Supporting Information

Methoxyl modification in furo[3,2-c]pyridine based iridium complexes towards highly efficient green- and orange-emitting electrophosphorescent devices

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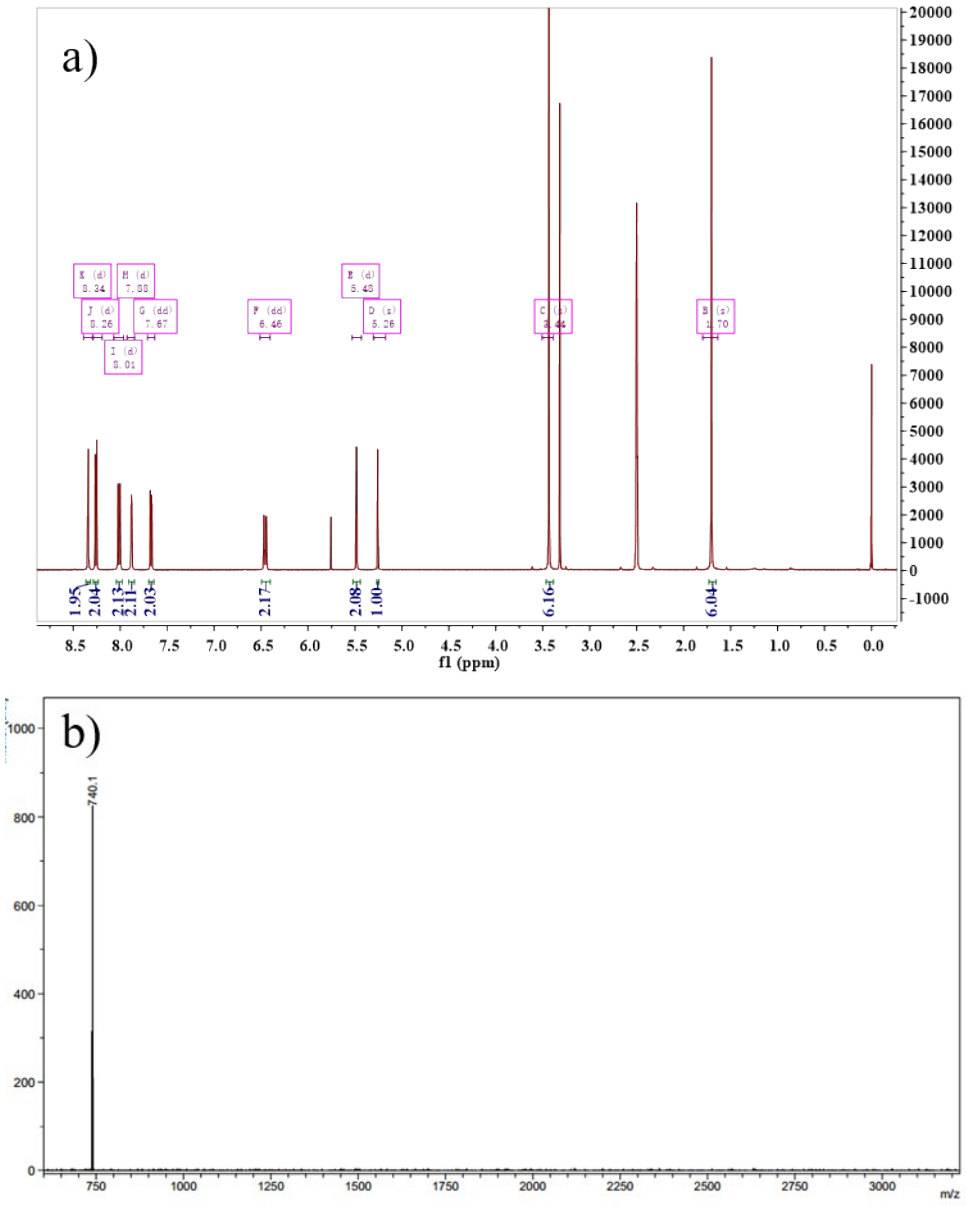

Figure S1. ^{1}H NMR (a) and MALDI-TOF spectra (b) for (4-MeOpfupy)$_2$Ir(acac).

