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Support information

Synthesis and luminescent properties of three excellent yellow emissive Cu(I) complexes based on the diphosphine ligand and diimine ligand

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Caption of Figure

Caption of Table

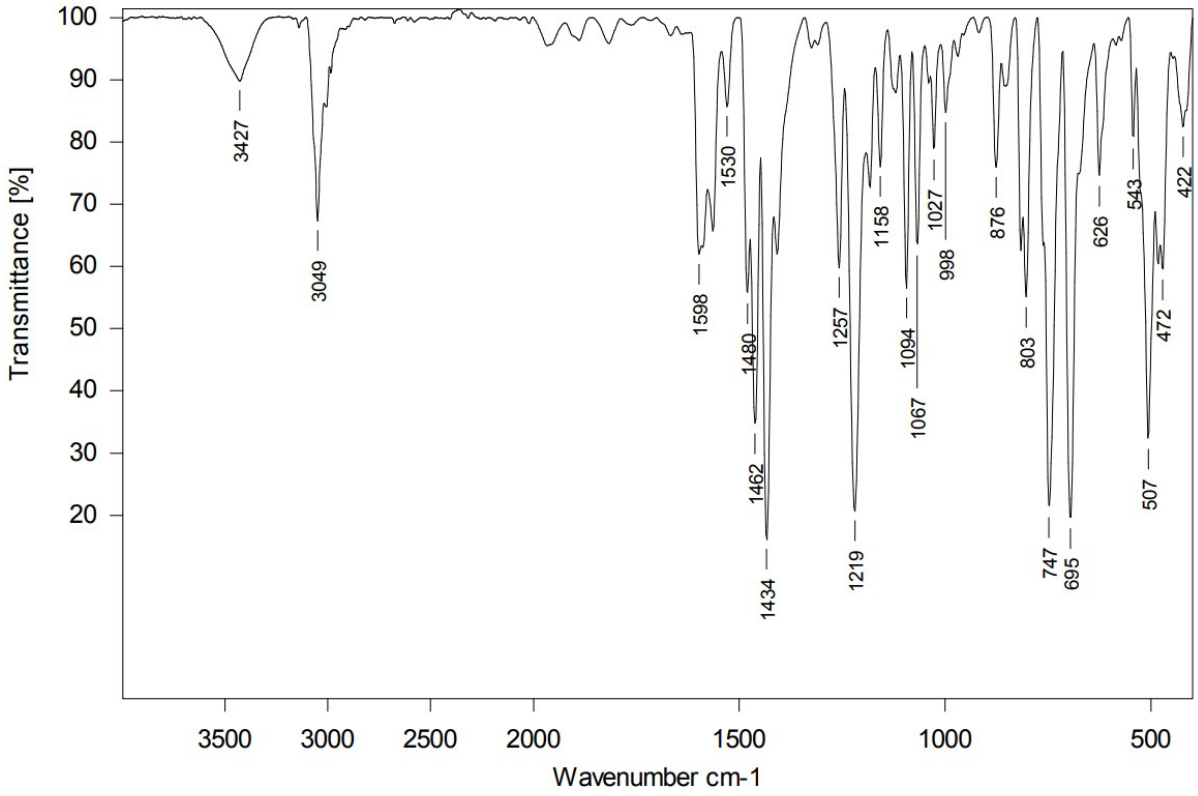

Fig. S1 The IR spectra for complex **1**

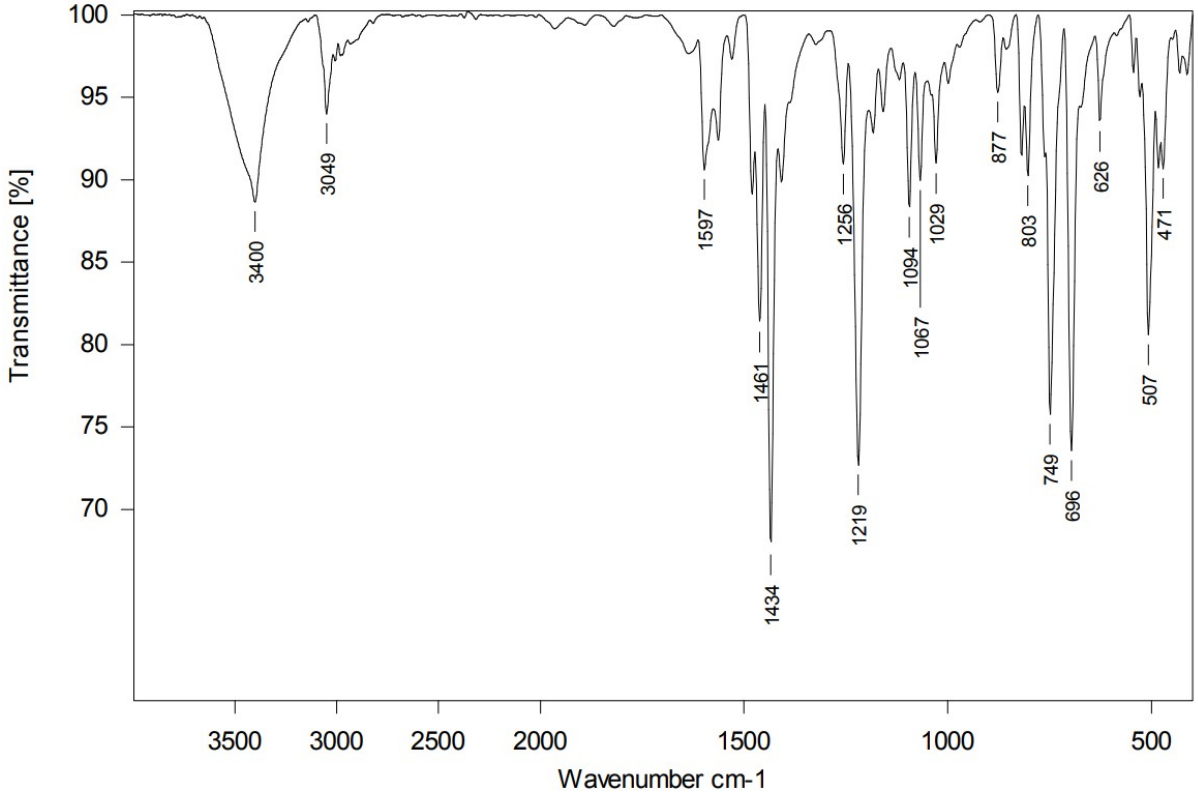

