

Color Tuning of Iridium Complexes by Using Conjugative Effect of Pyridine-derived Cyclometalated Ligands

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Note: Wu and Xue are co-first authors.

1. ESI-MS spectra of ligands

1.1. npy

1.2. pnpyp

1.3. Htpip

2. MALDI-TOF spectra of complexes

2.1 Ir(ppy)₂tpip

2.2 Ir(npy)₂tpip

2.3. Ir(pnpyp)₂tpip

3. H NMR spectra of ligands and complexes

3.1 npy

3.2 pnpyp

3.3 Ir(ppy)₂tpip

3.4 Ir(npy)₂tpip

3.5 Ir(pnpyp)₂tpip

4. Table S1 Parameters associated with the crystal diffraction data collection for Ir(ppy)₂tpip.

5. Table S2 Selected bond lengths(Å) and angles(deg) for Ir(ppy)₂tpip

6. TG-DSC curves of complexes

3.1 Ir(ppy)₂tpip

3.2 Ir(npy)₂tpip

3.3 Ir(pnpyp)₂tpip

1. ESI-MS spectra of ligands

1.1. npy

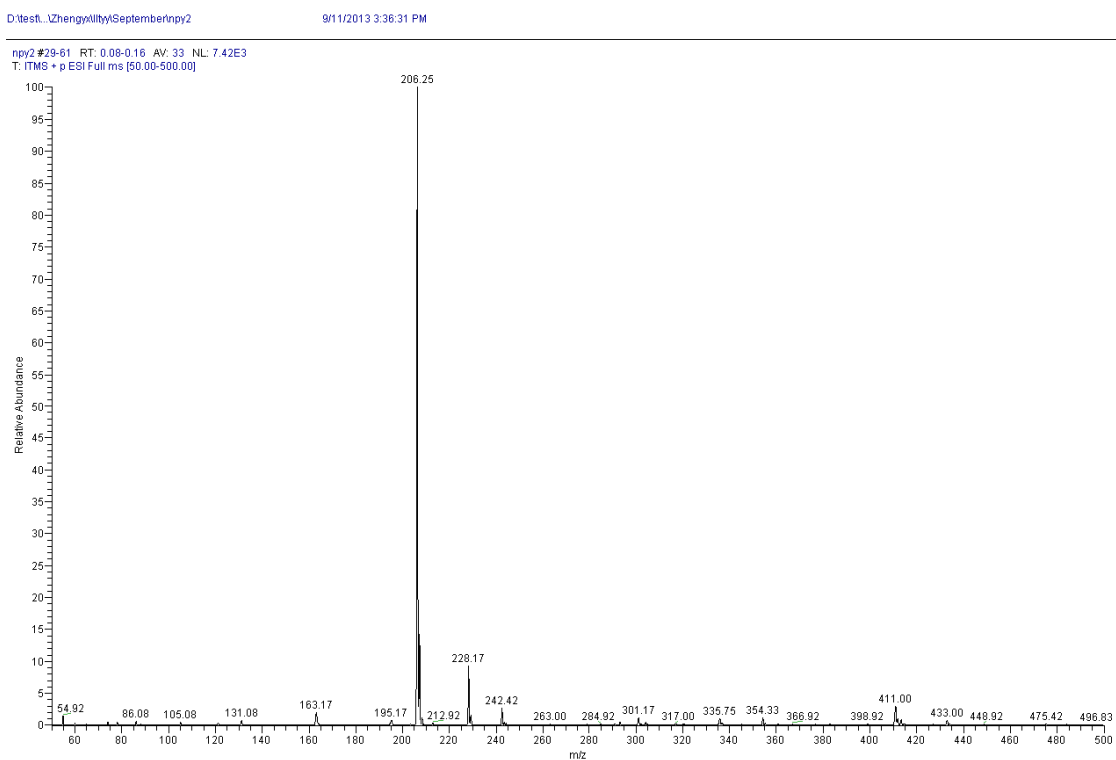


Fig. S1. The ESI-MS spectrum of npy.

1.2. pnp_y

pnp_y2 #22 RT: 0.07 AV: 1 NL: 1.25E3
T: ITMS + p ESI Full ms [50.00-500.00]

