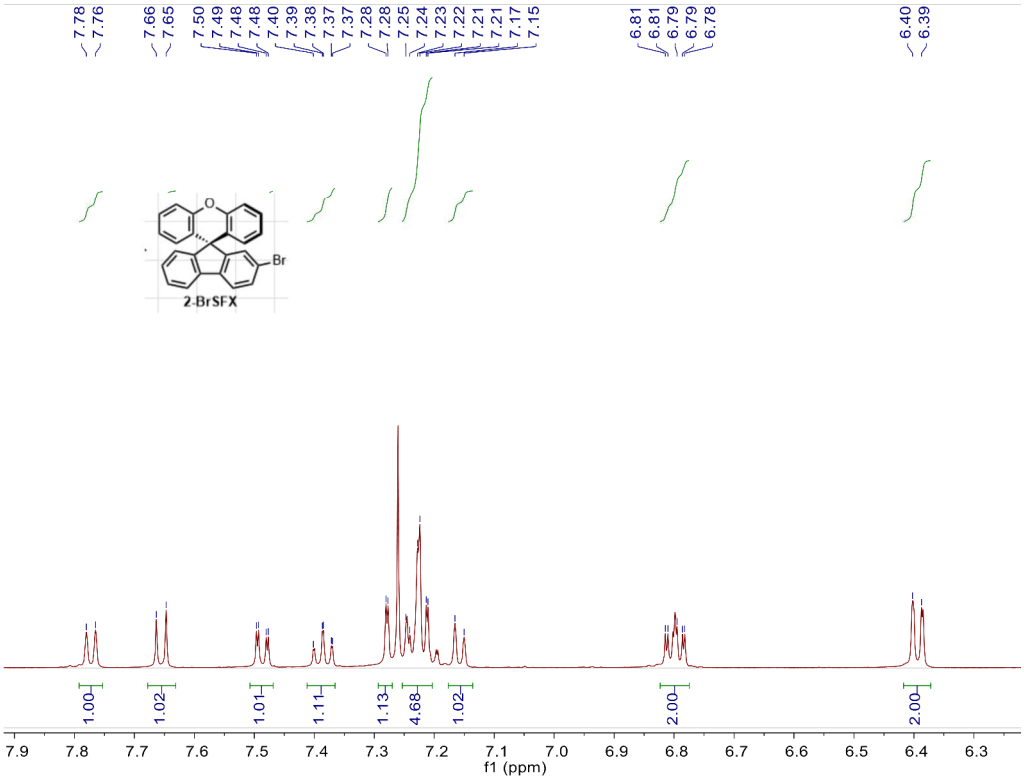

Figure S6. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of 2-BrSFX.

