Electronic Supplementary Information (ESI)

Synthesis, structure, and photophysical properties of copper(I) triphenylphosphine complexes with functionalized 3-(2′-pyrimidinyl)-1,2,4-triazole ligands

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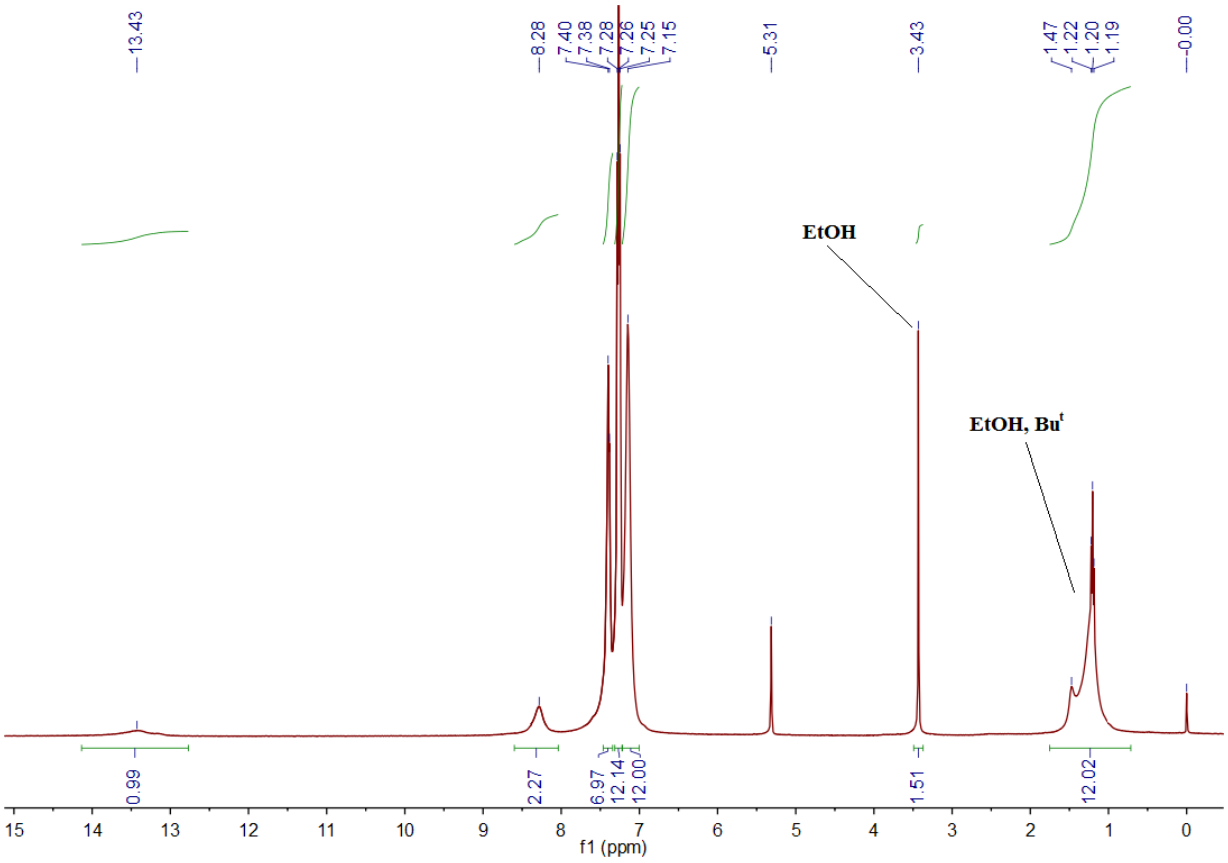


Fig. S1 ^{1}H NMR spectrum of **1** in CD_2Cl_2.