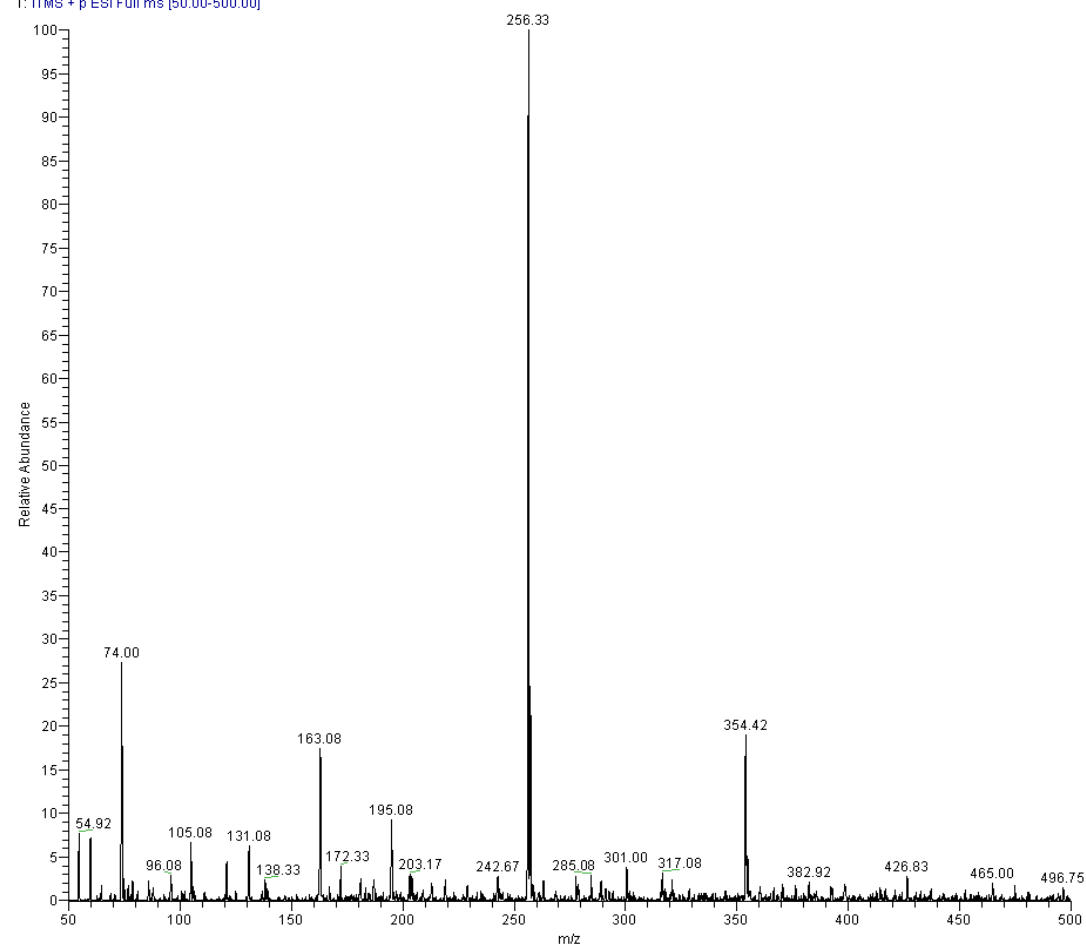


Fig. S2. The ESI-MS spectrum of pnp_y.

1.3. Htpip

D:\test\...September\Ktpip_130905155846

9/5/2013 3:58:46 PM

Ktpip_130905155846 #4-8 RT: 0.04-0.09 AV: 5 NL: 4.81E1
T: ITMS - p ESI Full ms [120.00-1000.00]

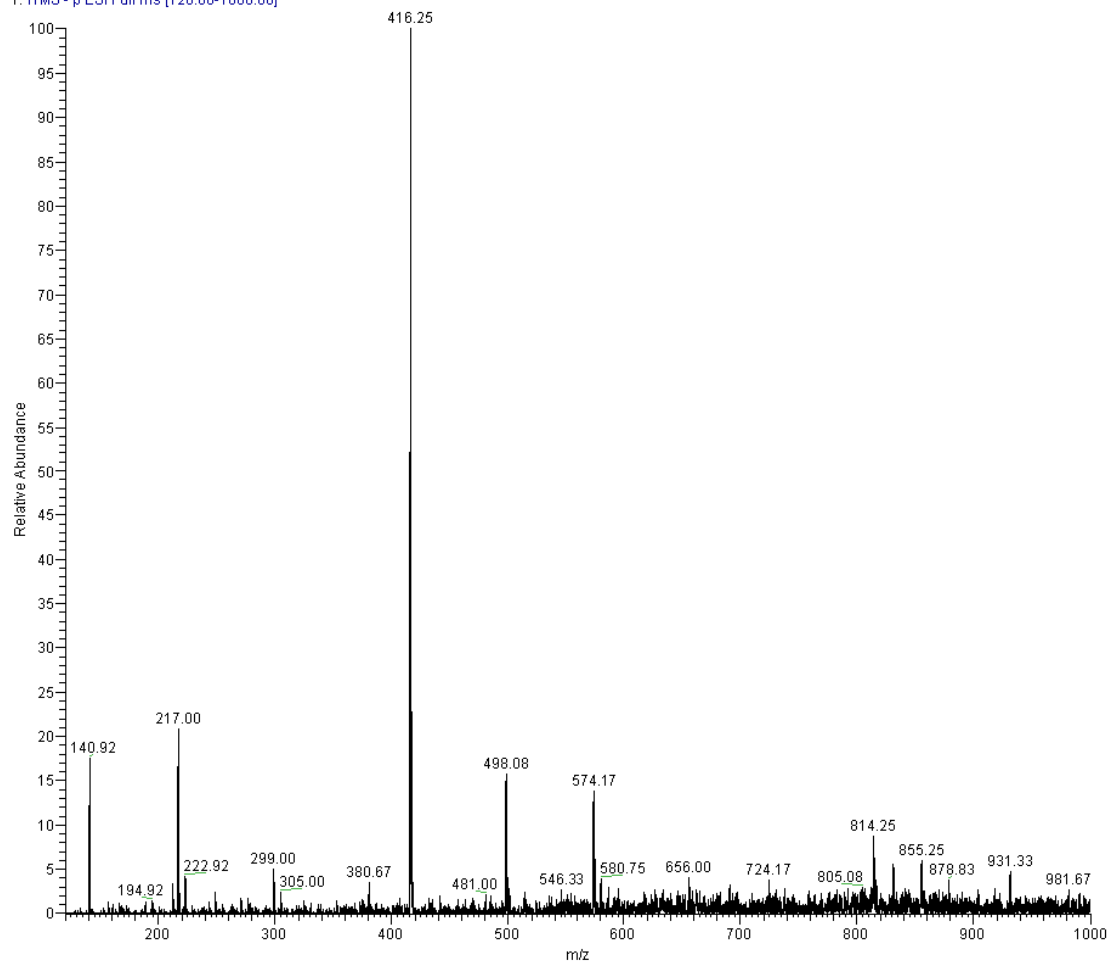


Fig. S3. The ESI-MS spectrum of Htpip.