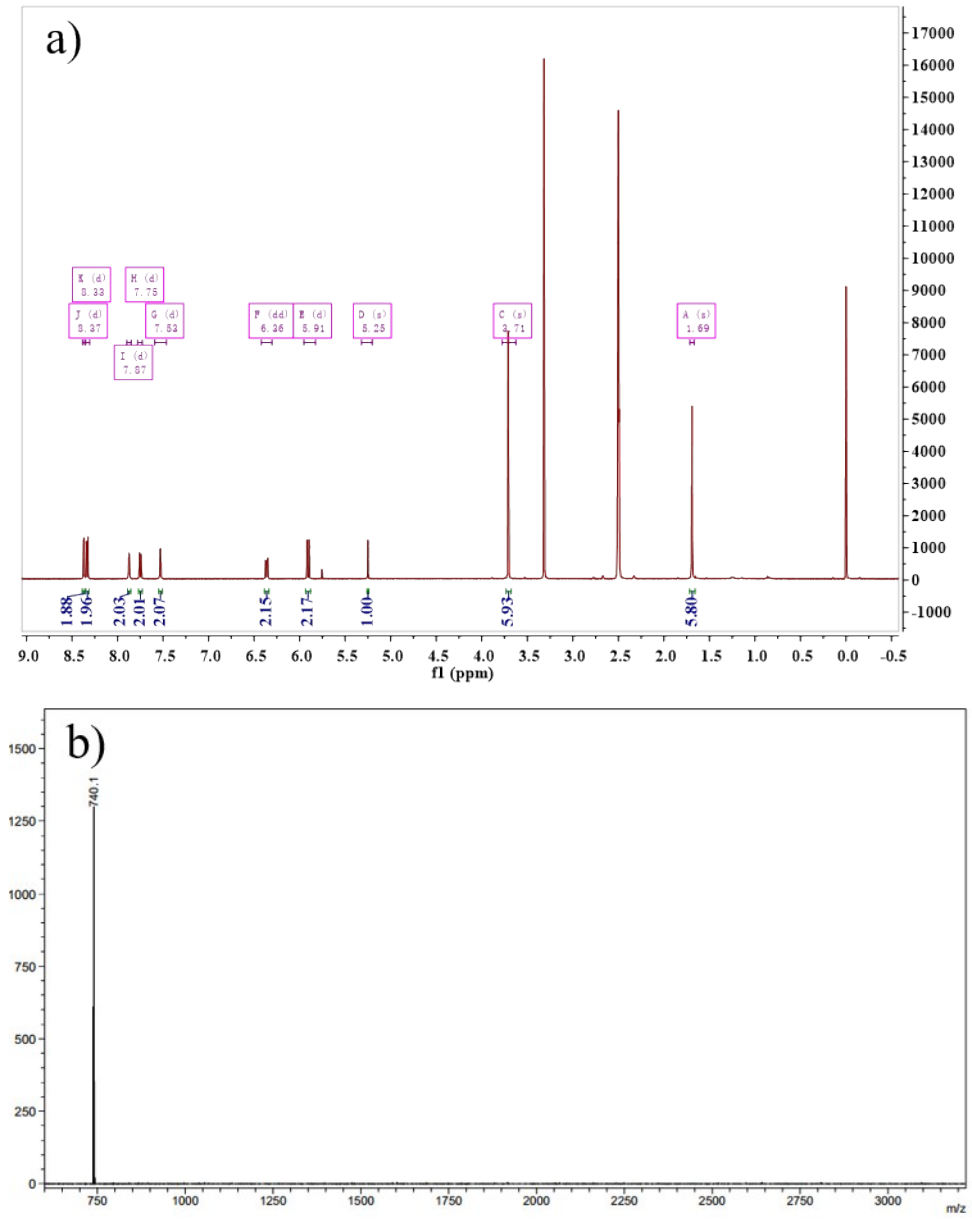

Figure S2. ^{1}H NMR (a) and MALDI-TOF spectra (b) (3-MeOpfupy)$_2$Ir(acac).