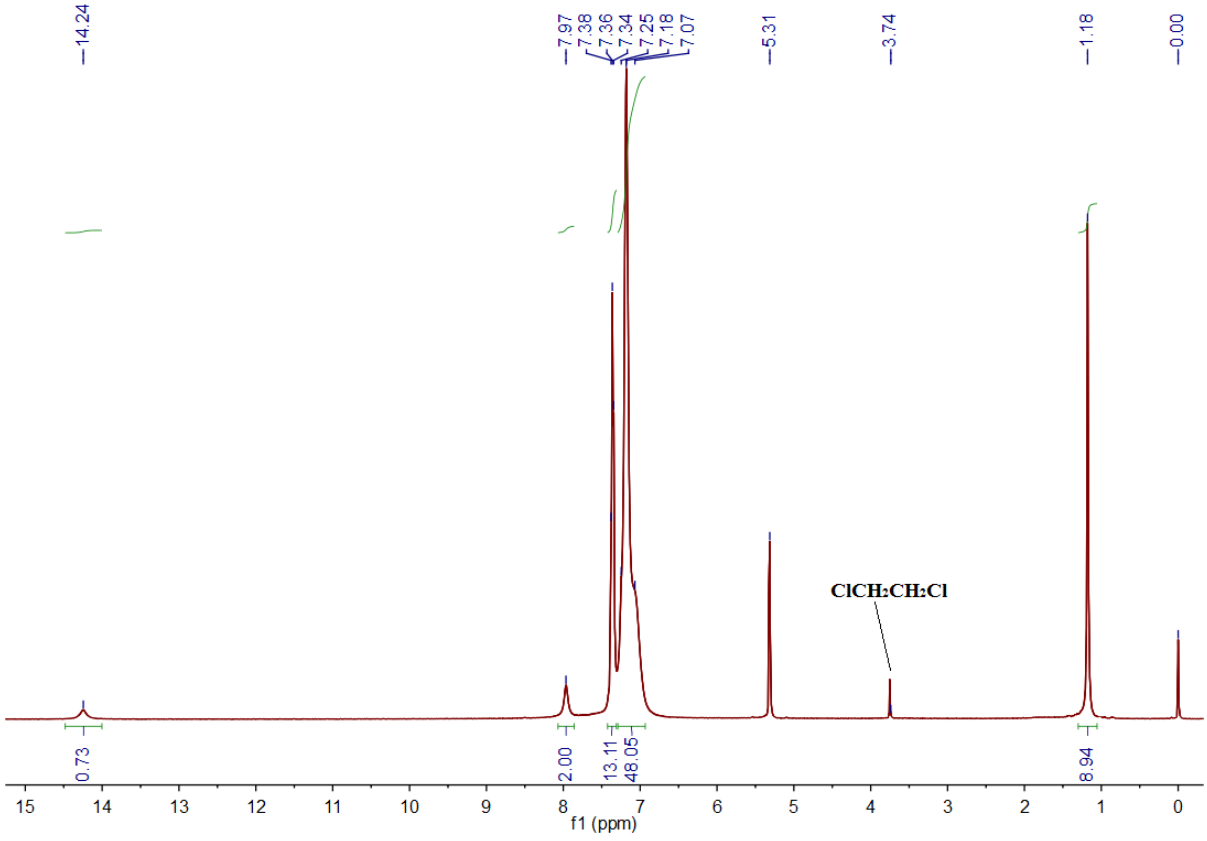


Fig. S2 ^{1}H NMR spectrum of **2** in CD_2Cl_2.

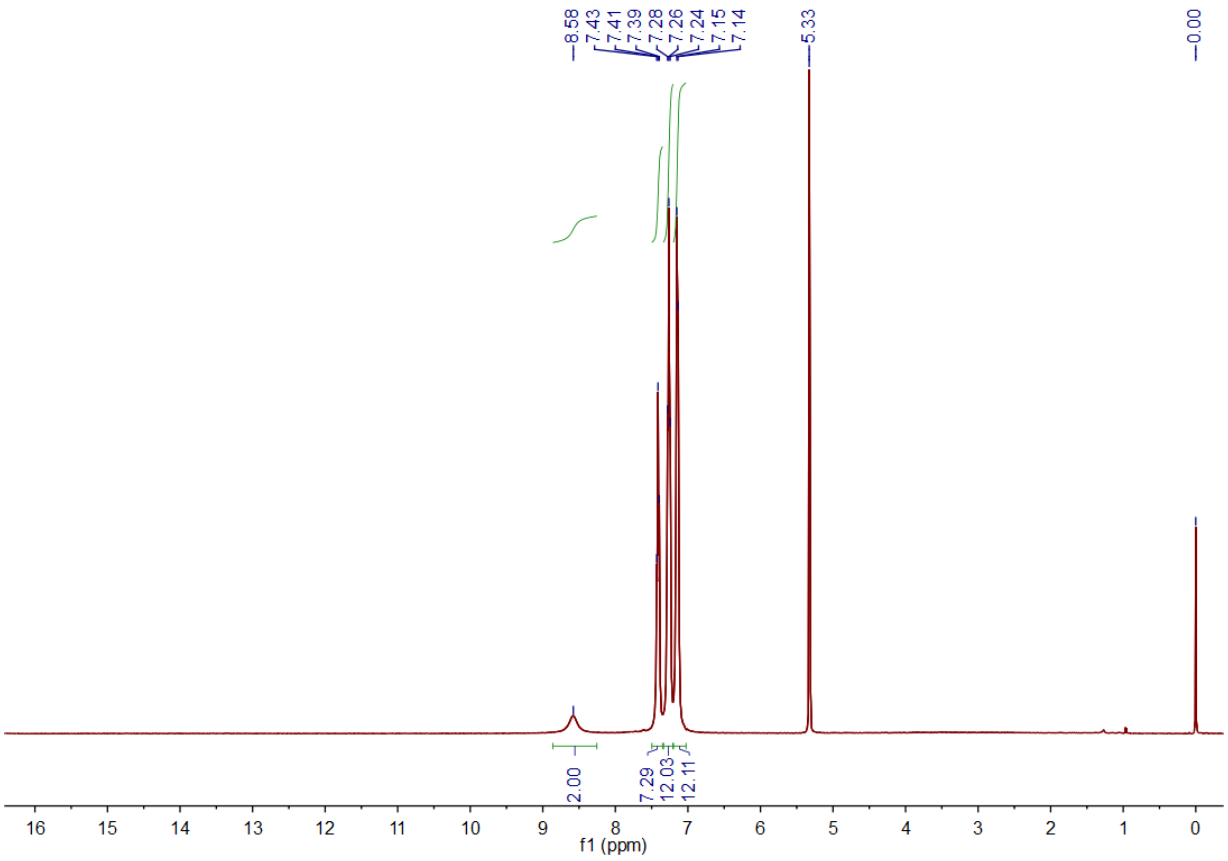


Fig. S3 ^{1}H NMR spectrum of **3** in CD_2Cl_2.

