

Electronic Supplementary Information (ESI) for

**Conjugated microporous polycarbazoles containing
tris(2-phenylpyridine)iridium(III) complex:
Phosphorescence, porosity, and heterogeneous
organic photocatalysis**

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Table S1. Crystal data and structure parameters for **Ir(*p*-PPC)₃**

Identification	code	Ir(<i>p</i>-PPC)₃
Empirical formula		C ₇₂ H ₄₅ Ir N ₃
Formular weight		1144.31
Crystal system		Cubic
Space group		Pa-3
Unit cell dimensions	<i>a</i> (Å)	22.825(3)
	<i>b</i> (Å)	22.825(3)
	<i>c</i> (Å)	22.825(3)
	α (°)	90.000
	β (°)	90.000
	γ (°)	90.000
Volume (Å ³)		11891(2)
<i>Z</i>		8
T (K)		293(2)
Calculated density (mg/m ³)		1.278
Absorption coefficient (mm ⁻¹)		2.288
Theta range for data collection (°)		1.55-27.56
Limiting indices		-29<= <i>h</i> <=29
		-29<= <i>k</i> <=29
		-29<= <i>l</i> <=29
Data / restraints / parameters		4585 / 0 /229
Final	R indices	<i>R</i> ₁ 0.0239
[I>2sigma(I)] ^a		<i>wR</i> ₂ 0.0873
R indices (all data)	<i>R</i> ₁	0.0255
	<i>wR</i> ₂	0.0891
Largest diff. Peak and hole (e·Å ⁻³)		3.182 and -0.480

Table S2. Selected bond lengths [Å] and angles [°] for **Ir(*p*-PPC)₃**

Ir(1)–C(11)	2.011(7)	Ir(1)–N(1)	2.135(6)	N(1)–C(5)	1.335(10)	N(1)–C(1)	1.338(10)
C(11)–Ir(1)–C(11)	93.2(3)	C(11)–Ir(1)–N(1)	79.1	C(11)–Ir(1)–N(1)	169.4	C(11)–Ir(1)–N(1)	94.5
C(5)–N(1)–C(1)	119.5(7)	C(5)–N(1)–Ir(1)	125.9(6)	C(1)–N(1)–Ir(1)	114.5(5)	C(6)–C(11)–Ir(1)	125.9(6)
C(10)–C(11)–Ir(1)	126.8(5)						

Table S3. Porosity Properties of **CPOP-20** and **CPOP-21**

Polymers	S_{BET}^a (m ² g ^{−1})	S_{Langmuir}^b (m ² g ^{−1})	S_{micro}^c (m ² g ^{−1})	V_{total}^d (cm ³ g ^{−1})	D_{pore}^e (nm)
CPOP-20	460	600	254	0.32	0.73
CPOP-21	480	610	308	0.38	0.68

^a Specific surface area calculated from the nitrogen adsorption isotherm using the BET method. ^b Specific surface area calculated from the nitrogen adsorption isotherm using the Langmuir method. ^c surface area calculated from the adsorption branch of the nitrogen adsorption–desorption isotherm using the t-plot method. ^d Total pore volume at $P/P_0=0.99$. ^e Data calculated from nitrogen adsorption isotherms with the NLDFT method.

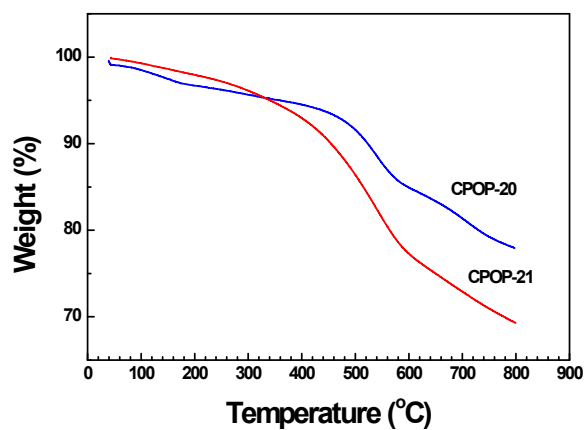


Fig. S1. Thermogravimetric analysis (TGA) curves for the **CPOP-20** and **CPOP-21** networks under a nitrogen atmosphere with a heating rate of 10 °C/min.

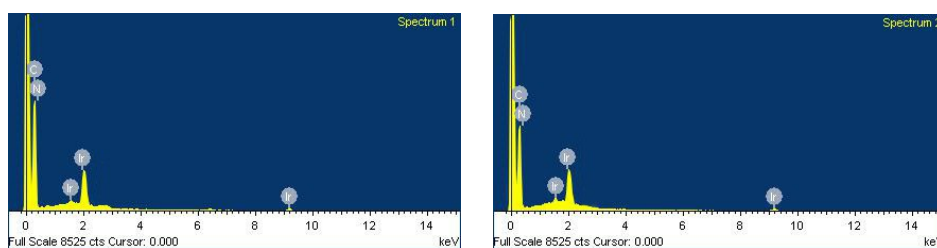


Fig. S2. Energy dispersive X-ray spectrum of **CPOP-20** and **CPOP-21**.