2. MALDI-TOF spectra of complexes

2.1 Ir(ppy)₂tpip

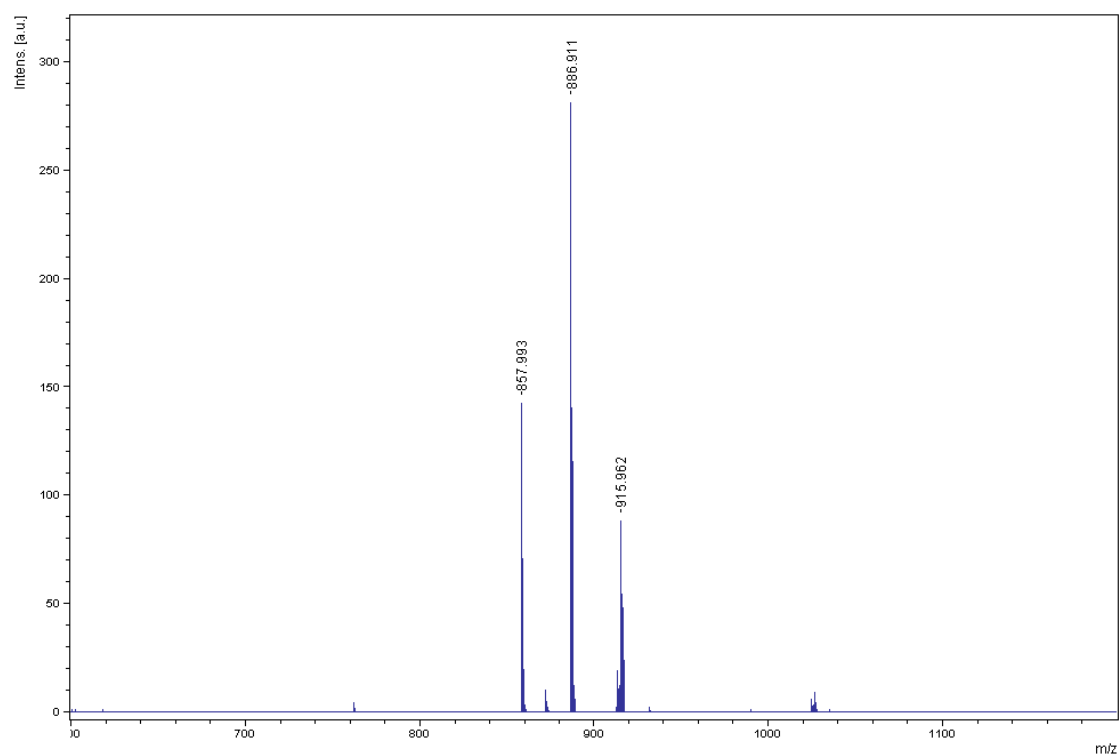


Fig. S4. The MALDI-TOF spectrum of Ir(ppy)₂tpip.

2.2 Ir(npy)₂tpip

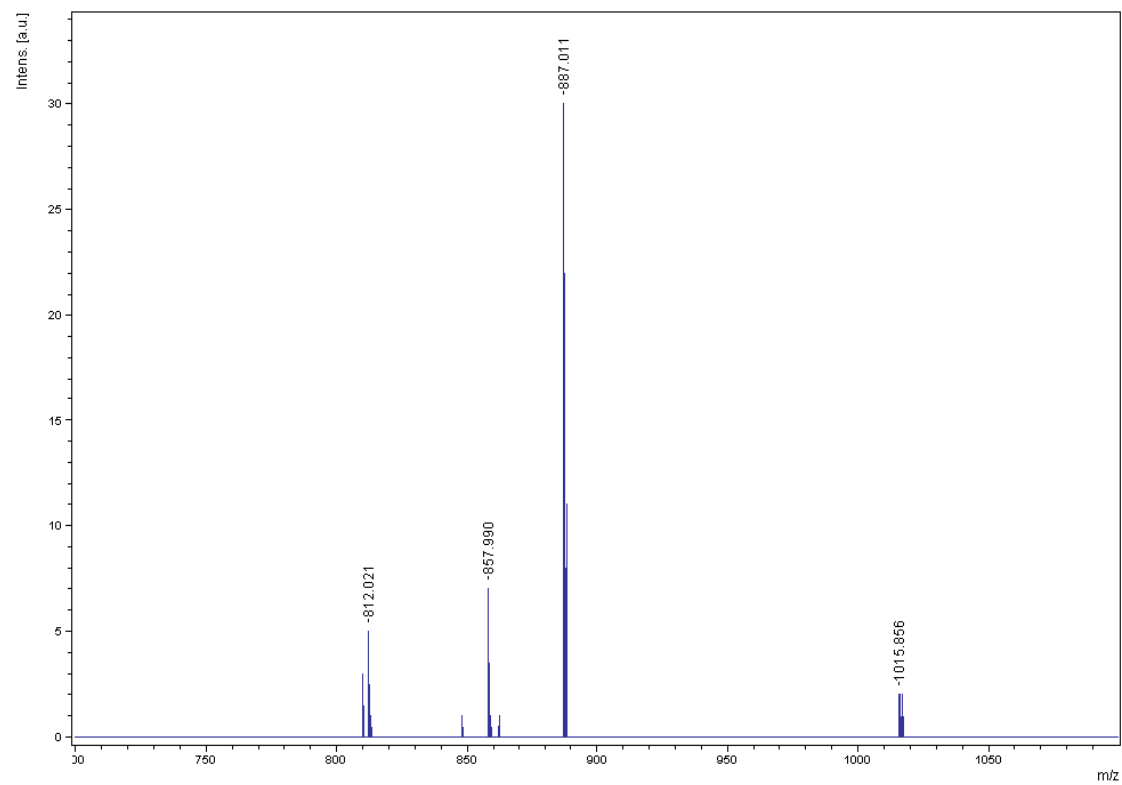


Fig. S5. The MALDI-TOF spectrum of Ir(npy)₂tpip.