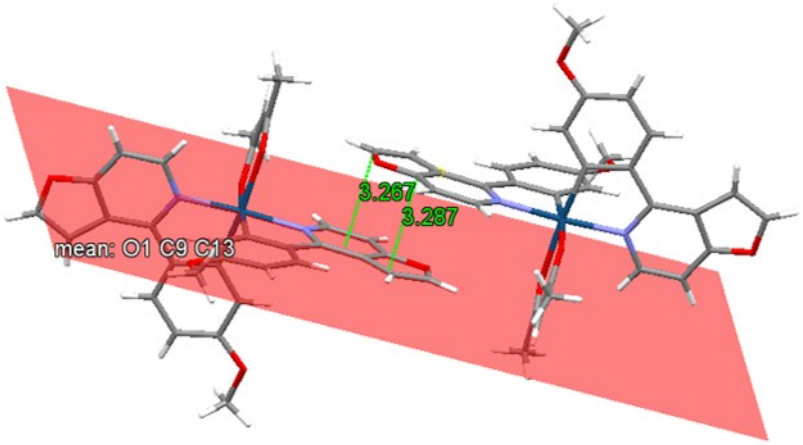

Figure S3. The intermolecular packing in the crystal of $(4\text{-MeOpfupy})_2\text{Ir(acac)}$.

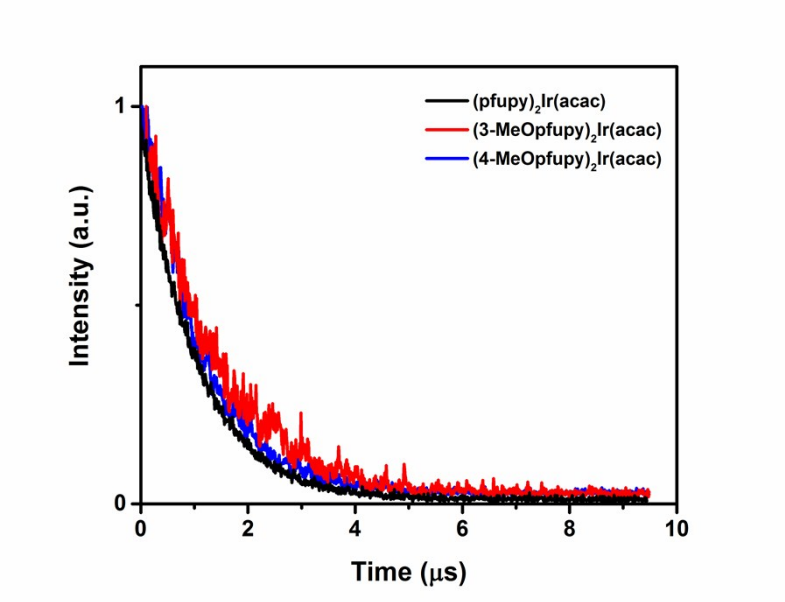

Figure S4. Transient PL spectra in N_2-saturated toluene solutions of (4-MeOpfupy)$_2$Ir(acac) and (3-MeOpfupy)$_2$Ir(acac) compared with (pfupy)$_2$Ir(acac).