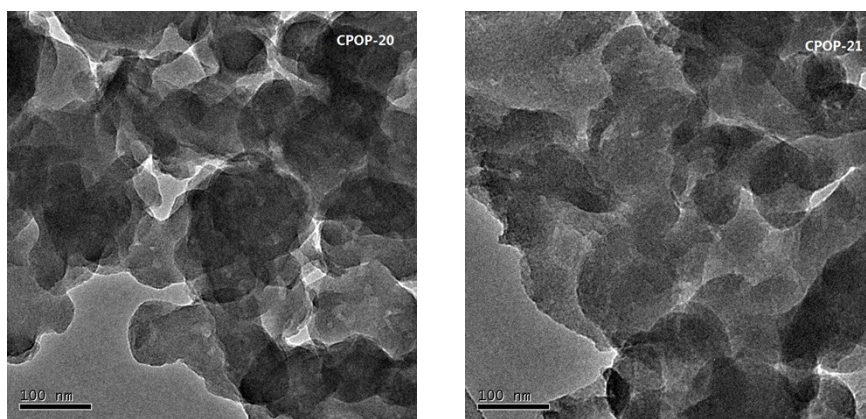


Fig. S3. TEM images of **CPOP-20** and **CPOP-21**

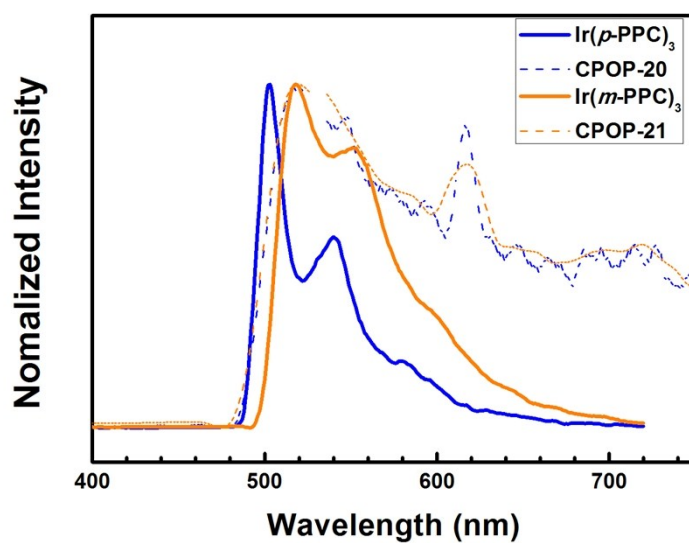


Fig. S4. Photoluminescence emission spectra of the complexes in dichloromethane solution and the polymers in solid state at 77 K.

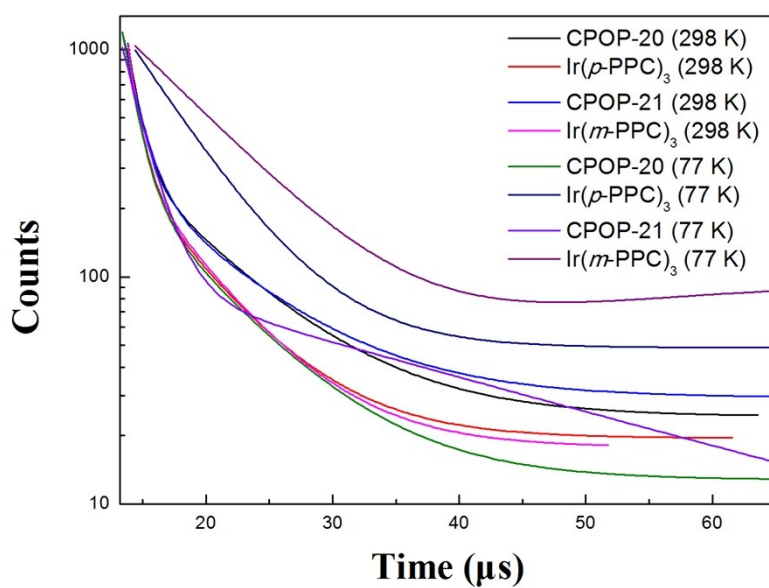


Fig. S5. The photoluminescence decay curves of the complexes in dichloromethane and the polymers in the solid state at 298 K and 77K.