2.3. Ir(pnpy)₂tpip

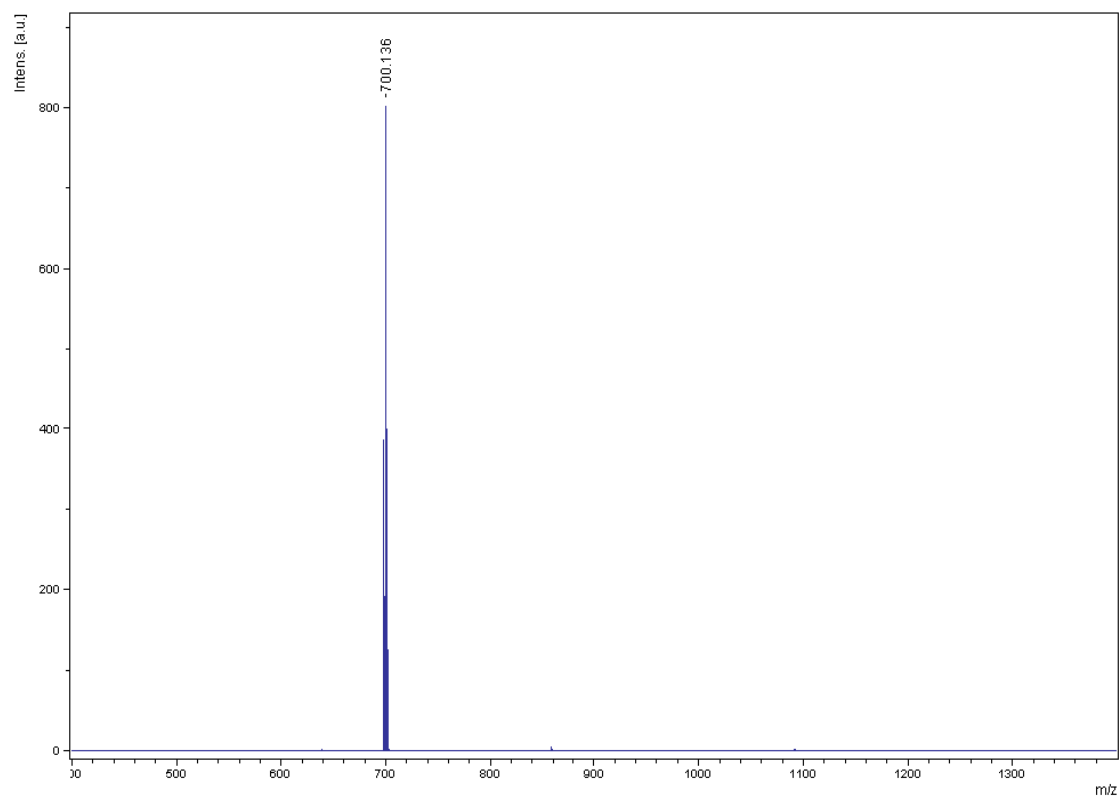


Fig. S6. The MALDI-TOF spectrum of Ir(pnpy)₂tpip.

3. ¹H NMR spectra of ligands and complexes

3.1 npy

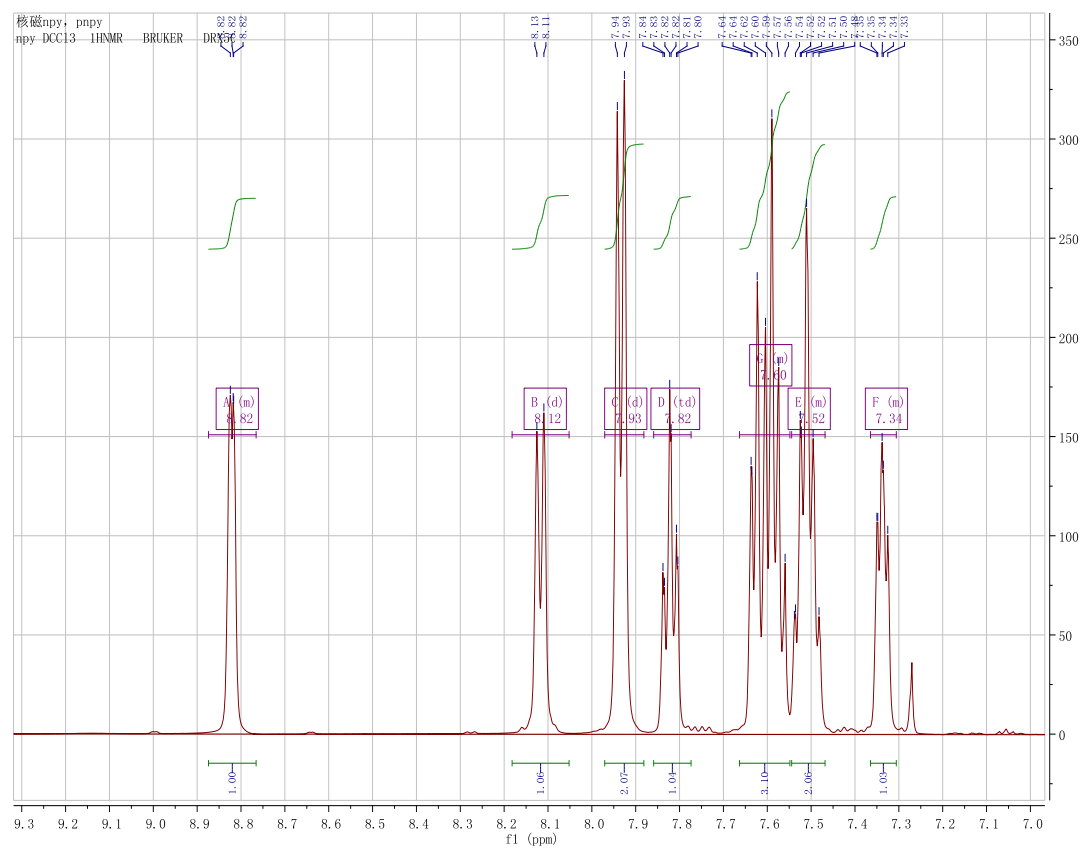


Fig. S7. The ¹H NMR spectrum of npy.