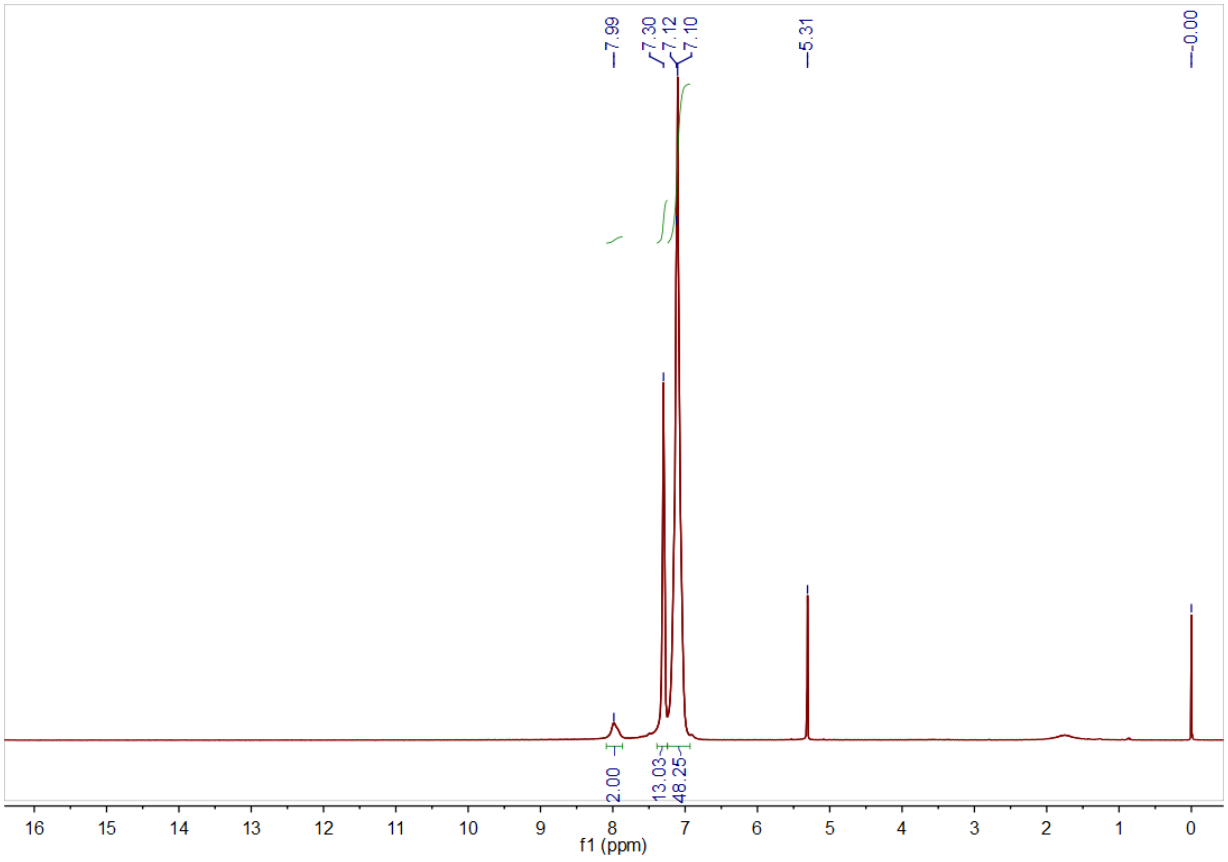


Fig. S4 ^{1}H NMR spectrum of **4** in CD_2Cl_2.

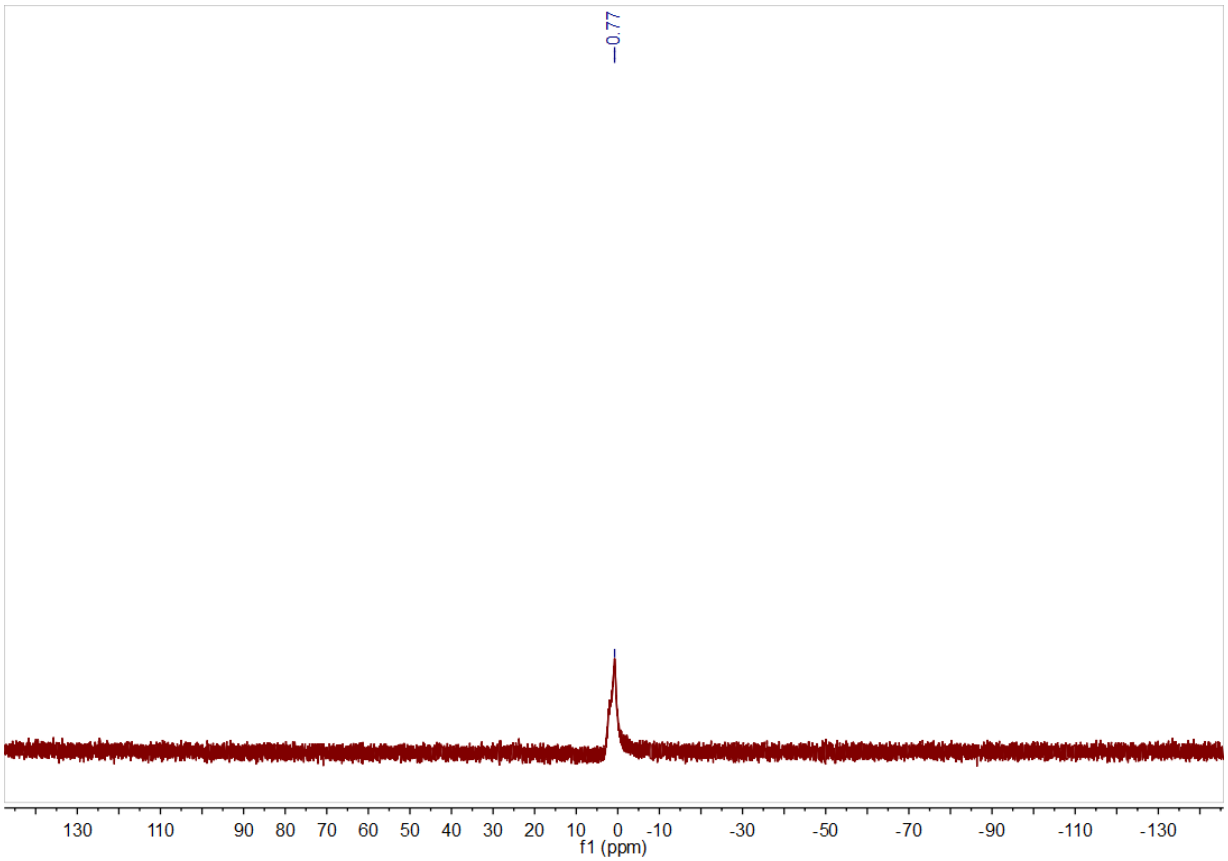


Fig. S5 ^{31}P NMR spectrum of **1** in CD_2Cl_2.