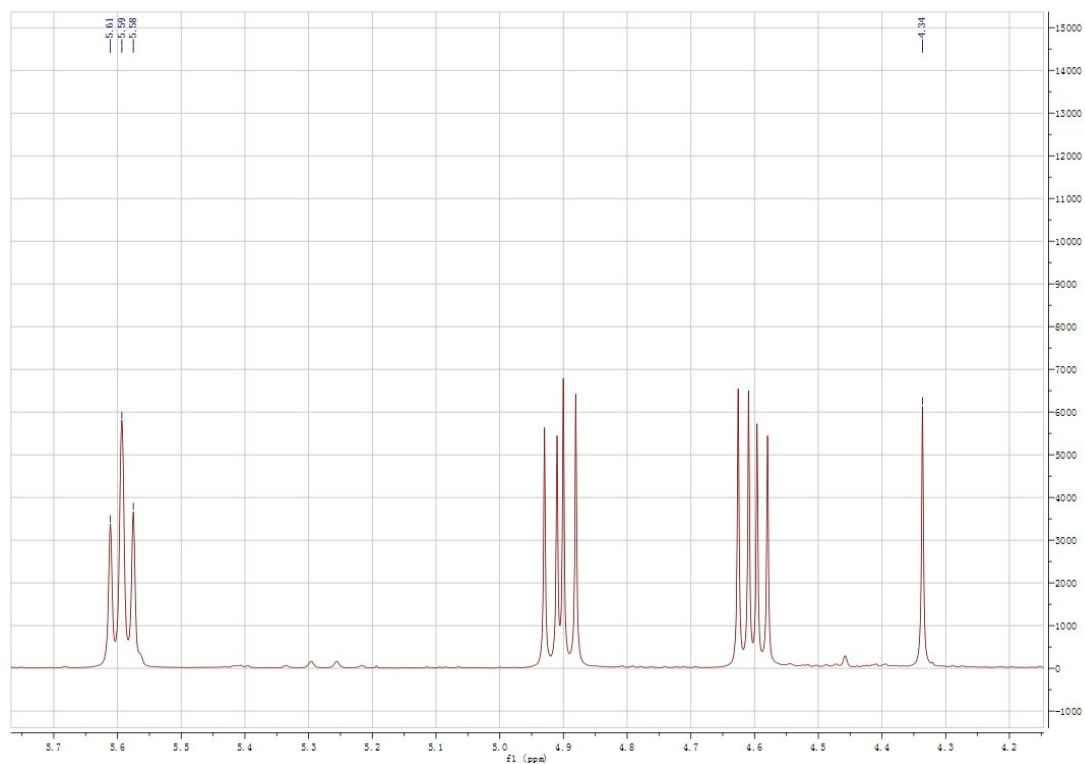
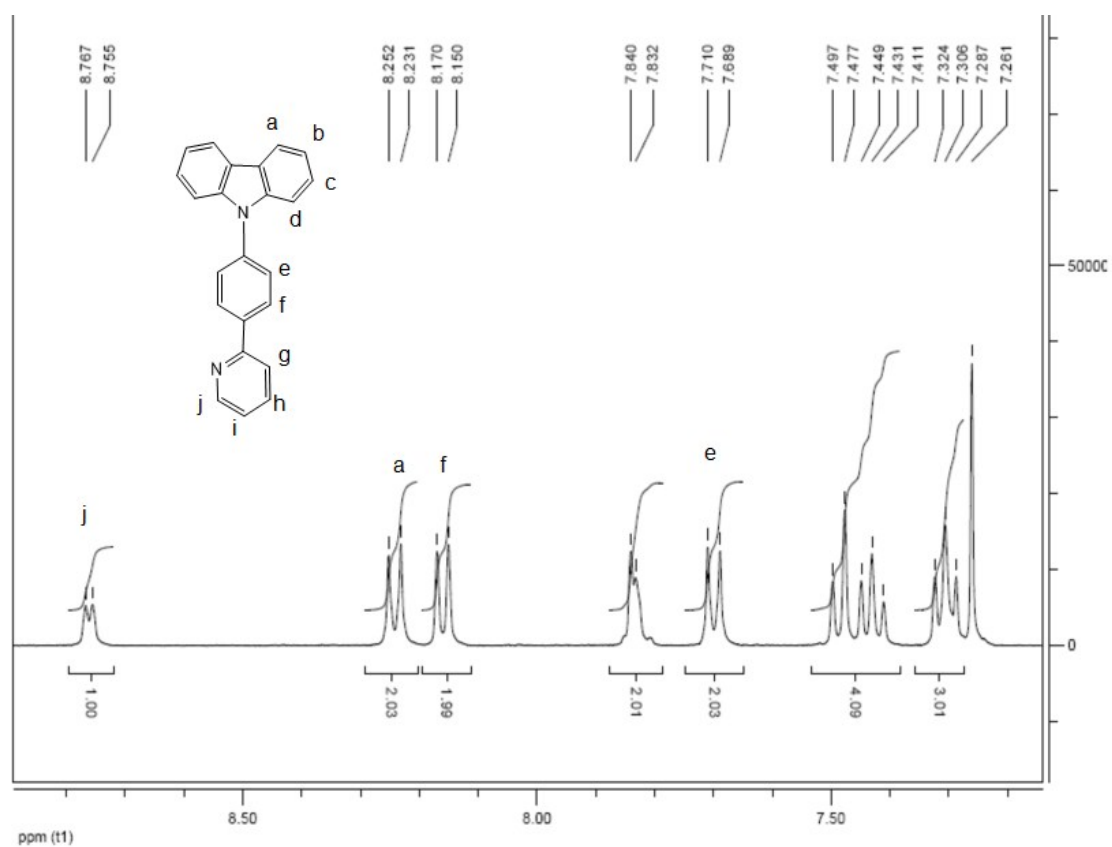


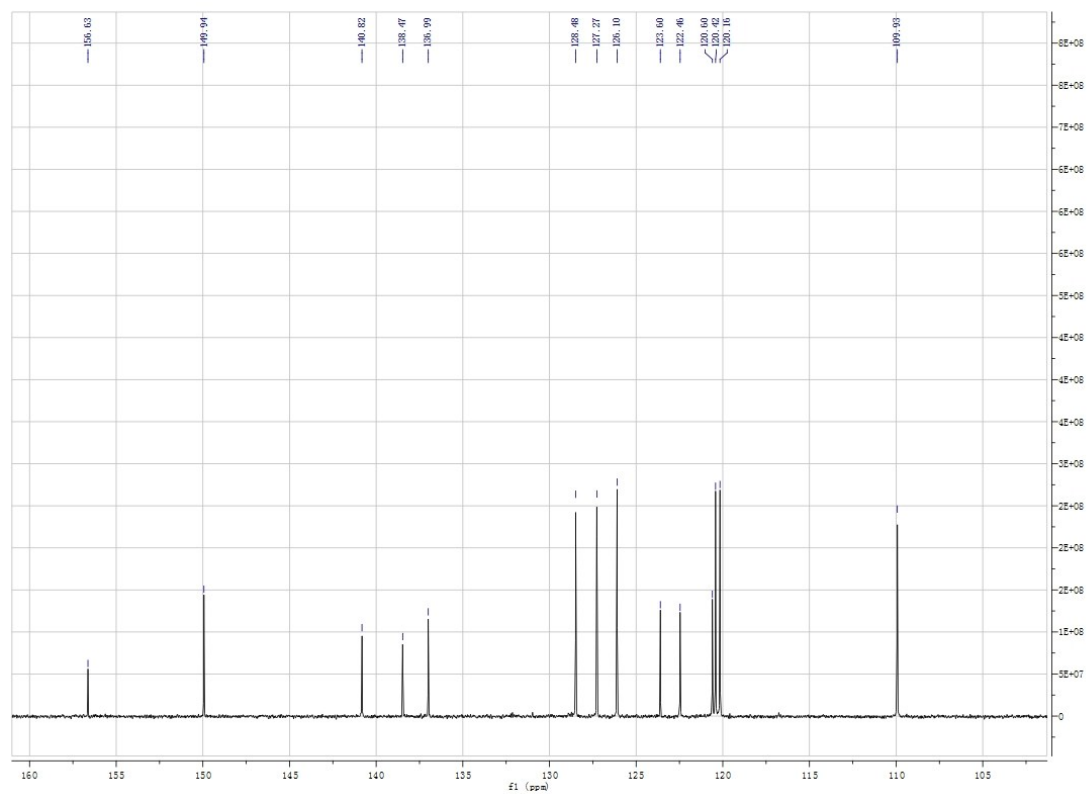
Fig. S6. ^1H -NMR spectrum for aza-Henry reaction of **CPOP-20** with substrate **a**. The substrate peak at 4.34 ppm and the product peak at 5.59 ppm were used to calculate the conversion.