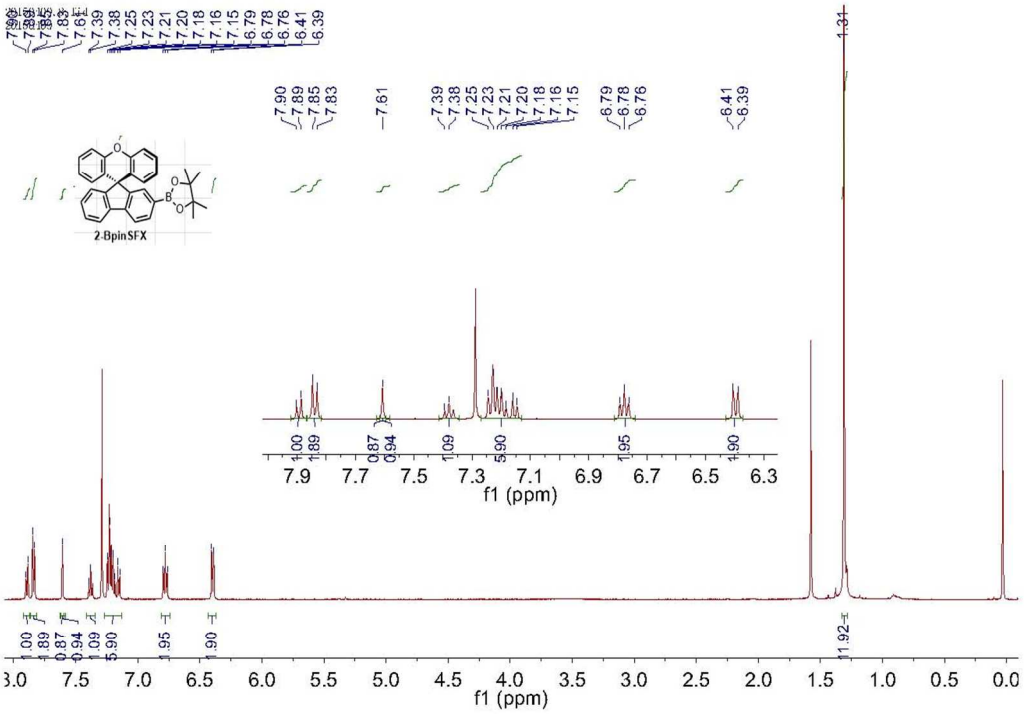

Figure S7. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of 2-BpinSFX.

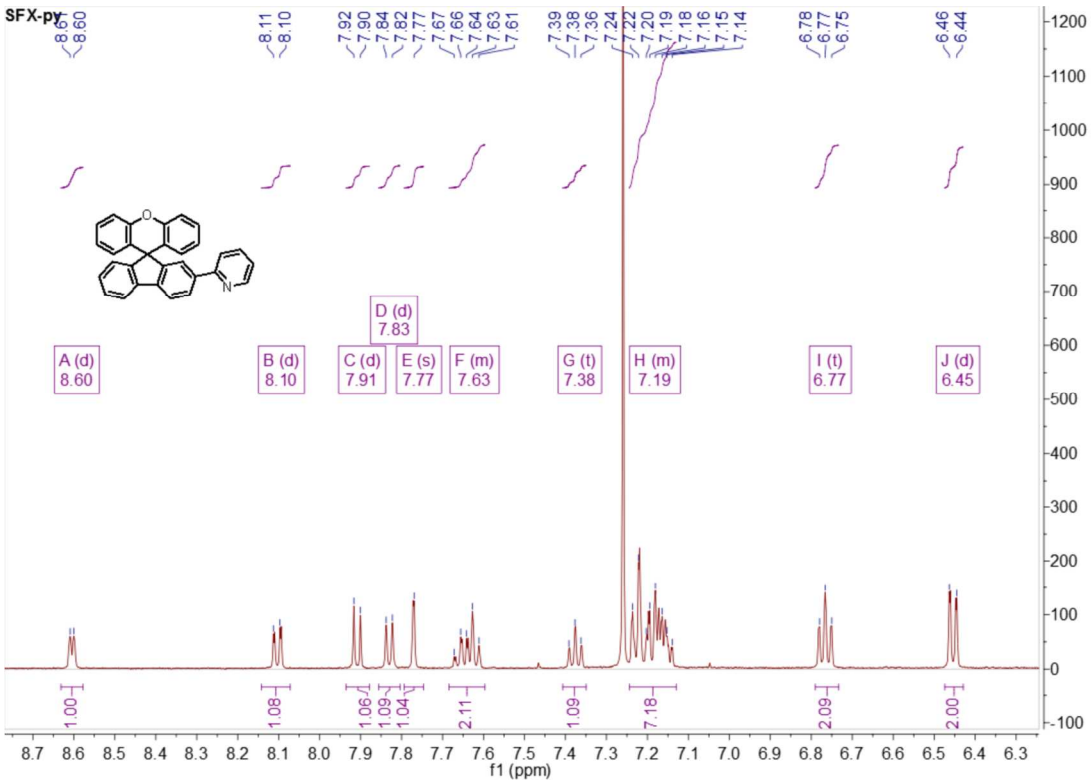

Figure S8. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of SFXpy.