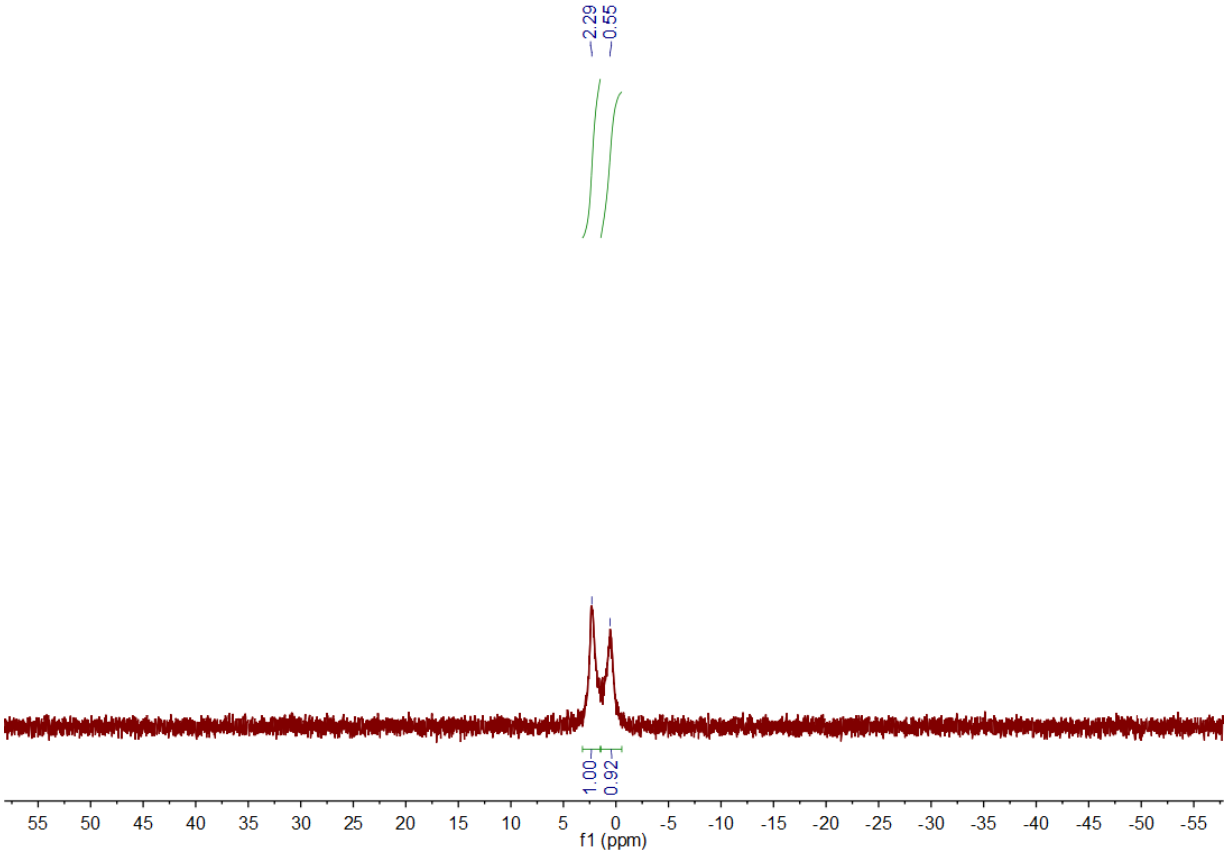


Fig. S6 ^{31}P NMR spectrum of **2** in CD_2Cl_2.

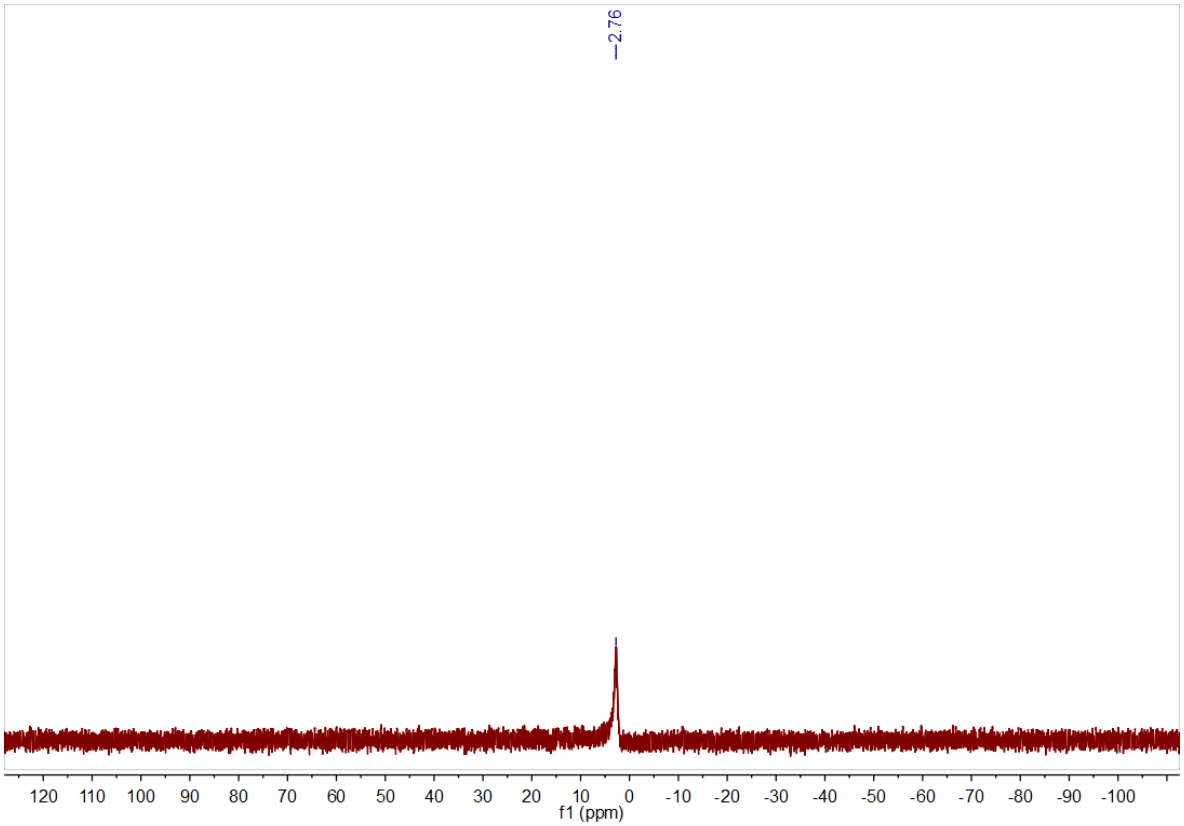


Fig. S7 ^{31}P NMR spectrum of **3** in CD_2Cl_2.