3.2 pnpv

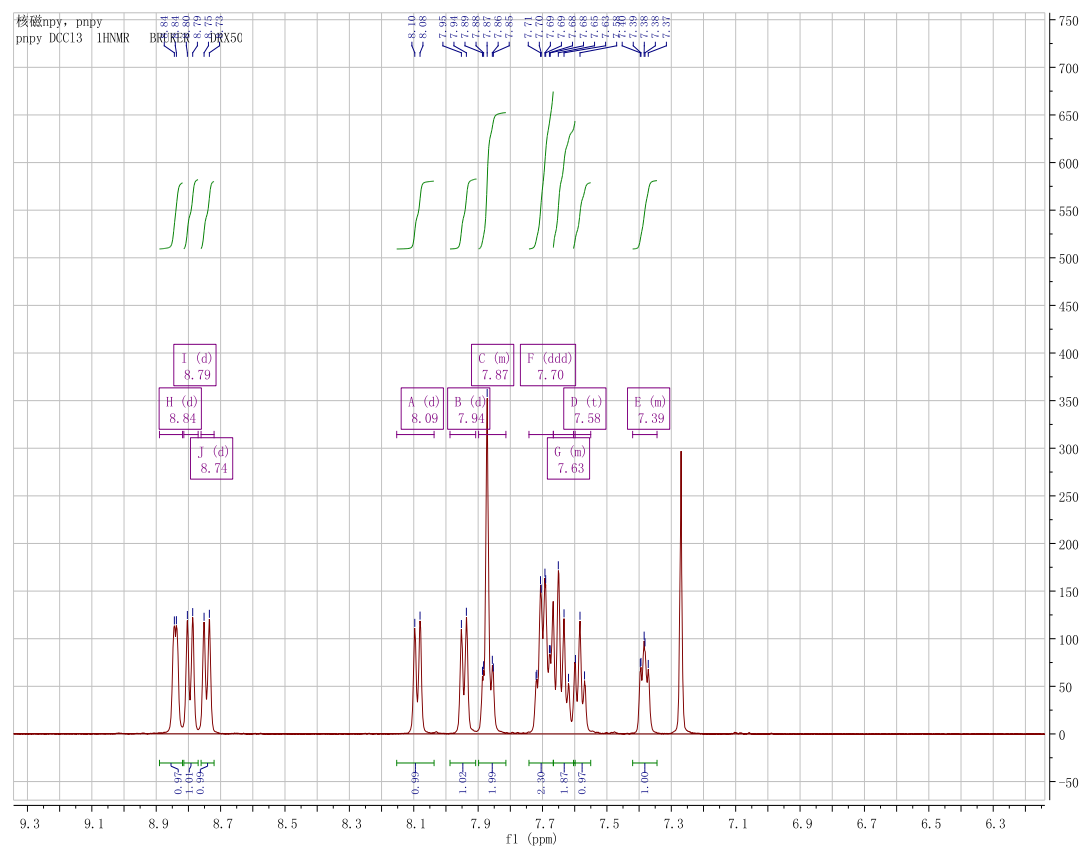


Fig. S8. The ^1H NMR spectrum of pnpv.

3.3 Ir(ppy)₂tpip

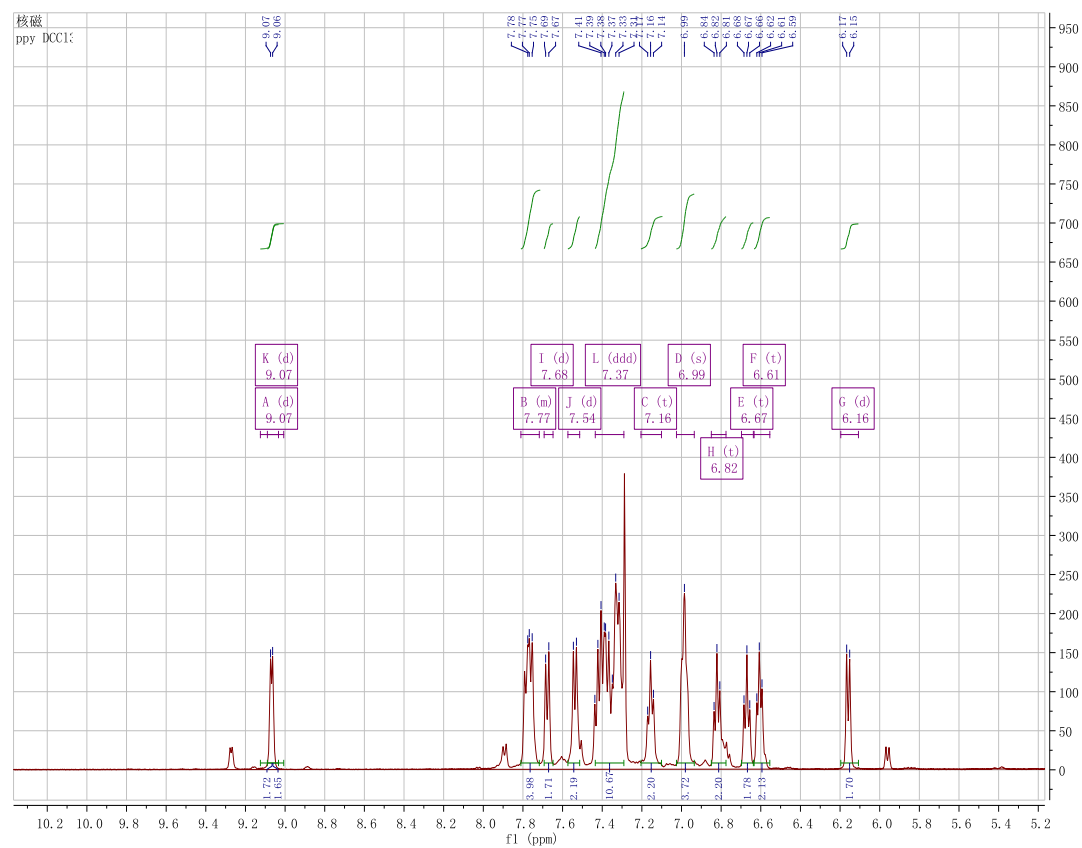


Fig. S9. The ¹H NMR spectrum of Ir(ppy)₂tpip.