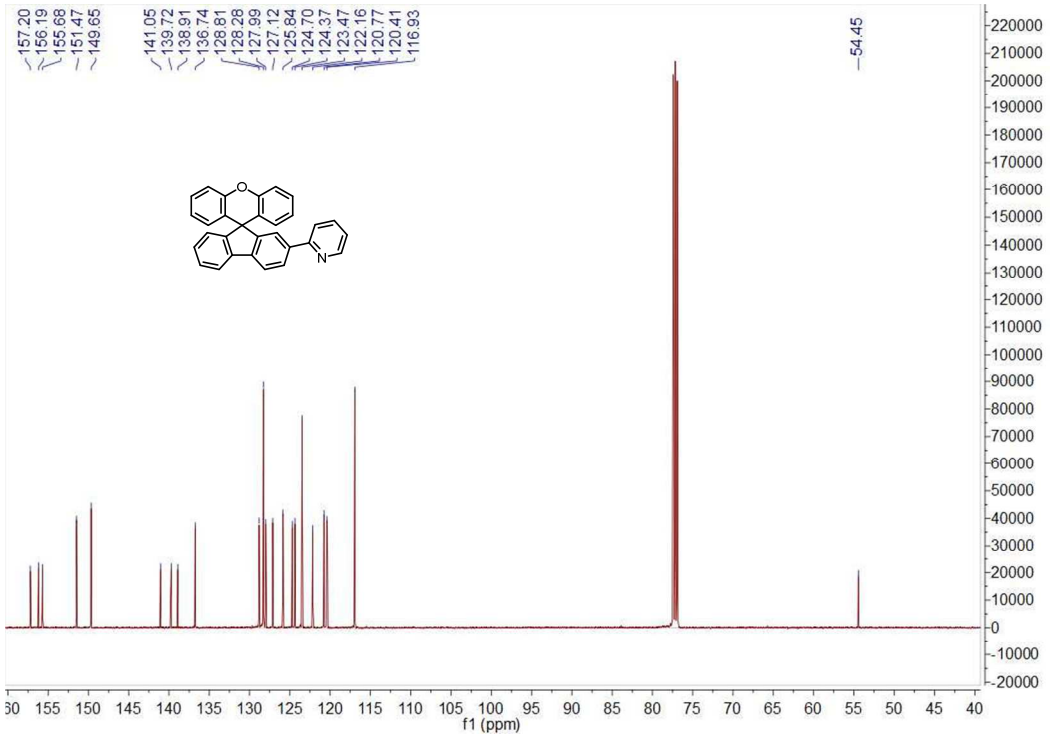

Figure S9. ^{13}C NMR spectrum ($CDCl_3$ 125 MHz, 298 K)of SFXpy.

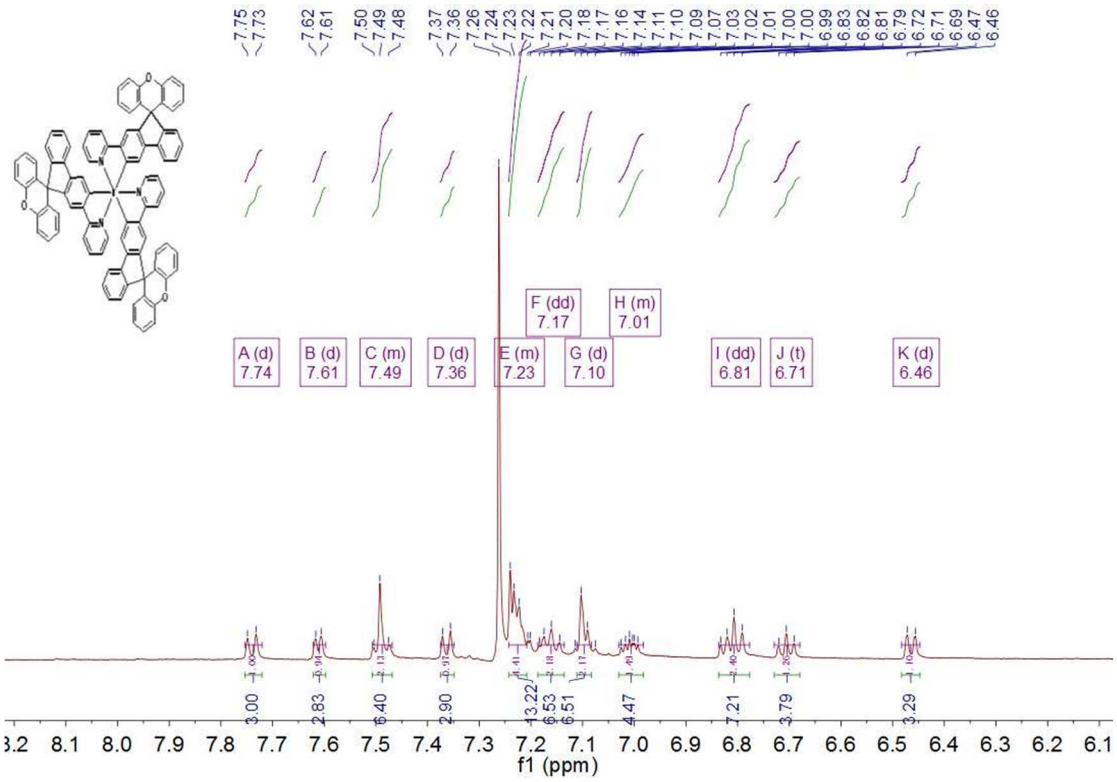

Figure S10. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz, 298 K) of *fac*-Ir(SFXpy)$_3$.