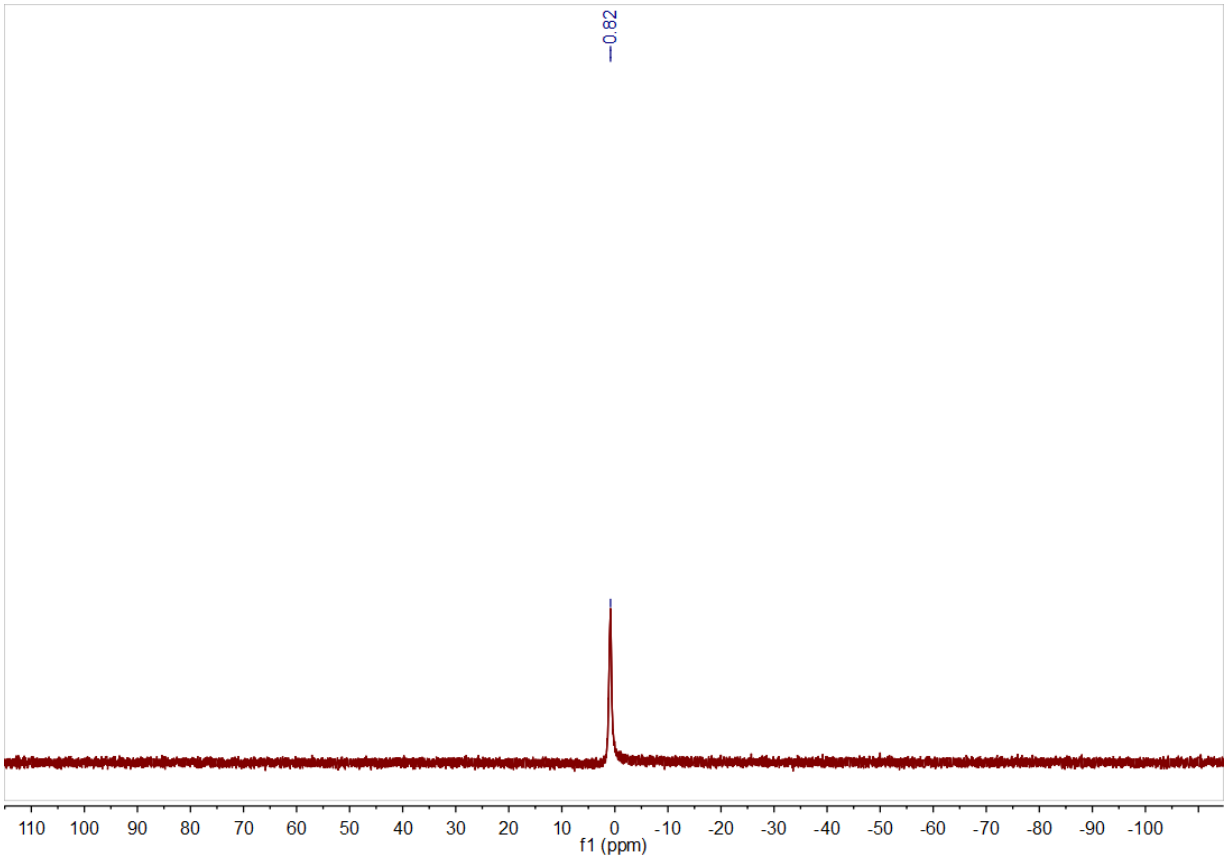


Fig. S8 ^{31}P NMR spectrum of **4** in CD_2Cl_2.

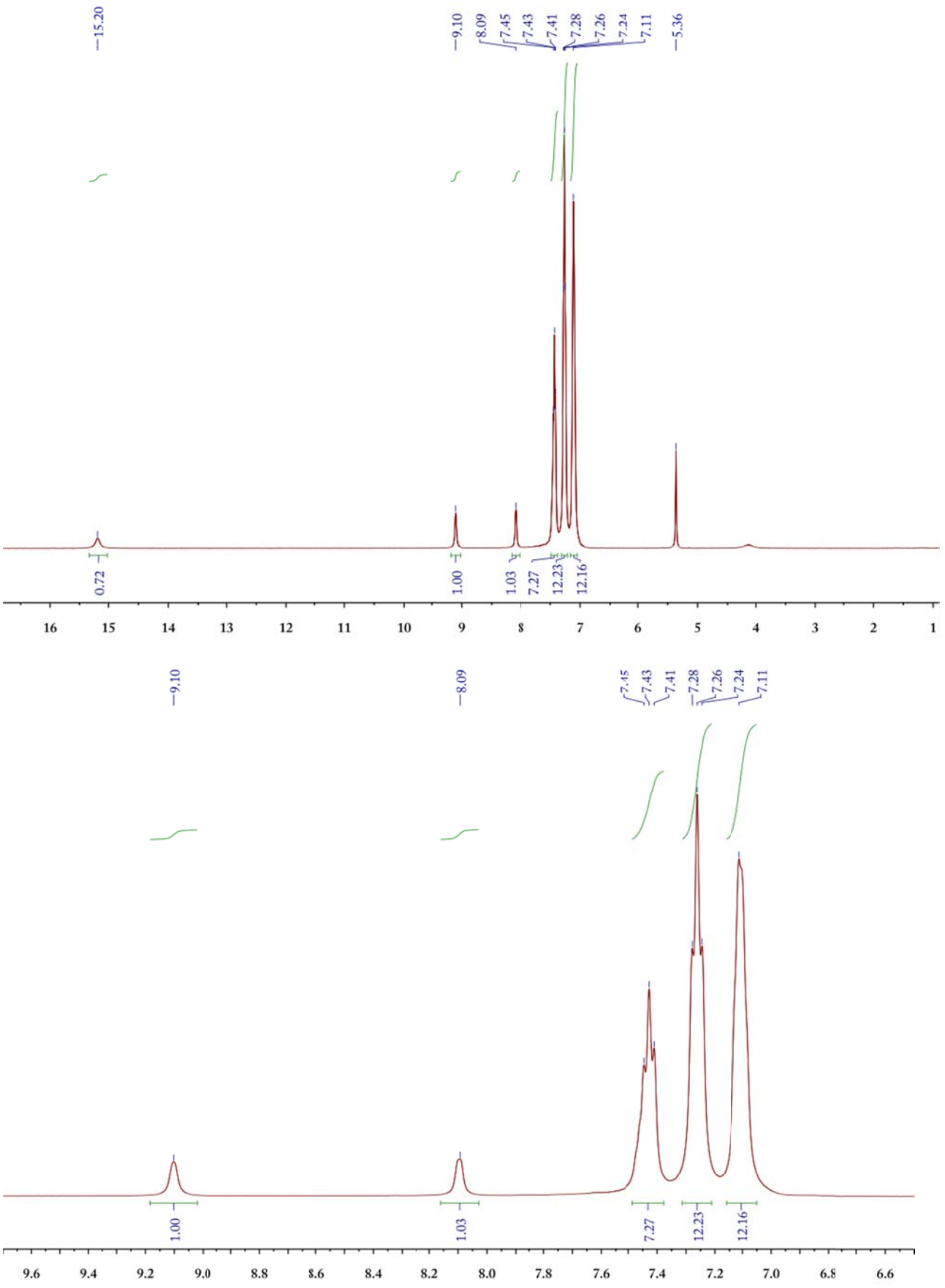


Fig. S9 ^{1}H NMR spectra of **3** in CD_2Cl_2 at 218 K.