Fig. S2 The IR spectra for complex **2**

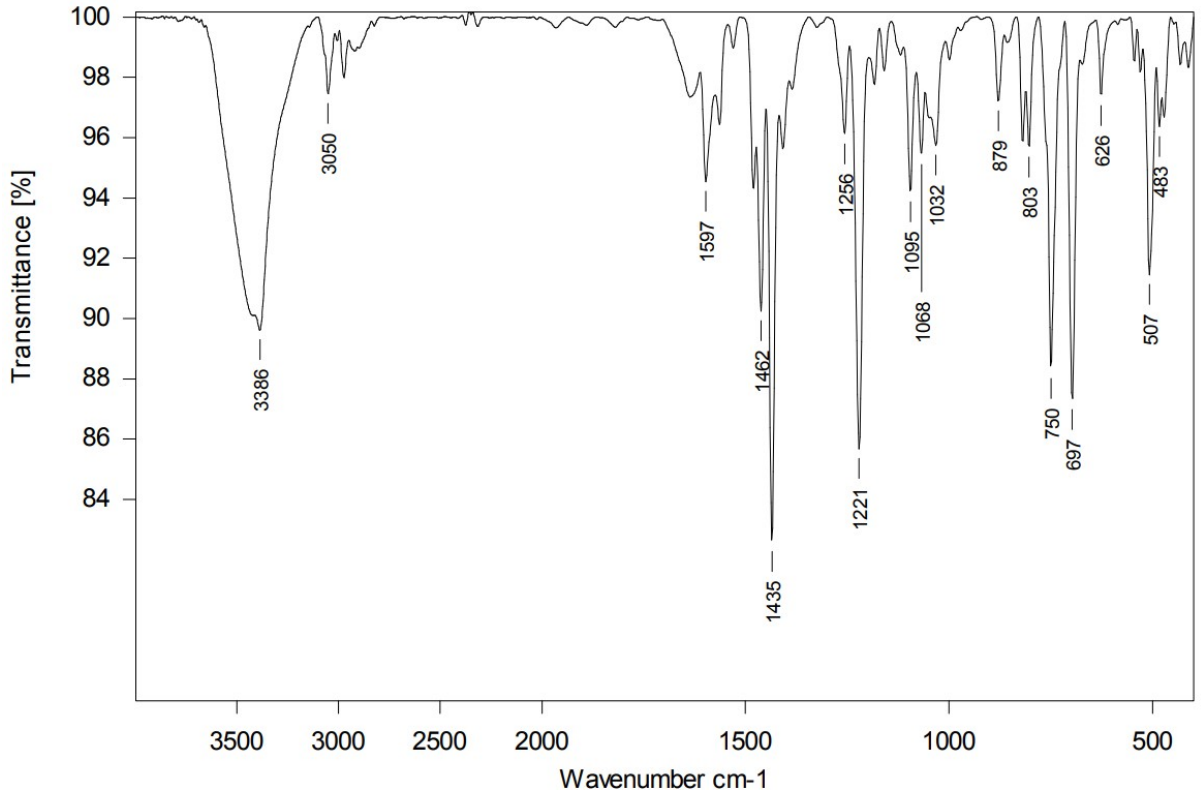

Fig. S3 The IR spectra for complex **3**

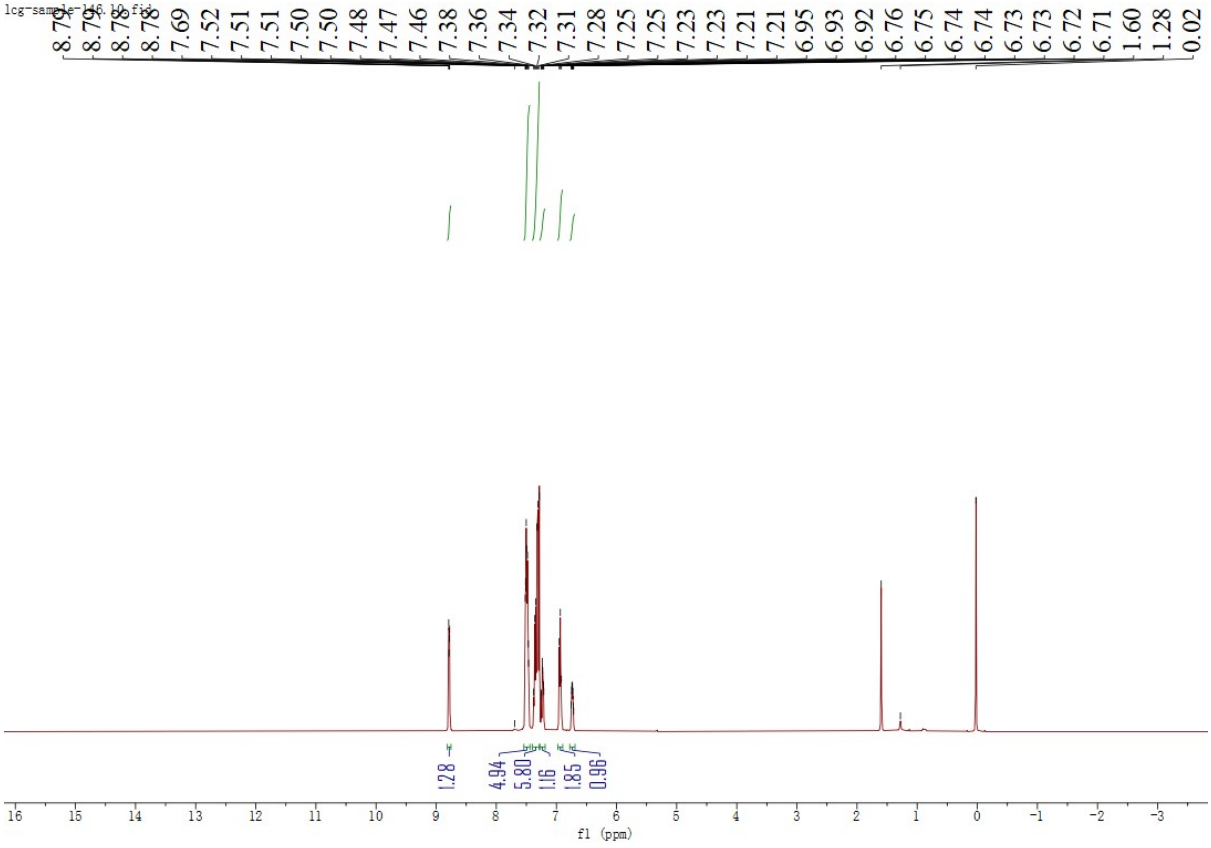

Fig. S4 The ^{1}H NMR spectra for complex **1**

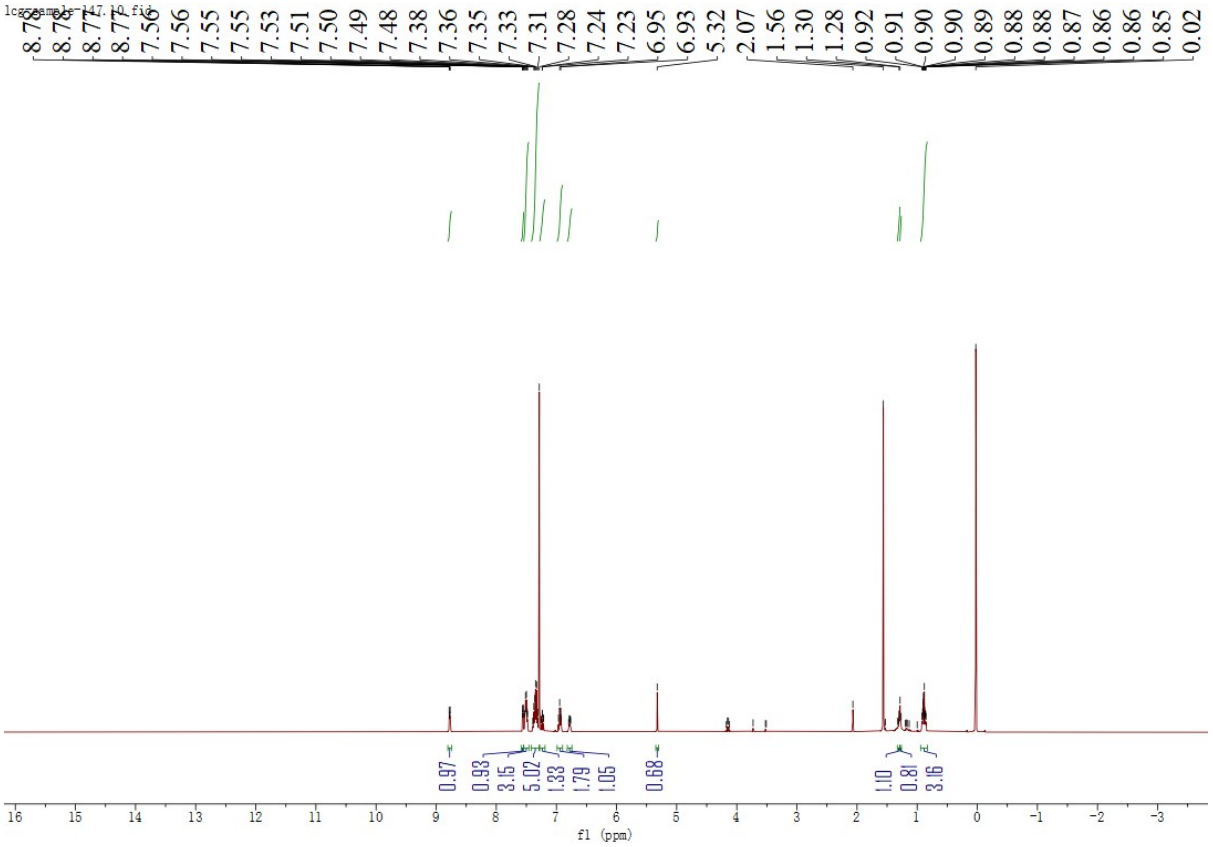

Fig. S5 The ^{1}H NMR spectra for complex **2**

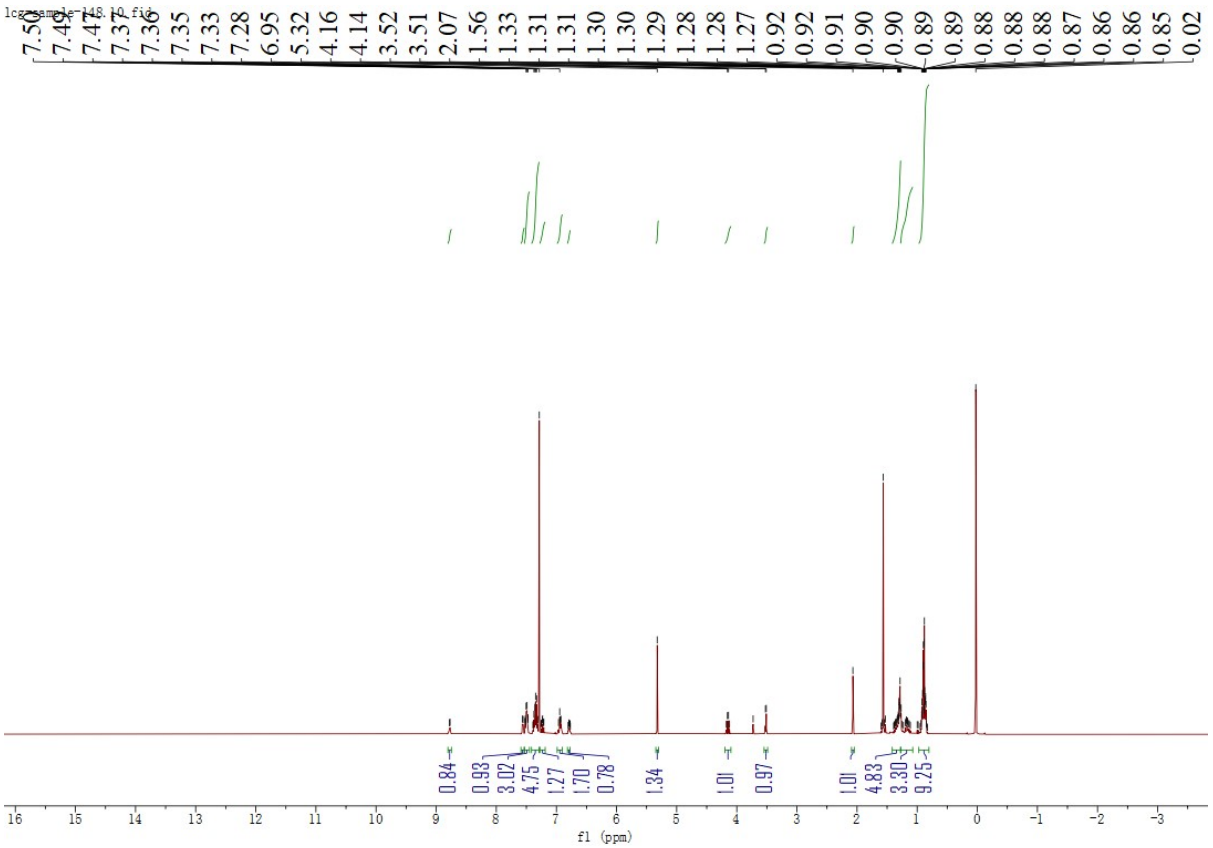

Fig. S6 The ^{1}H NMR spectra for complex **3**