3.4 Ir(npv)₂tpip

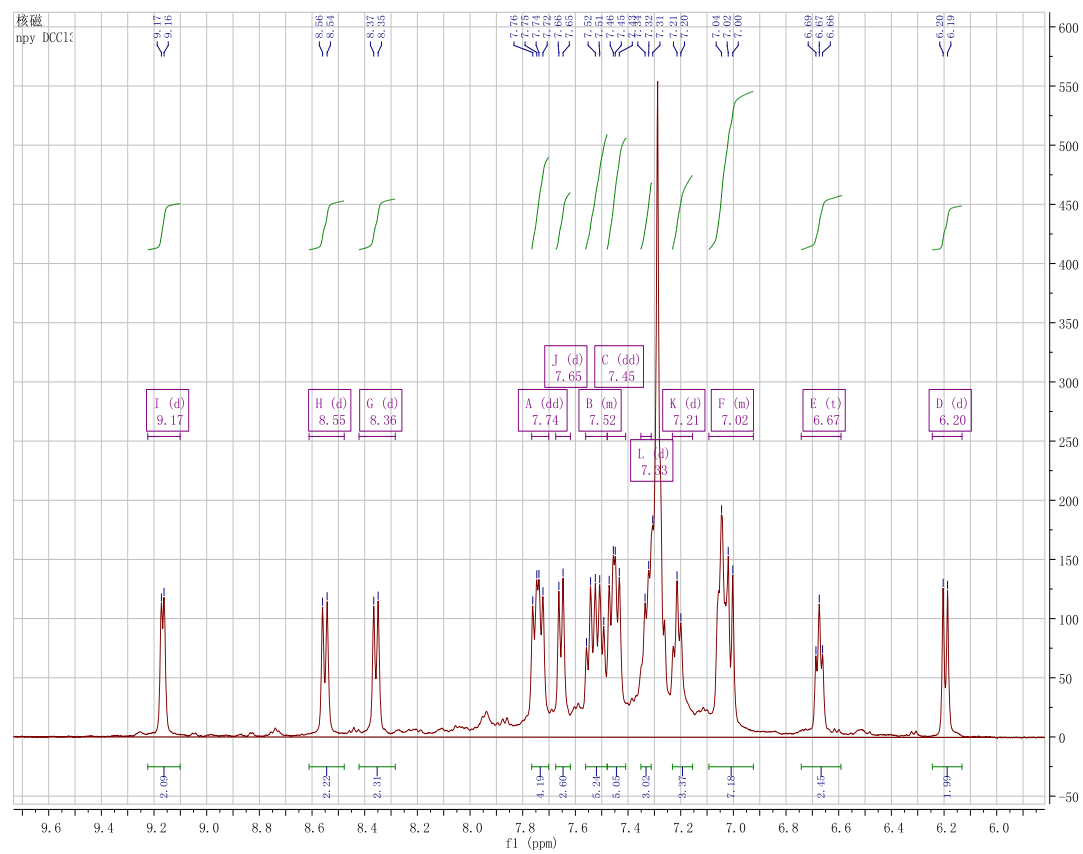


Fig. S10. The ¹H NMR spectrum of Ir(npv)₂tpip.

3.5 Ir(pnpy)₂tpip

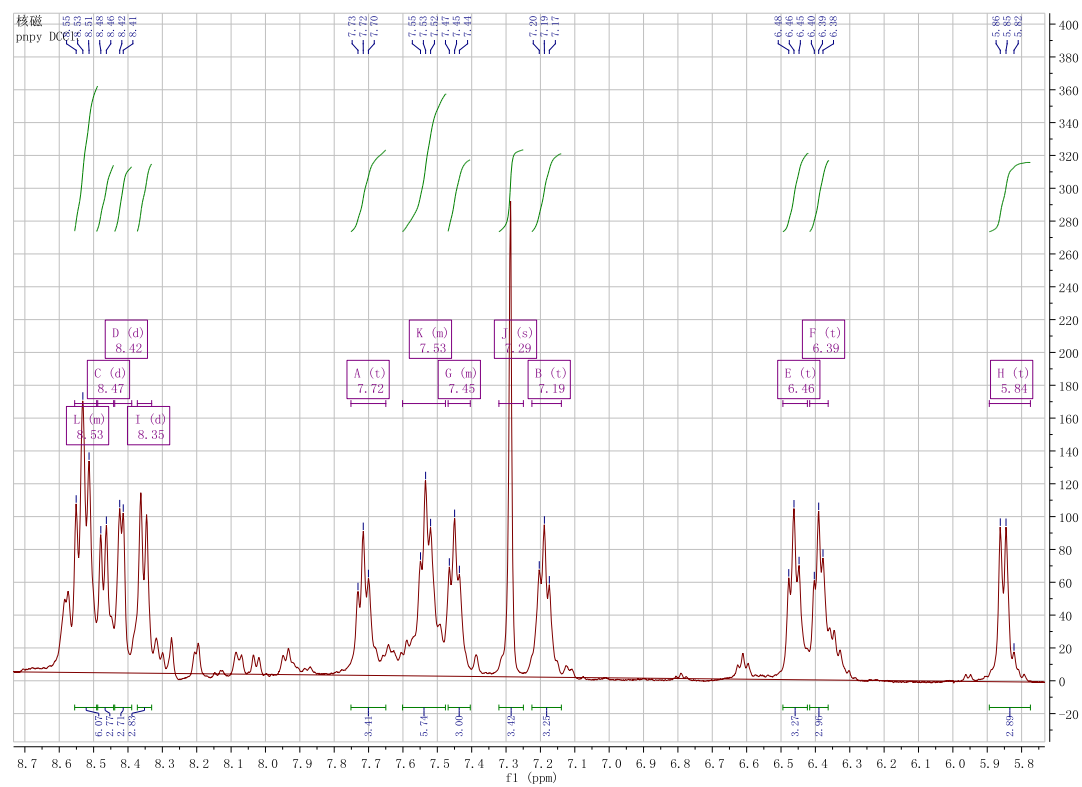


Fig. S11. The ¹H NMR spectrum of Ir(pnpy)₂tpip.