Table S4. Comparison of the catalysis property among various porous materials for the aza-Henry reaction

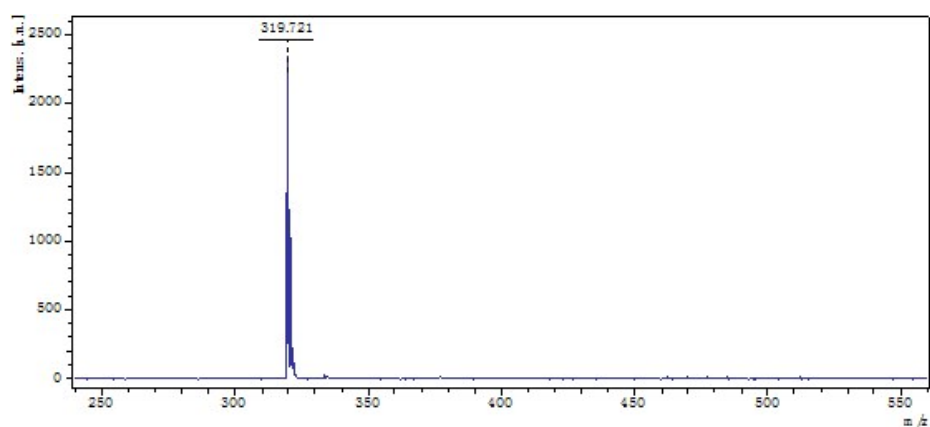
Entry	Catalyst	ref	Substrate	Conv'n (%)
1	CPOP-20	–	a	88
2	CPOP-20	–	c	94
3	CPOP-21	–	a	70
4	CPOP-21	–	c	89
5	MOF 5	34	a	59
6	MOF 5	34	c	96
7	MOF 6	34	a	86
8	MOF 6	34	c	97
9	RB-CMP1	15	a	95
10	RB-CMP1	15	c	97
11	Ir-PCP	35	a	94
12	Ir-PCP	35	c	91