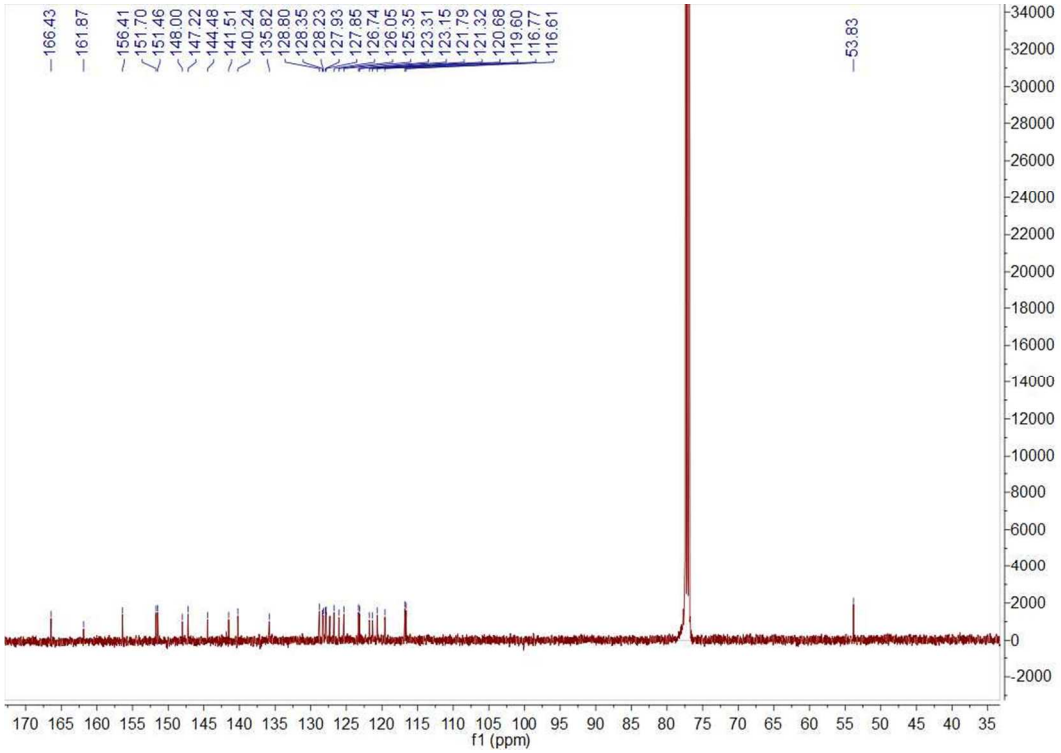

Figure S11. ^{13}C NMR spectrum ($CDCl_3$ 125 MHz, 298 K)of *fac*-Ir(SFXpy)$_3$.