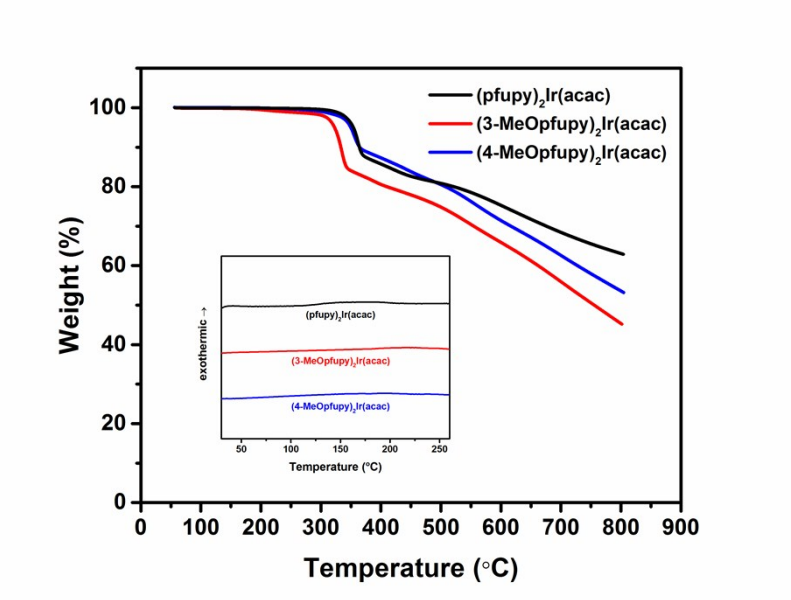

Figure S5. TGA curves of (4-MeOpfupy)$_2$Ir(acac) and (3-MeOpfupy)$_2$Ir(acac) compared with (pfupy)$_2$Ir(acac). Inset: DSC curves.

Table S1. Crystallographic data for $(4\text{-MeOpfupy})_2\text{Ir(acac)}$.

	$(4\text{-MeOpfupy})_2\text{Ir(acac)}$
Empirical formula	C33 H27 Ir N2 O6
Formula weight	739.79
Temperature [K]	186(2)
Wavelength [Å]	0.71073
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions:	
a [Å]	14.3281(9)
b [Å]	19.2115(12)
c [Å]	10.7242(7)
a [°]	90°
b [°]	111.5112(8)
g [°]	90°
Volume [$Å^3$]	2746.4(3)
Z	4
Density (calculated) [Mg/m^3]	1.789
Absorption coefficient [mm^{-1}]	4.913
F(000)	1456
Crystal size [mm^3]	0.28 x 0.18 x 0.10
Theta range for data collection [°]	1.86 to 25.35
Index ranges	-17<=h<=17
	-15<=k<=23
	-12<=l<=12
Reflections collected	8083
Independent reflections	5031 [R(int) = 0.0313]
Completeness to theta =25.35	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6393 and 0.3400
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2520 / 0 / 192
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0208, wR2 = 0.0495
R indices (all data)	R1 = 0.0231, wR2 = 0.0506
Largest diff. peak and hole [e. $Å^3$]	0.742 and -0.361

Table S2. Selected bond lengths, angle and torsion angles for (4-MeOpfupy)$_2$Ir(acac).

Bond lengths [Å]	
Ir(1)-C(2)	1.978(3)
Ir(1)-C(1)	1.978(3)
Ir(1)-N(2)	2.046(3)
Ir(1)-N(1)	2.046(3)
Ir(1)-O(4)	2.151(2)
Ir(1)-O(3)	2.151(2)
Bond Angles [°]	
C(1)-Ir(1)-N(1)	80.59(12)
C(2)-Ir(1)-N(2)	80.59(12)
O(4)-Ir(1)-O(3)	87.73(13)
N(2)-Ir(1)-N(1)	176.01(15)
C(2)-Ir(1)-O(4)	174.87(10)
C(1)-Ir(1)-O(3)	174.87(10)
Torsion Angles [°]	
N(1)-C(4)-C(3)-C(1)	-3.84
N(2)-C(6)-C(5)-C(2)	-3.84