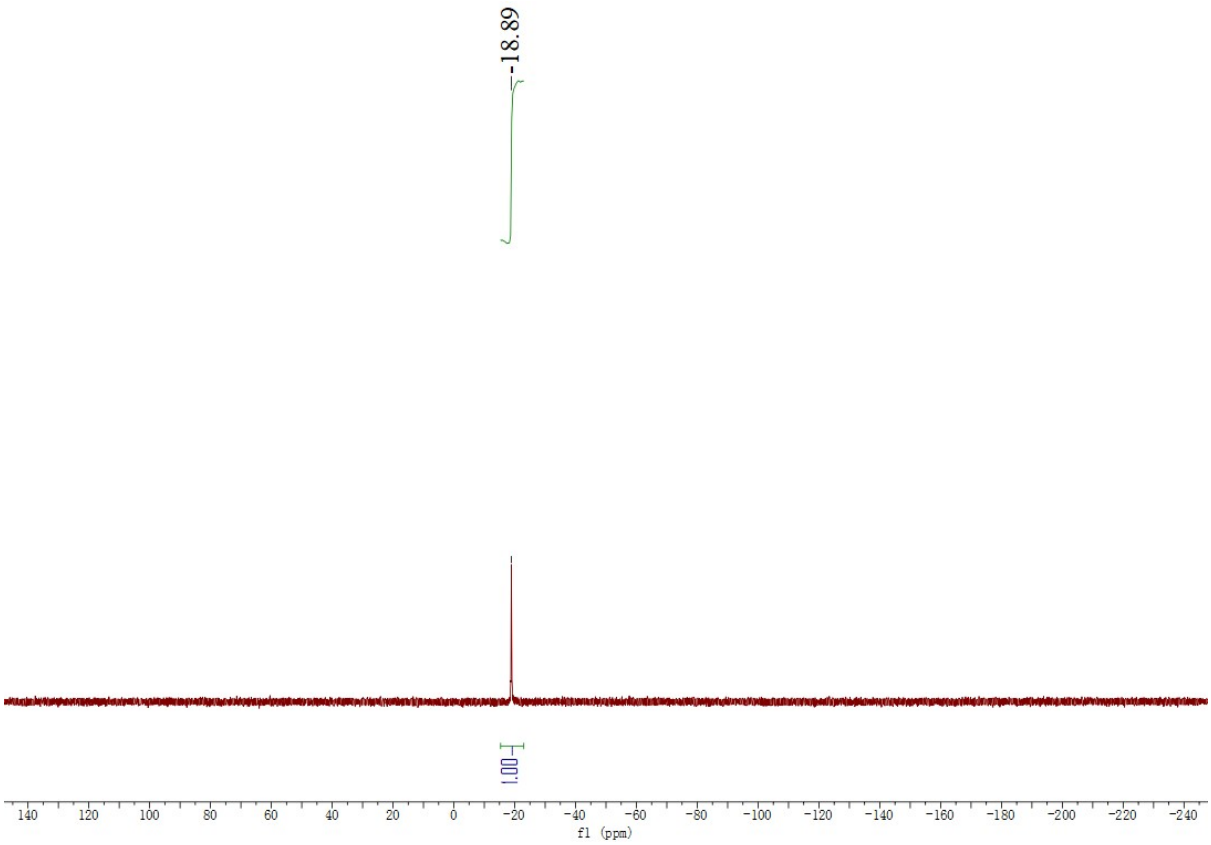

Fig. S7 The ^{31}P NMR spectra for complex **1**

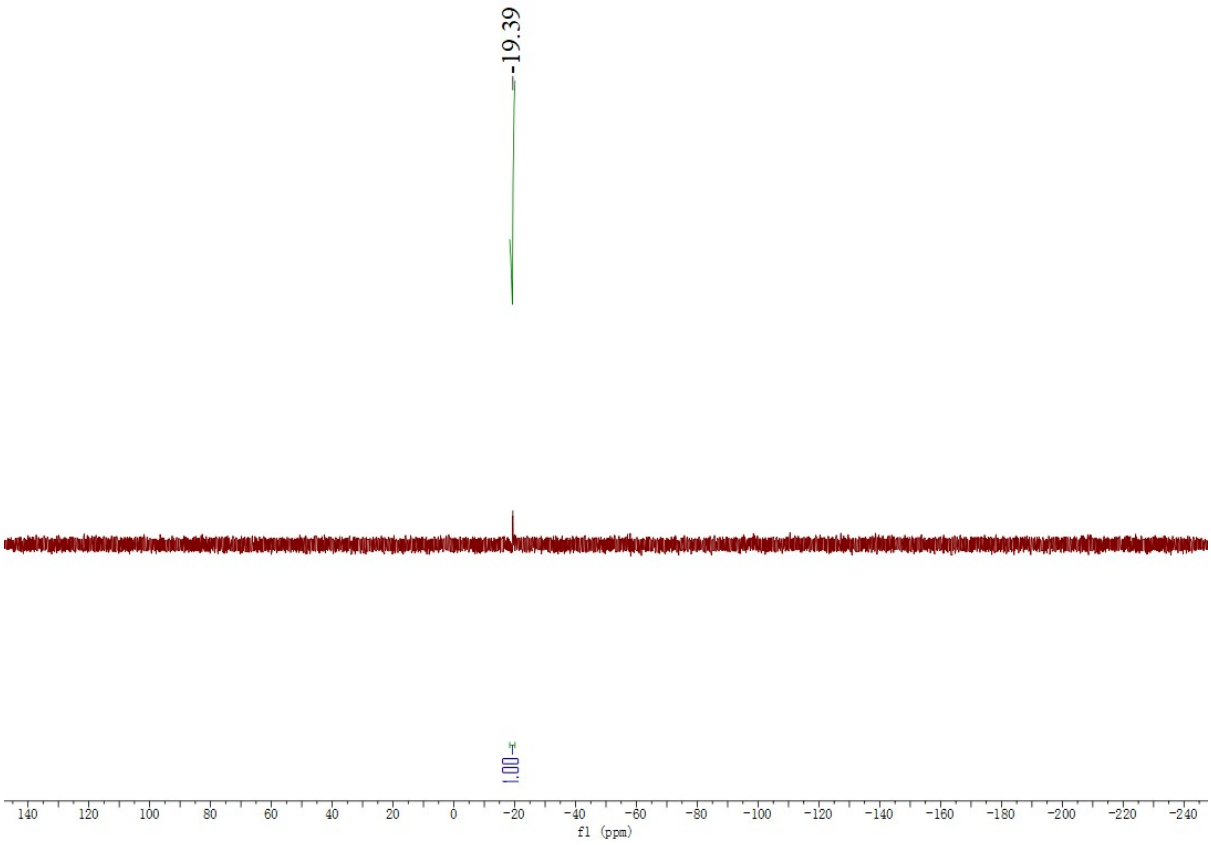

Fig. S8 The ^{31}P NMR spectra for complex **2**

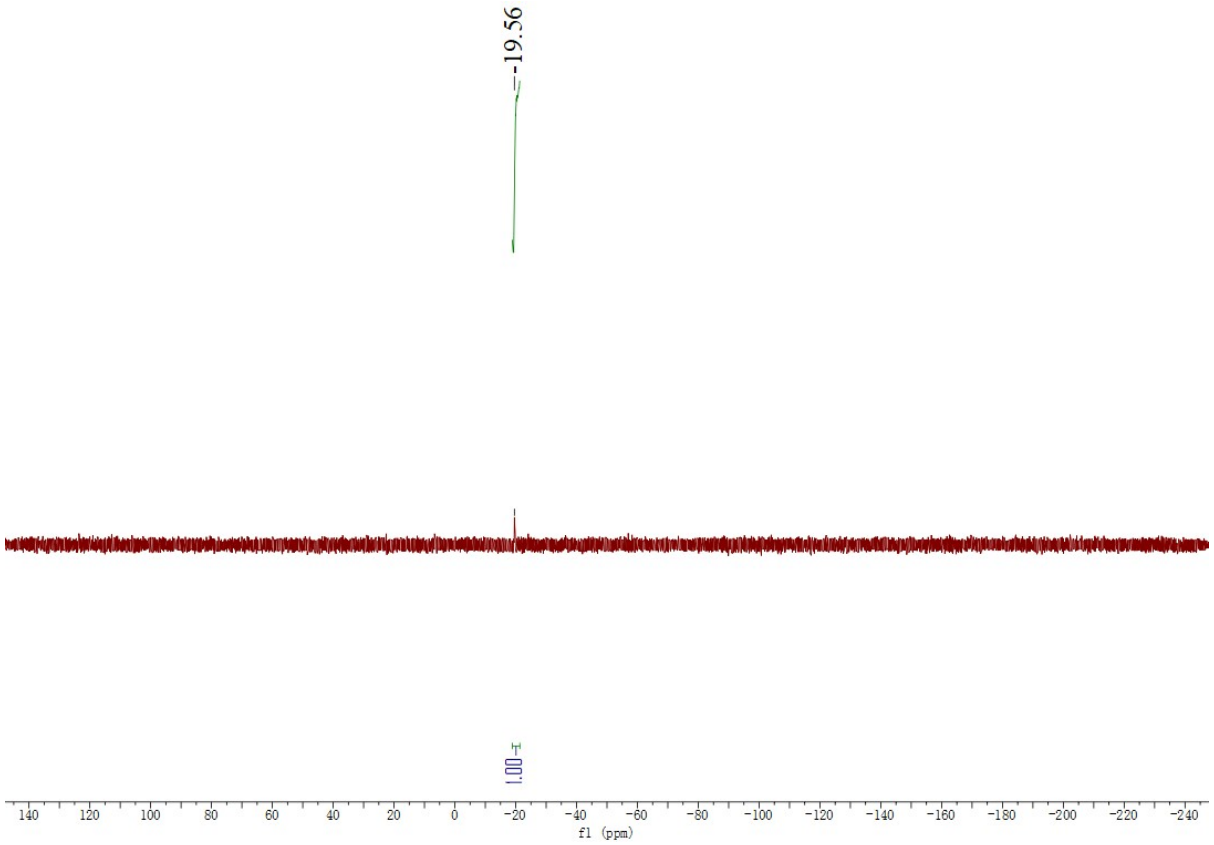

Fig. S9 The ^{31}P NMR spectra for complex **3**

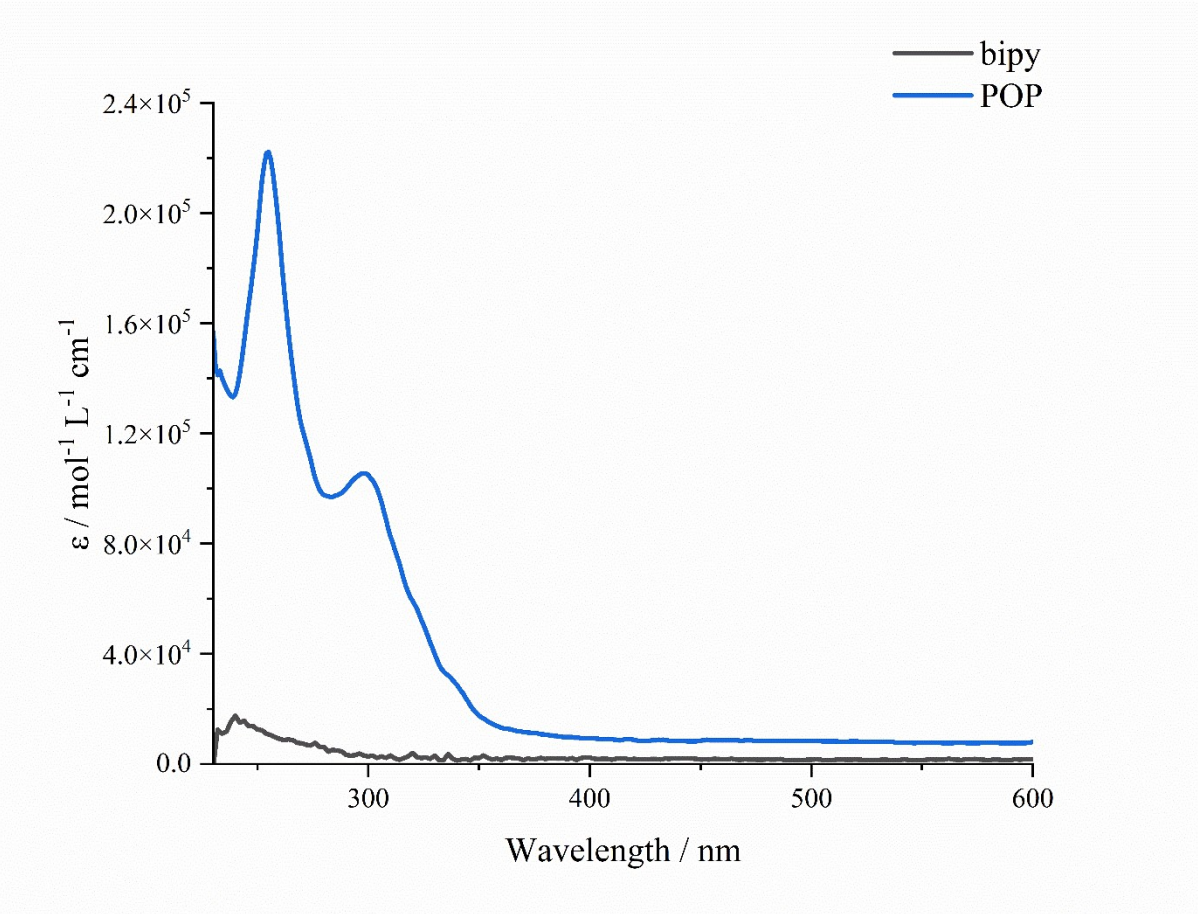

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Fig. S10 UV-vis spectra of bipy and POP at room temperature