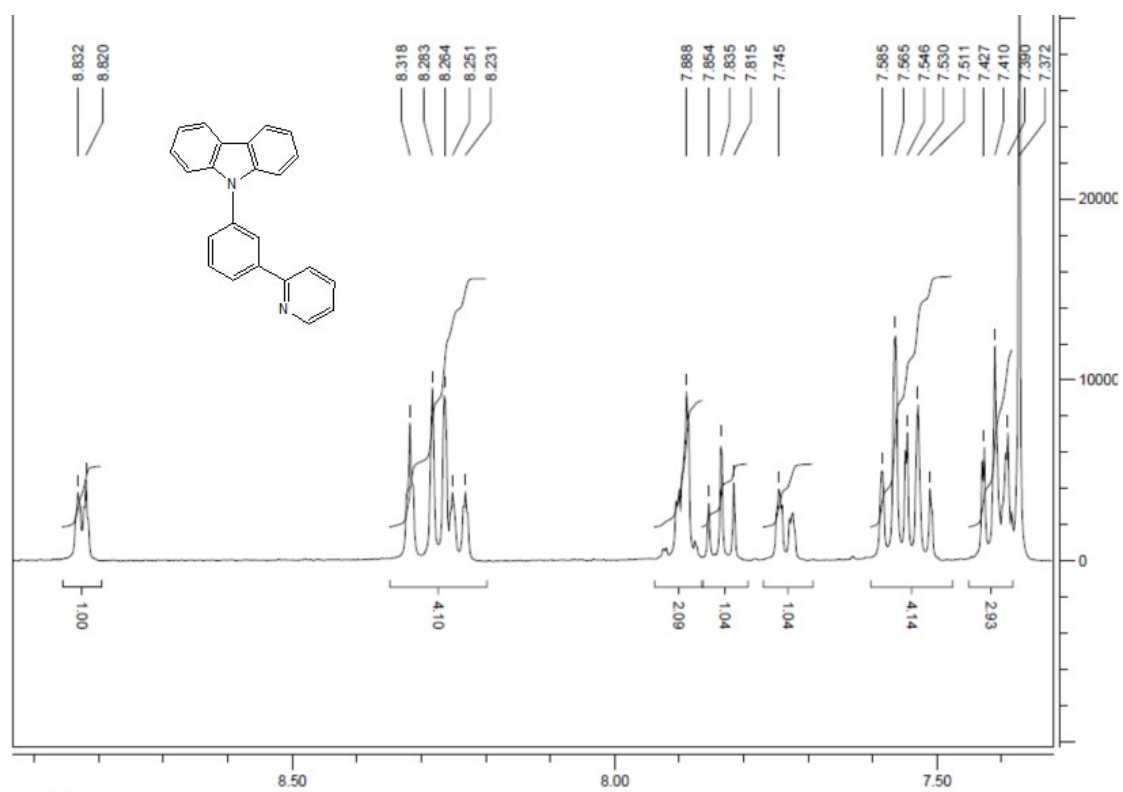
¹H NMR of ligand *p*-PPC



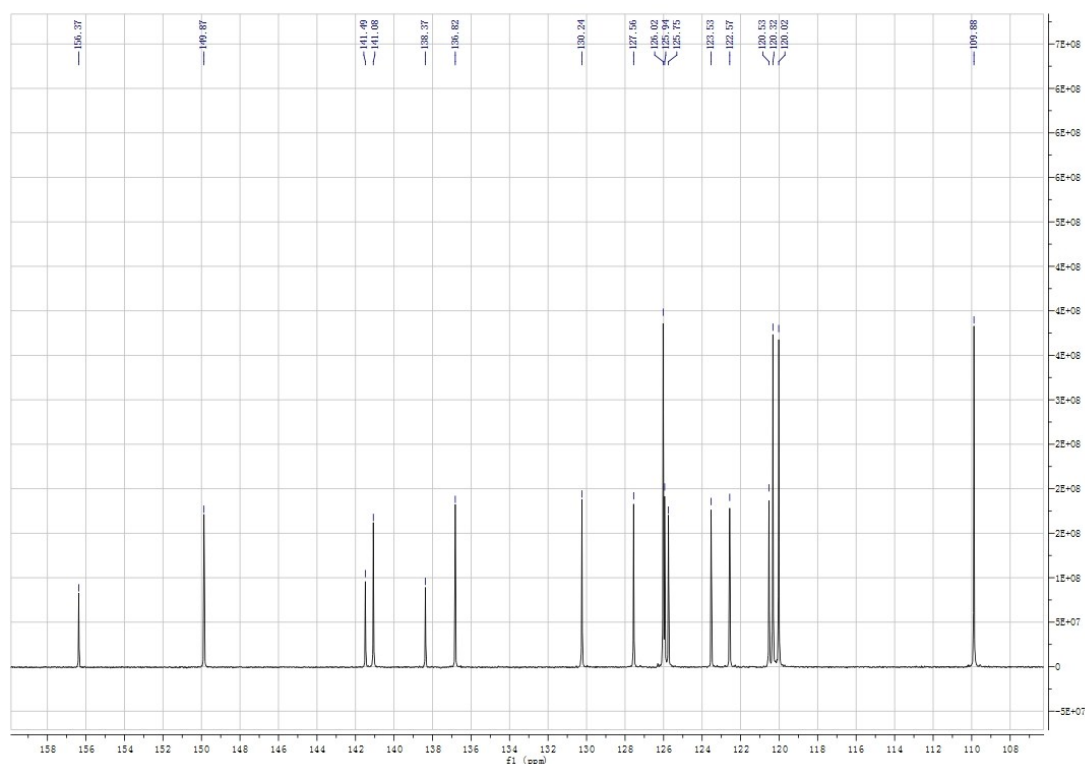
¹³C NMR of ligand *p*-PPC



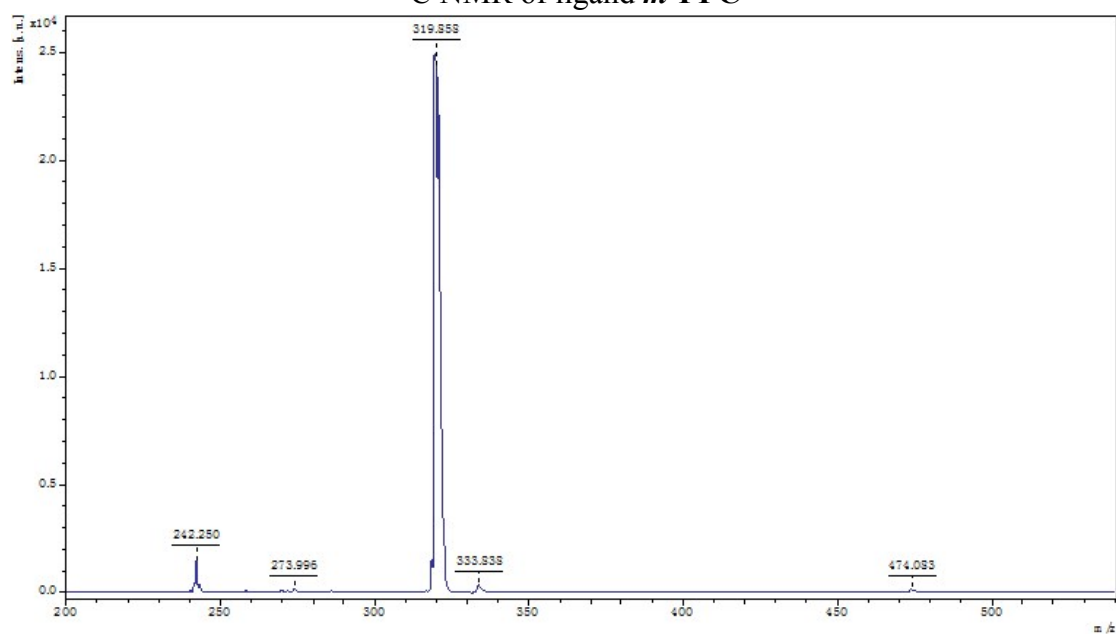