4. Table S1 1 Parameters associated with the crystal diffraction data collection for Ir(ppy)₂tpip.

	Ir(ppy) ₂ tpip
Formula	C ₄₆ H ₃₆ IrN ₃ O ₂ P ₂
FW	916.94
T (K)	296(2)
Wavelength (Å)	0.71073
Cryst syst	Monoclinic
Space group	P2(1)/c
<i>a</i> (Å)	15.5516(12)
<i>b</i> (Å)	11.1611(9)
<i>c</i> (Å)	23.4952(18)
α (deg)	90.00
β (deg)	106.5230(10)
γ (deg)	90.00
<i>V</i> (Å ³)	3909.7(5)
<i>Z</i>	4
ρ_{calcd} (g/cm ³)	1.558
μ (Mo K α) (mm ⁻¹)	3.539
<i>F</i> (000)	1824
Range of transm factors (deg)	1.37-28.28
Reflns collected	27514
Unique	9697
Data/restraints/params	9697/0/487
GOF on <i>F</i> ²	1.000
<i>R</i> ₁ ^{<i>a</i>} , <i>wR</i> ₂ ^{<i>b</i>} (<i>I</i> > 2 σ (<i>I</i>))	0.0383, 0.0766
<i>R</i> ₁ ^{<i>a</i>} , <i>wR</i> ₂ ^{<i>b</i>} (all data)	0.0561, 0.0801
CCDC NO.	966232

$$R_1^a = \Sigma ||F_o| - |F_c|| / \Sigma F_o$$

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

5. Table S2 Selected bond lengths(Å) and angles(deg) for Ir(ppy)₂tpip

Ir(1)-C(46)	1.992(4)
Ir(1)-N(2)	2.030(4)
Ir(1)-C(35)	1.989(4)
Ir(1)-O(1)	2.219(2)
Ir(1)-N(3)	2.029(3)
Ir(1)-O(2)	2.199(3)
C(46)-Ir(1)-C(35)	92.17(17)
C(46)-Ir(1)-N(2)	98.66(17)
C(46)-Ir(1)-O(1)	92.00(14)
C(46)-Ir(1)-N(3)	80.81(17)
C(46)-Ir(1)-O(2)	170.53(16)
C(35)-Ir(1)-N(2)	80.72(15)
C(35)-Ir(1)-O(1)	172.73(14)
C(35)-Ir(1)-N(3)	98.06(15)
C(35)-Ir(1)-O(2)	87.74(14)
N(3)-Ir(1)-N(2)	178.67(12)
N(3)-Ir(1)-O(1)	88.49(12)
N(2)-Ir(1)-O(1)	92.76(12)
N(3)-Ir(1)-O(2)	89.83(13)
N(2)-Ir(1)-O(2)	90.67(12)
O(1)-Ir(1)-O(2)	89.13(10)

6. TG-DSC curves of complexes

6.1 Ir(ppy)₂tpip

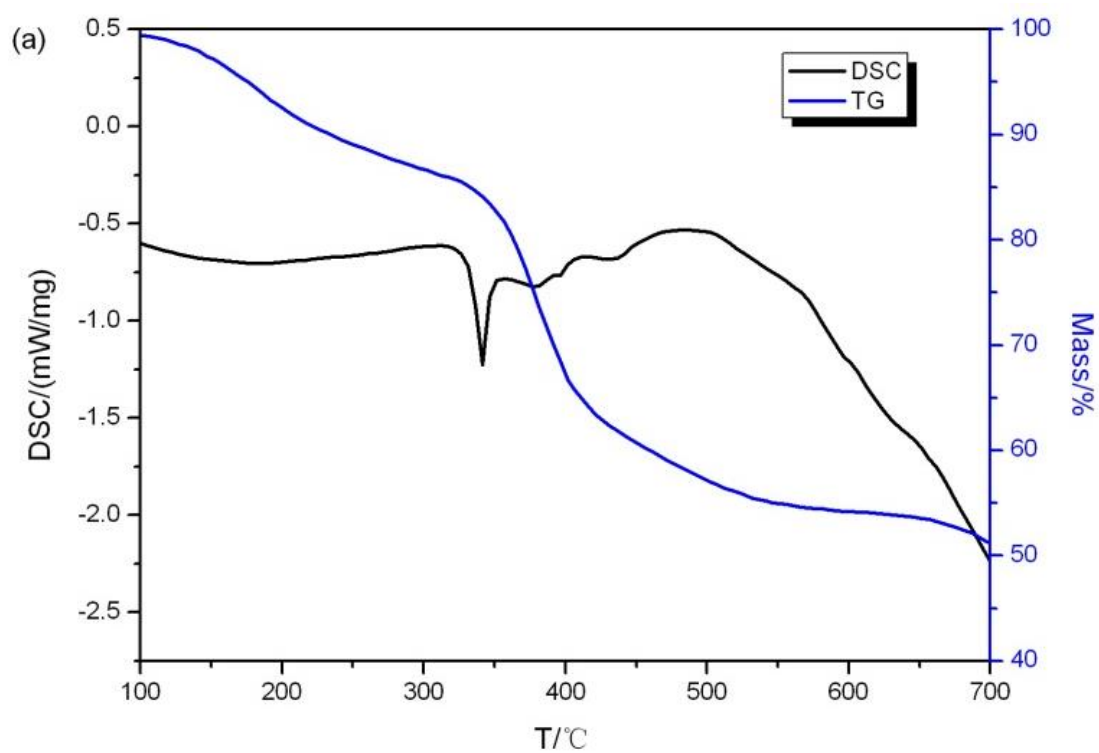


Fig. S12. The TG-DSC curves of Ir(ppy)₂tpip.