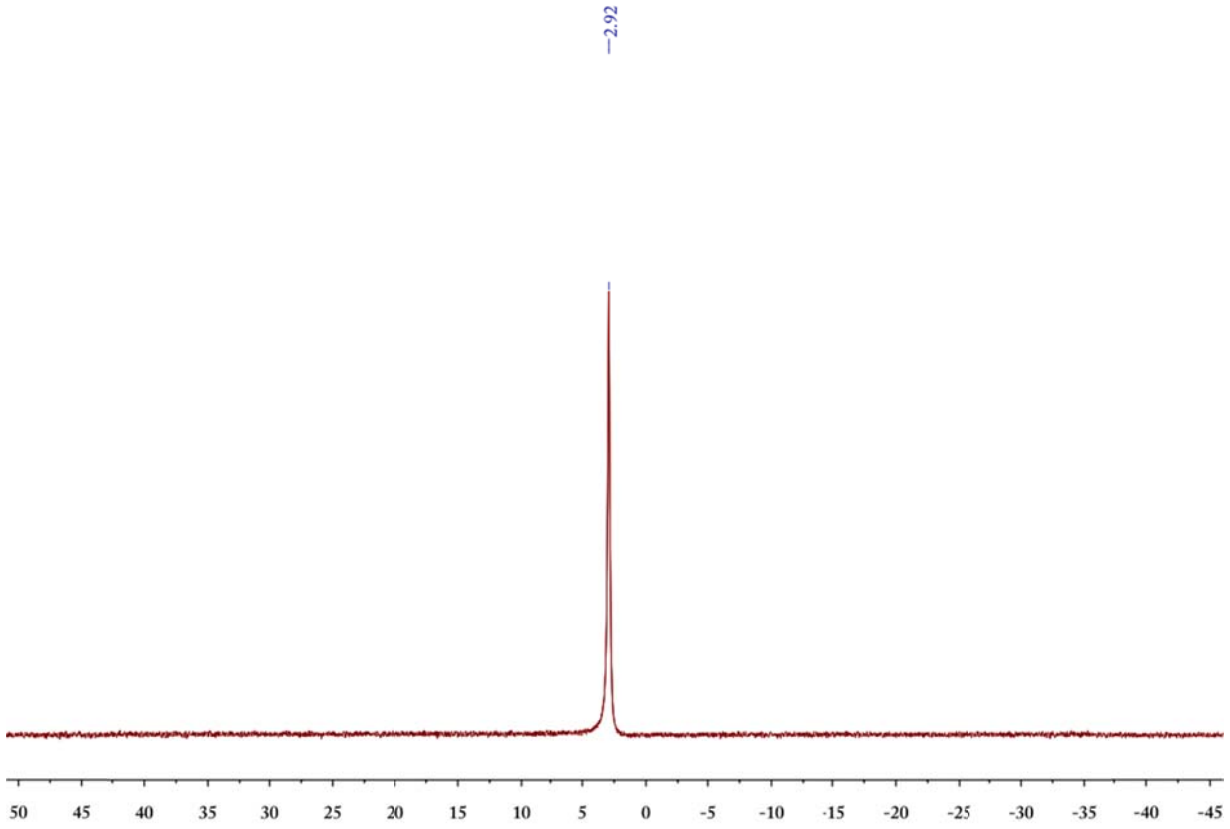


Fig. S10 ^{31}P NMR spectrum of **3** in CD_2Cl_2 at 218 K.