Table. S1 Selected bond lengths (Å) and angles (º) for complexes **1-3.**

1			
Cu(1)-P(1)	2.3057(9)	P(1)-Cu(1)-P(2)	112.30(3)
Cu(1)-P(2)	2.2645(9)	P(1)-Cu(1)-I(1)	107.80(3)
Cu(1)-I(1)	2.6115(6)	P(1)-Cu(1)-N(1)	106.53(8)
Cu(1)-N(1)	2.1056(24)	P(2)-Cu(1)- I(1)	114.09(3)
		P(2)-Cu(1)-N(1)	109.73(7)
		I(1)-Cu(1)-N(1)	105.93(7)
2			
Cu(1)-P(1)	2.2734(9)	P(1)-Cu(1)-P(2)	111.45(3)
Cu(1)-P(2)	2.2837(9)	P(1)-Cu(1)-Br(1)	115.74(3)
Cu(1)-Br(1)	2.4551(6)	P(1)-Cu(1)-N(1)	109.42(8)
Cu(1)-N(1)	2.1231(24)	P(2)-Cu(1)-Br(1)	109.24(3)
		P(2)-Cu(1)-N(1)	105.86(7)
		Br(1)-Cu(1)-N(1)	104.46(8)
3			
Cu(1)-P(1)	2.2726(10)	P(1)-Cu(1)-P(2)	111.58(3)
Cu(1)-P(2)	2.2578(8)	P(1)-Cu(1)-Cl(1)	106.24(4)
Cu(1)-Cl(1)	2.3357(11)	P(1)-Cu(1)-N(1)	108.68(8)
Cu(1)-N(1)	2.0785(25)	P(2)-Cu(1)-Cl(1)	116.95(4)
		P(2)-Cu(1)-N(1)	110.97(8)