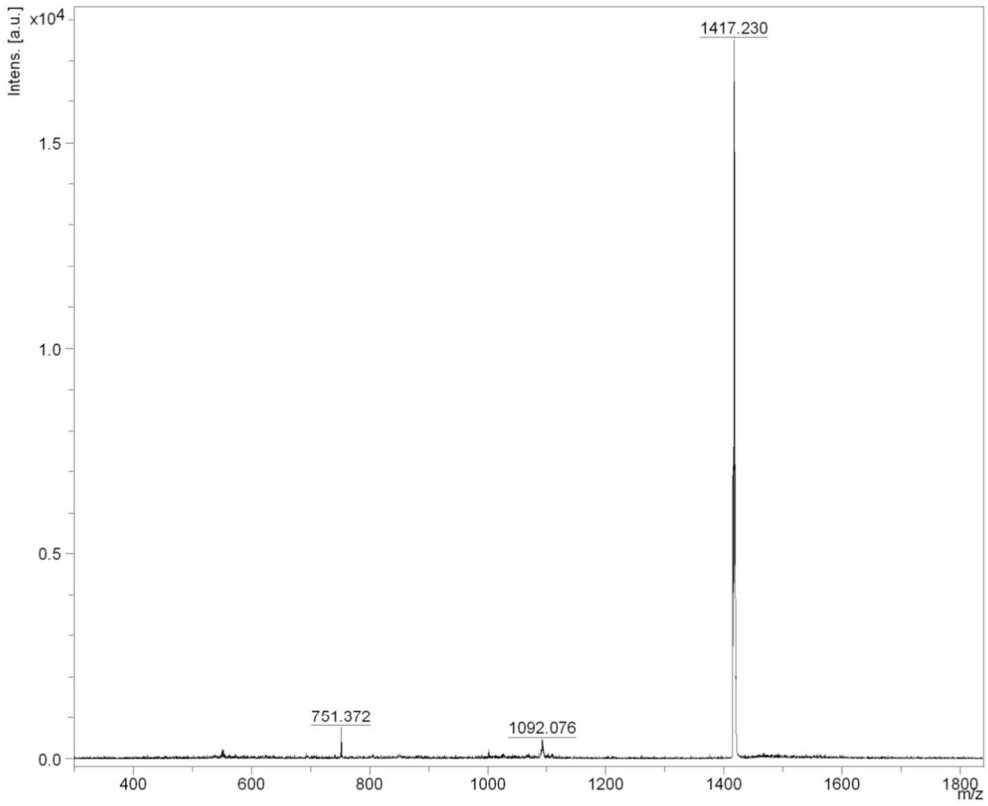

Figure S12. MALDI-TOF MS spectrum of *fac*-Ir(SFXpy)$_3$.

Table S1. Selected Bond Lengths for *fac*-Ir(SFXpy)$_3$

Atom	Atom	Length/Å
C_7	Ir_1	2.006(8)
C_{41}	Ir_1	2.018(8)
C_{71}	Ir_1	2.024(7)
N_3	Ir_1	2.120(7)
N_2	Ir_1	2.119(7)
N_1	Ir_1	2.113(7)

Table S2. Selected Bond Angles for *fac*-Ir(SFXpy)$_3$

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_8	C_7	Ir_1	129.2(6)	C_{61}	N_3	Ir_1	125.1(6)
C_6	C_7	Ir_1	115.8(6)	C_{65}	N_3	Ir_1	115.0(5)
C_{40}	C_{41}	Ir_1	128.1(6)	C_{31}	N_2	Ir_1	125.8(6)
C_{36}	C_{41}	Ir_1	115.5(6)	C_{35}	N_2	Ir_1	115.6(5)
C_{66}	C_{71}	Ir_1	114.8(5)	C_5	N_1	Ir_1	115.4(5)

C_{70}	C_{71}	Ir_1	128.0(5)	C_1	N_1	Ir_1	125.5(7)
C_{71}	Ir_1	N_3	79.2(3)	C_7	Ir_1	N_1	79.5(3)
C_{71}	Ir_1	N_2	90.4(3)	C_{41}	Ir_1	C_{71}	97.5(3)
C_{71}	Ir_1	N_1	171.0(3)	C_{41}	Ir_1	N_3	173.6(3)
C_7	Ir_1	C_{71}	94.1(3)	C_{41}	Ir_1	N_2	79.1(3)
C_7	Ir_1	C_{41}	95.0(3)	C_{41}	Ir_1	N_1	89.4(3)
C_7	Ir_1	N_3	90.8(3)	N_3	Ir_1	N_2	95.3(3)
C_7	Ir_1	N_2	173.0(3)	N_1	Ir_1	N_3	94.5(3)
N_1	Ir_1	N_2	96.6(3)				

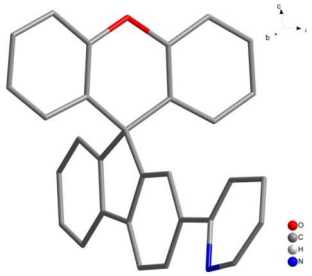

Figure S13. Stick representation of the crystal structure of SFXpy. The hydrogen atoms were omitted for clarity.