MS of ligand *p*-PPC



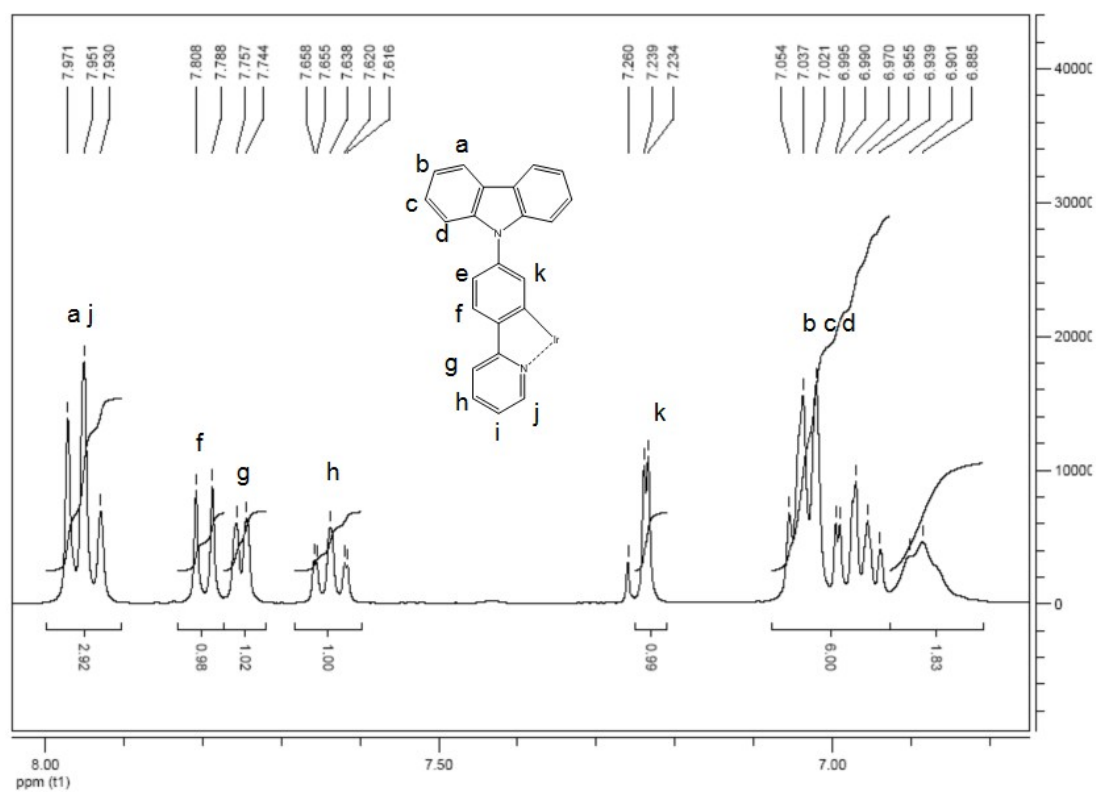
¹H NMR of ligand *m*-PPC



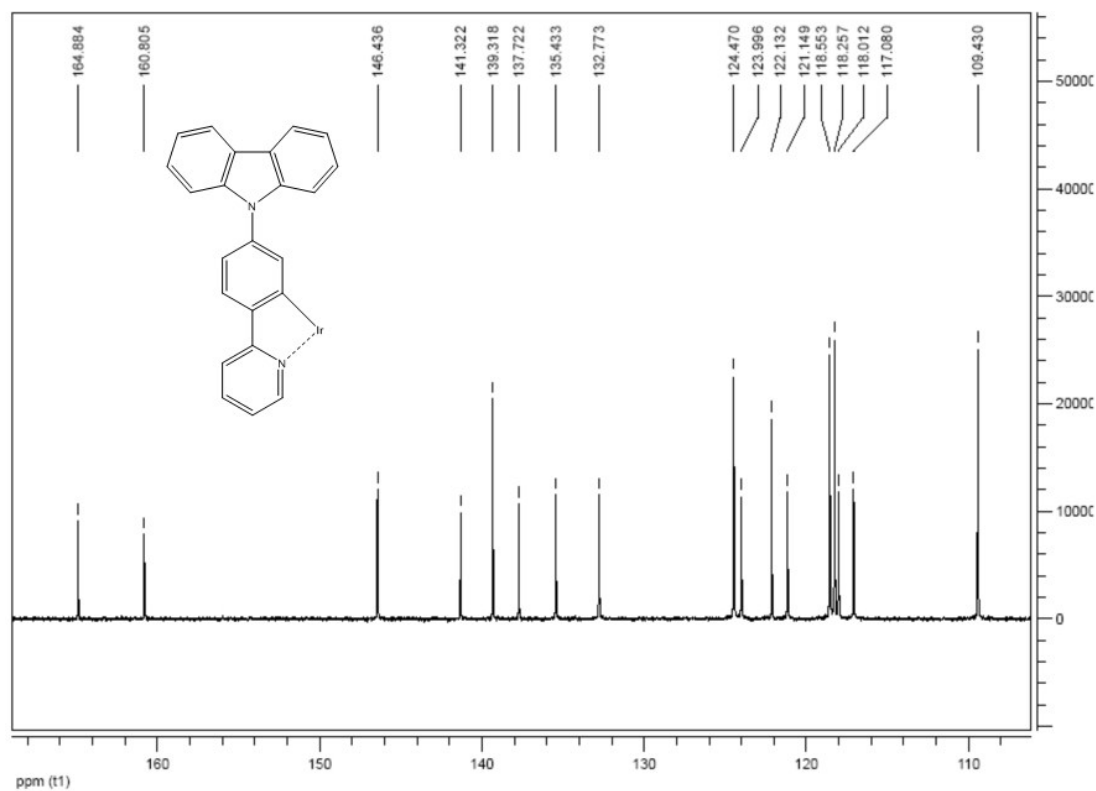
¹³C NMR of ligand *m*-PPC