		Cl(1)-Cu(1)-N(1)	101.74(8)

Table. S2 Intermolecular weak interactions for complexes **1** and **3.**

	Cg(i)/C-H→Cg(i)/(A)	Cg	Symmetry code	Cg(A)/H···Cg(B)/Å
1	C38-H38A→Cg(6)	C25-C26-C27-C28-C29-C30	x, -1+y, z	2.87
3	Cg(4)···Cg(6)	Cg(4): C7-C8-C9-C10-C11-C12 Cg(6): C19-C20-C21-C22-C23-C24	x, y, z	3.8358
	C16-H16→Cg(6)	C19-C20-C21-C22-C23-C24	x, 1/2-y, -1/2+z	2.85
	O2-H2A→Cl1	/	1-x, -y, 1-z	2.36
	C35-H35→Cl2	/	/	2.79
	C47-H47B→Cl1	/	1-x, 1/2+y, 1-z	2.67

Table. S3 The composition of the S-state HOMO and LUMO orbitals for **1**, **2** and **3** in the optimized S_0 structure.

		Cu / %	X/ %	Ligand N/ %	Ligand P/ %
Complex **1**	HOMO-6	27.70	6.61	3.26	62.42
	LUMO	2.73	0.02	90.34	6.90
Complex **2**	HOMO-6	35.34	7.92	4.50	52.24
	LUMO	3.24	0.01	89.54	7.21
Complex **3**	HOMO-3	43.06	2.11	5.56	49.27
	LUMO	2.26	0.03	92.52	5.19

Table. S4 Energy, oscillator strength and major contribution of the calculated transitions for complexes **1**-**3**.

	Energy		Oscillator strength	Contribution %			
1	2.1412 eV	579.04 nm	0.2957	**HOMO-6**	→	**LUMO**	**95.18**
2	2.1506 eV	576.50 nm	0.2599	HOMO-7	→	LUMO	5.73
				HOMO-6	→	**LUMO**	**89.87**
3	2.2058Ev	562.09 nm	0.1523	**HOMO-3**	→	**LUMO**	**85.11**
				HOMO	→	LUMO+1	4.78
				HOMO	→	LUMO+2	2.15