6.2 Ir(npv)₂tpip

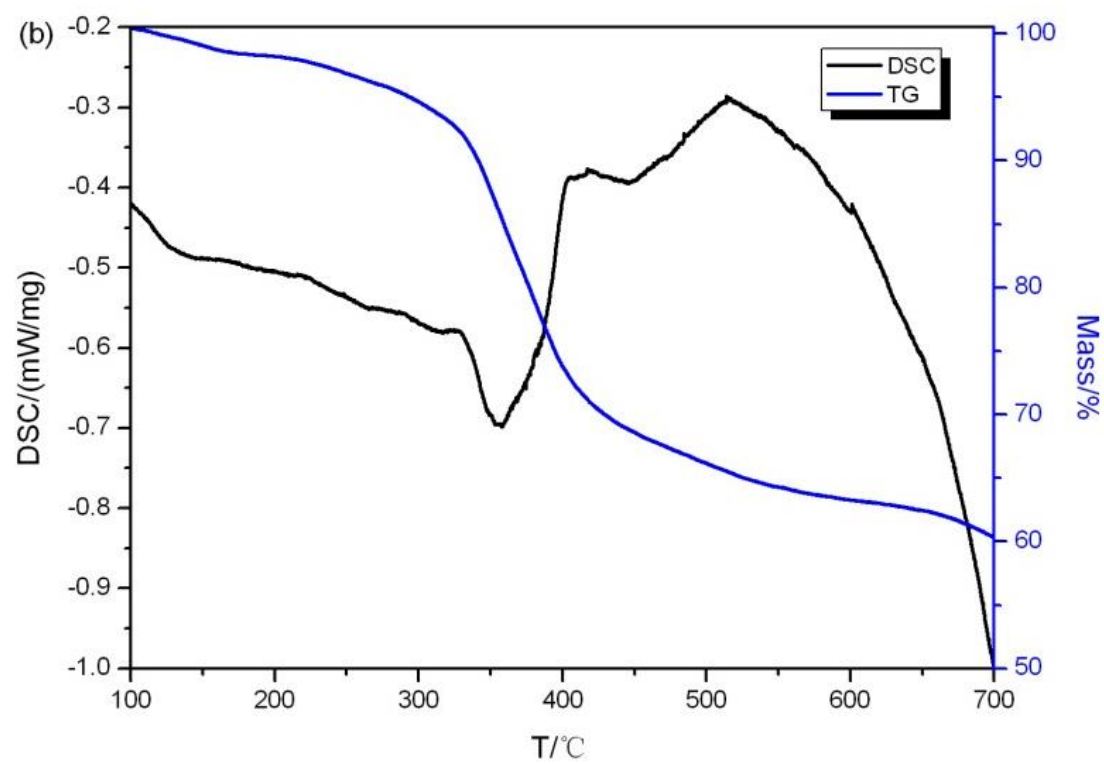


Fig. S13. The TG-DSC curves of Ir(npv)₂tpip.

6.3 Ir(pnpy)₂tpip

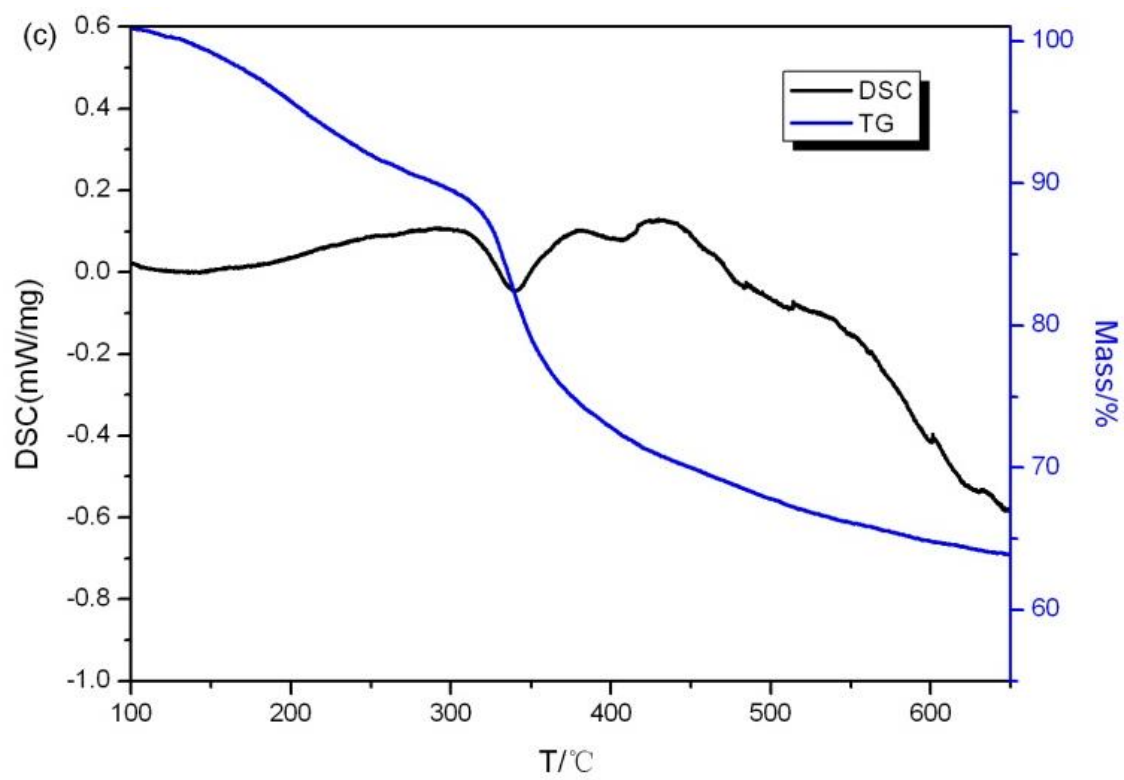


Fig. S14. The TG-DSC curves of Ir(pnpy)₂tpip.