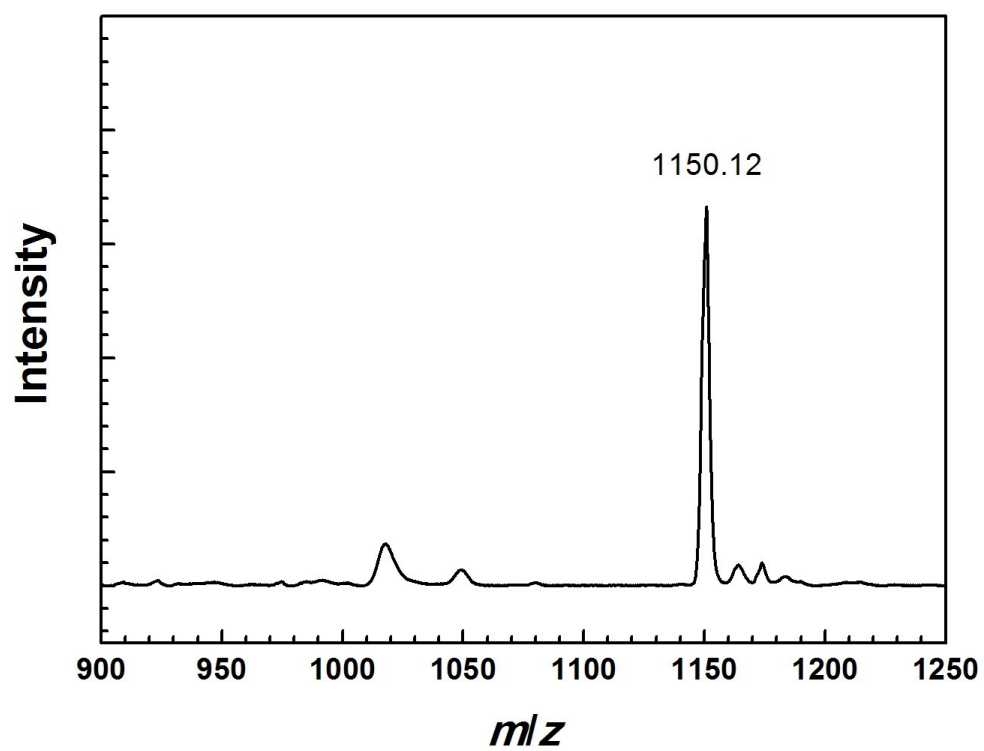
MS of ligand *m*-PPC



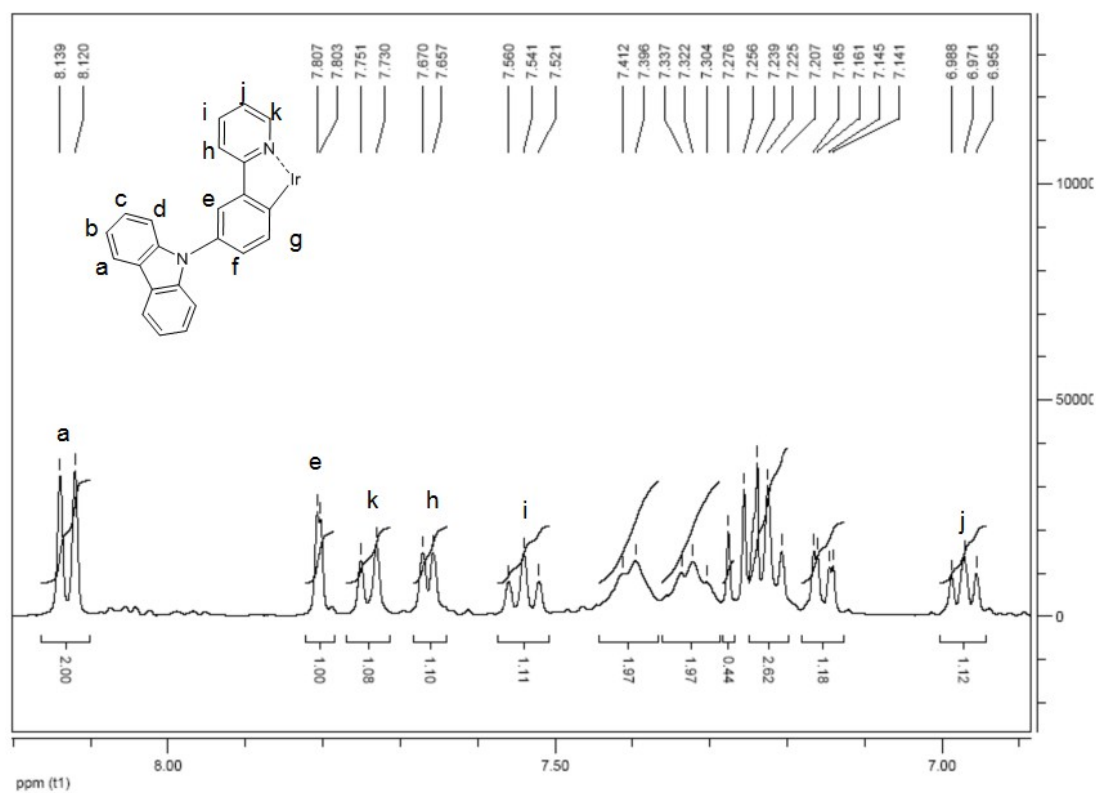
¹H NMR of Ir(*p*-PPC)₃



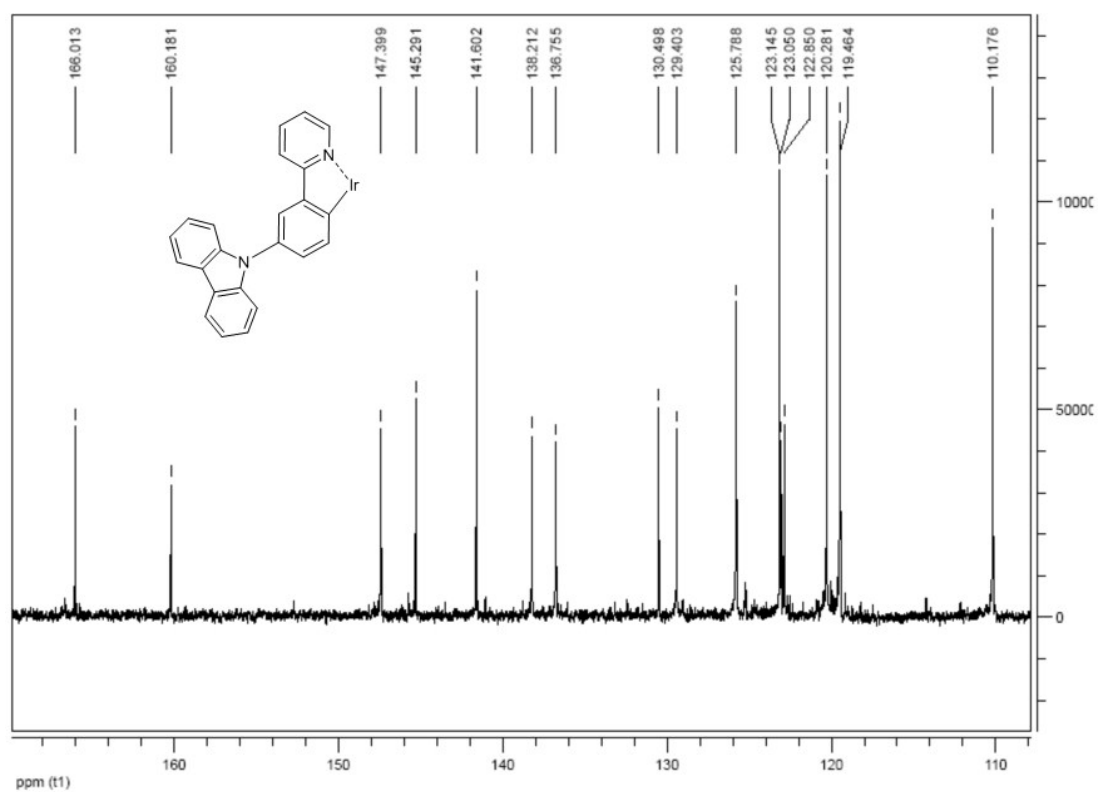
¹³C NMR of Ir(*p*-PPC)₃