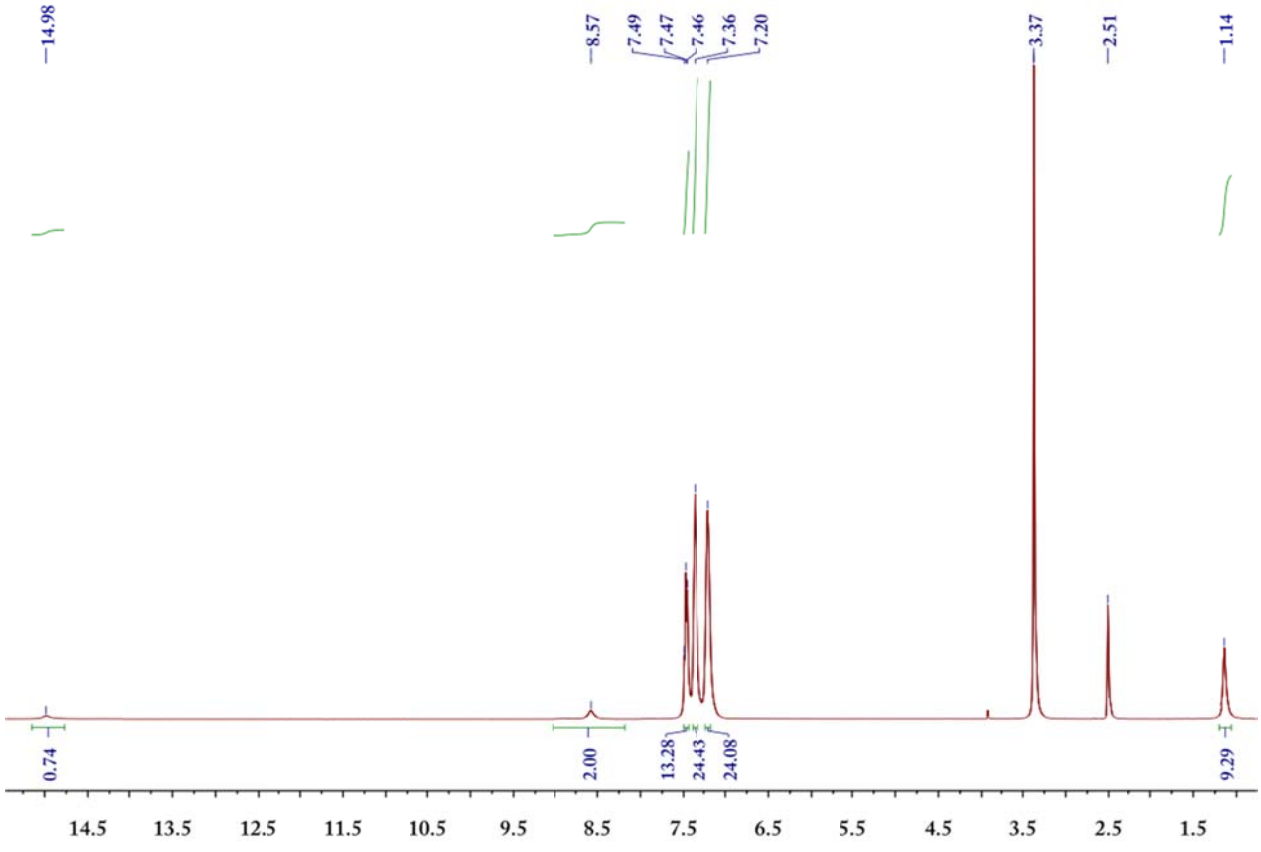


Fig. S11 ^{1}H NMR spectrum of **2** in DMSO-d_6 at 298 K.

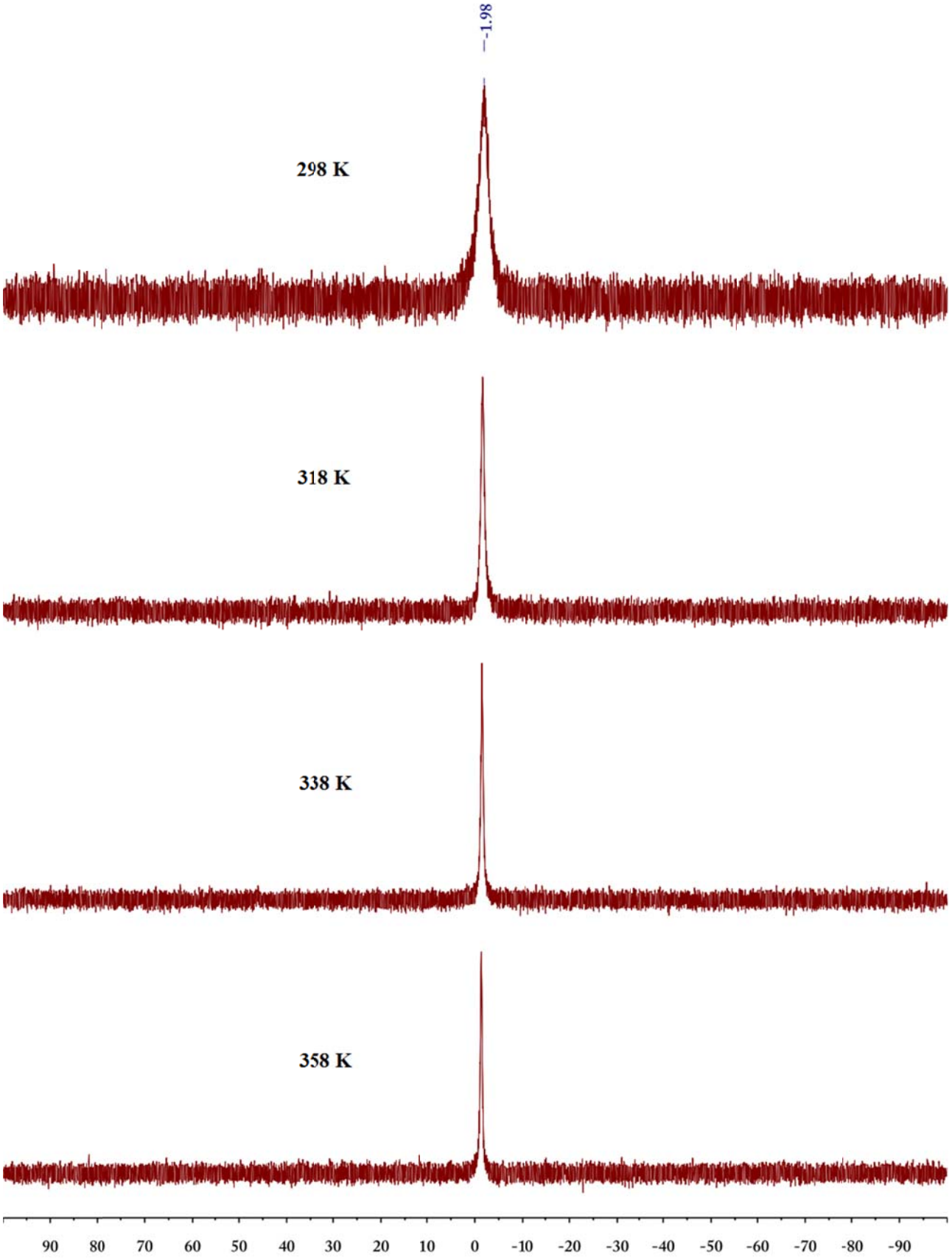


Fig. S12 Variable-temperature ^{31}P NMR spectra of **2** in DMSO-d_6 from 298 K to 358 K.