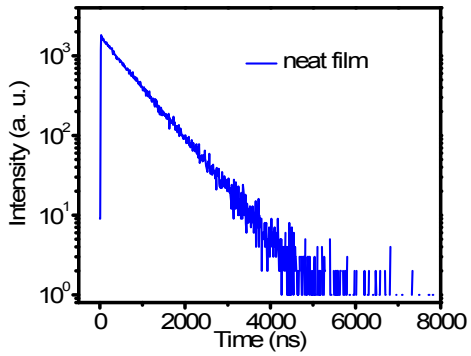

Figure S14. The phosphorescent lifetime (excited at 365 nm) curves under 298 K for the neat films of *fac*-Ir(SFXpy)$_3$.

Table S3. Crystal data and structure refinement of SFXpy ligand

Identification code	**CCDC 1522839**
Formula moiety	$C_{30}H_{19}NO$
Formula weight	243.22

Crystal system	orthorhombic
Space group	$P_{nca}(60)$
a	14.615(9)
b	16.663(10)
c	17.269(10)
a/Å	90.00
b/Å	90.00
c/Å	90.00
Volume/Å^3	4205(4)
Z	8
Crystal density	1.293
F(000)	1712
Crystal size	0.2

Table S4. The atomic coordinates of SFXpy ligand

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
O1	0.34747(14)	0.38808(13)	0.58862(10)	H19	0.5021	0.4083	0.5306
C1	0.35828(14)	0.35447(13)	0.83176(11)	C20	0.3956(6)	0.5897(4)	0.9265(5)
C2	0.36537(15)	0.43247(13)	0.85805(12)	H20	0.3927	0.5819	0.8732
H2	0.3671	0.475	0.8232	C21	0.1887(2)	0.40864(19)	0.59533(17)
C3	0.26626(16)	0.35431(13)	0.70725(12)	H21	0.1915	0.4286	0.5451
C4	0.35551(15)	0.29017(13)	0.88327(12)	C22	0.5924(2)	0.37698(18)	0.61200(17)
C5	0.35044(15)	0.21509(13)	0.83880(13)	H22	0.6444	0.3872	0.5825
C6	0.43651(16)	0.34650(13)	0.70034(12)	C23	0.6013(2)	0.34928(18)	0.68664(17)
C7	0.34827(15)	0.23369(14)	0.75994(13)	H23	0.659	0.3403	0.7077
C8	0.35242(15)	0.32462(13)	0.74752(12)	C24	0.3460(2)	0.07614(16)	0.8063(2)
C9	0.36989(16)	0.44686(14)	0.93798(12)	H24	0.3458	0.0226	0.8214
C10	0.37949(17)	0.52968(16)	0.96940(14)	C25	0.3434(2)	0.09470(17)	0.7285(2)
C11	0.26791(18)	0.38286(16)	0.63232(13)	H25	0.3407	0.0538	0.6919
C12	0.52394(17)	0.33507(17)	0.72983(15)	C26	0.1063(2)	0.40440(19)	0.63341(18)
H12	0.5304	0.3172	0.7805	H26	0.0532	0.4217	0.6089
C13	0.42976(18)	0.37427(15)	0.62500(14)	C27	0.1022(2)	0.3748(2)	0.70722(17)
C14	0.36606(19)	0.38195(16)	0.98841(13)	H27	0.0463	0.371	0.7326
H14	0.3685	0.3914	1.0414	C28	0.3931(3)	0.6796(2)	1.0295(3)
C15	0.35874(19)	0.30389(17)	0.96227(14)	H28	0.3964	0.7309	1.0505
H15	0.356	0.2614	0.9971	C29	0.4170(3)	0.6660(2)	0.9527(2)
C16	0.18138(18)	0.35065(18)	0.74373(15)	H29A	0.4449	0.7046	0.9218
H16	0.178	0.3313	0.7942	H29	0.4301	0.7104	0.9221
1	0.3624(4)	0.5301(3)	1.0502(3)	C30	0.3651(3)	0.6171(3)	1.0729(2)

C17	0.34877(17)	0.13513(15)	0.86236(17)	H30A	0.3451	0.6293	1.1226
H17	0.3495	0.1218	0.9147	H30	0.3557	0.6209	1.126
C18	0.34495(19)	0.17410(16)	0.70478(17)	N2	0.4229(4)	0.5897(4)	0.9183(4)
H18	0.3437	0.187	0.6524	C31	0.3533(5)	0.5568(4)	1.0375(4)
C19	0.5077(2)	0.38951(18)	0.58109(16)	H31	0.317	0.5202	1.0641