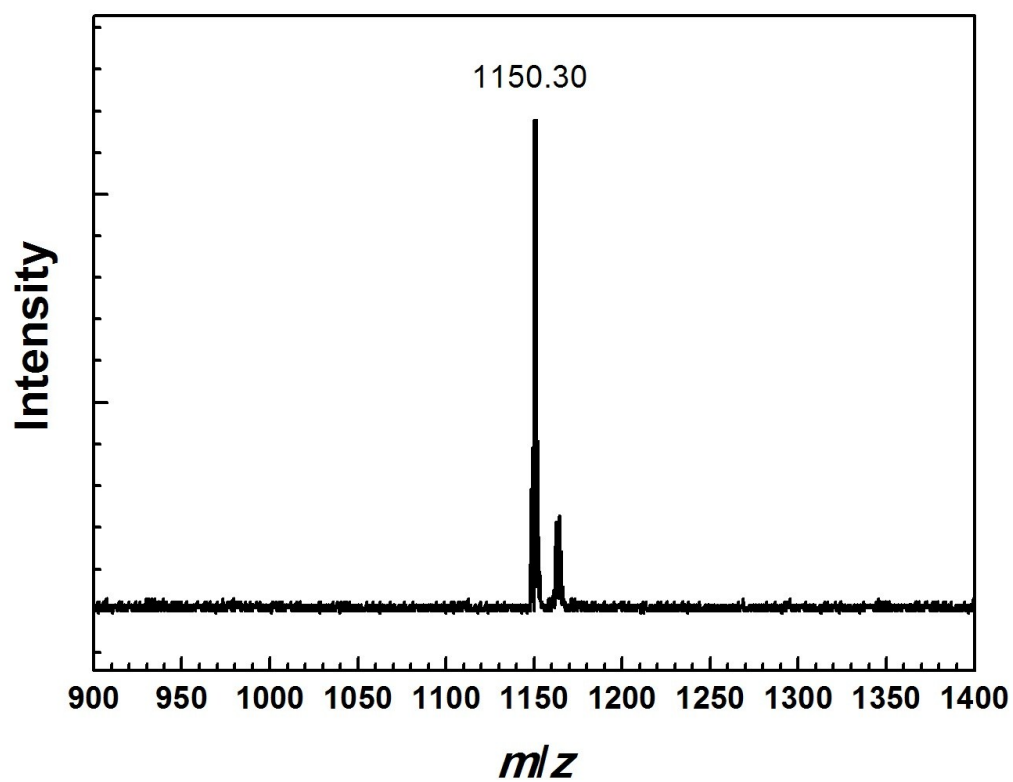
MS of $\text{Ir}(p\text{-PPC})_3$



^1H NMR of $\text{Ir}(m\text{-PPC})_3$



¹³C NMR of Ir(*m*-PPC)₃



MS of Ir(*m*-PPC)₃