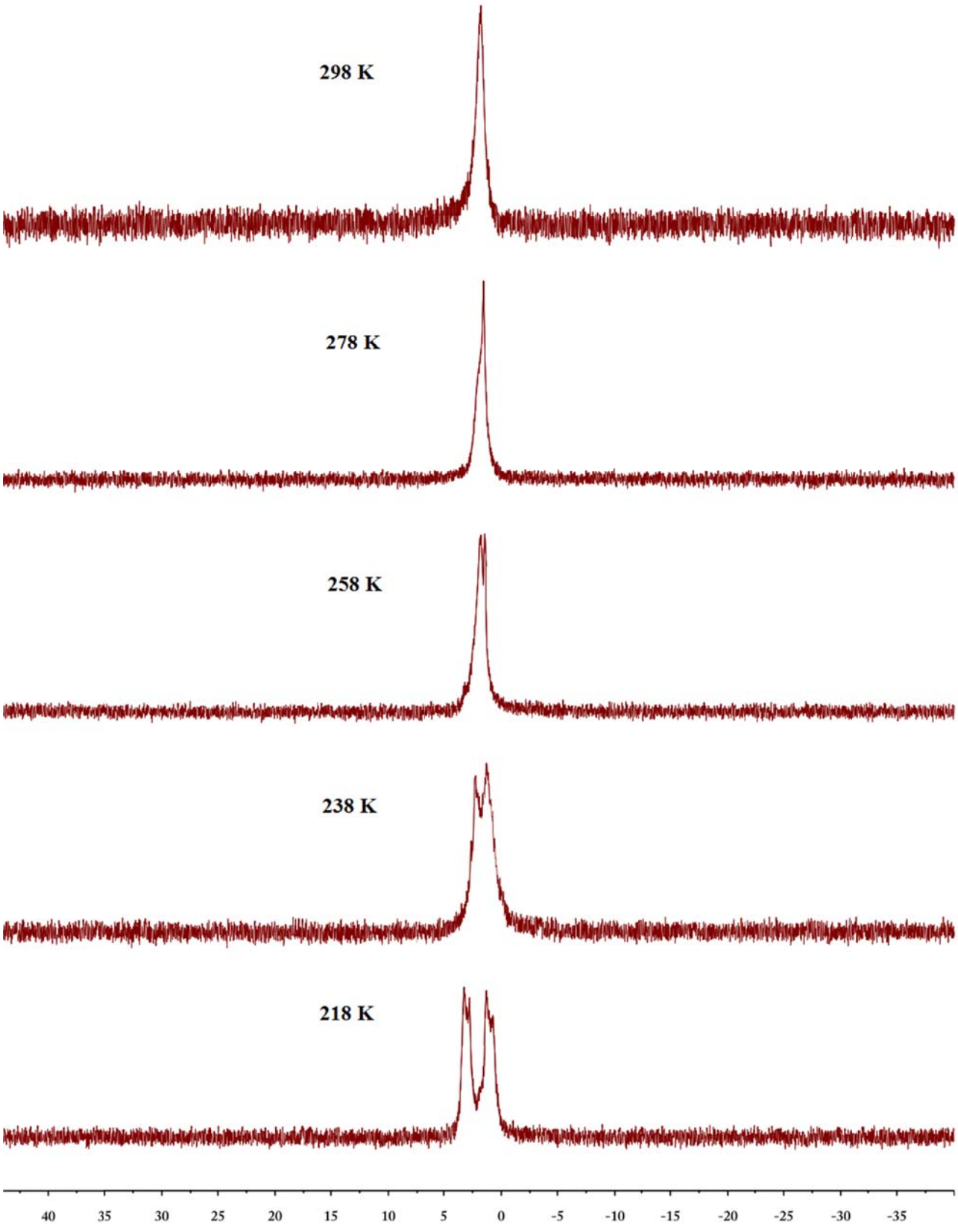


Fig. S13 Variable-temperature ^{31}P NMR spectra of **4** in CD_2Cl_2 from 298 K to 218 K.

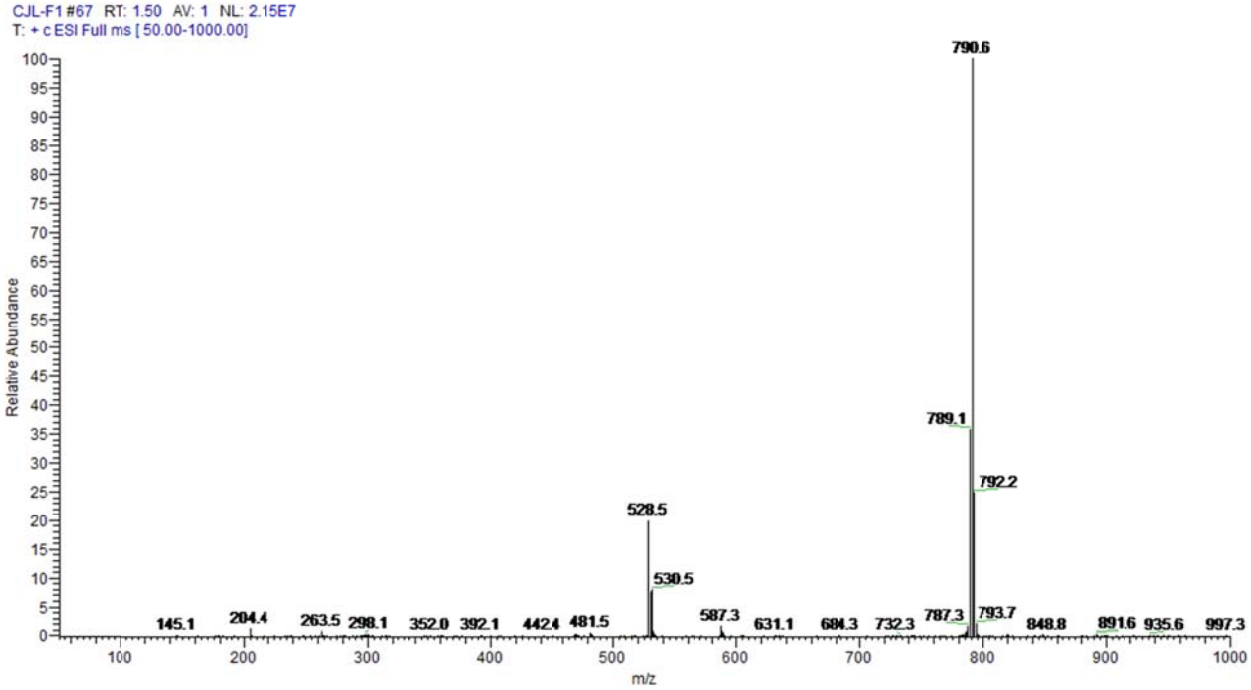


Fig. S14 ESI-MS of complex **1**.

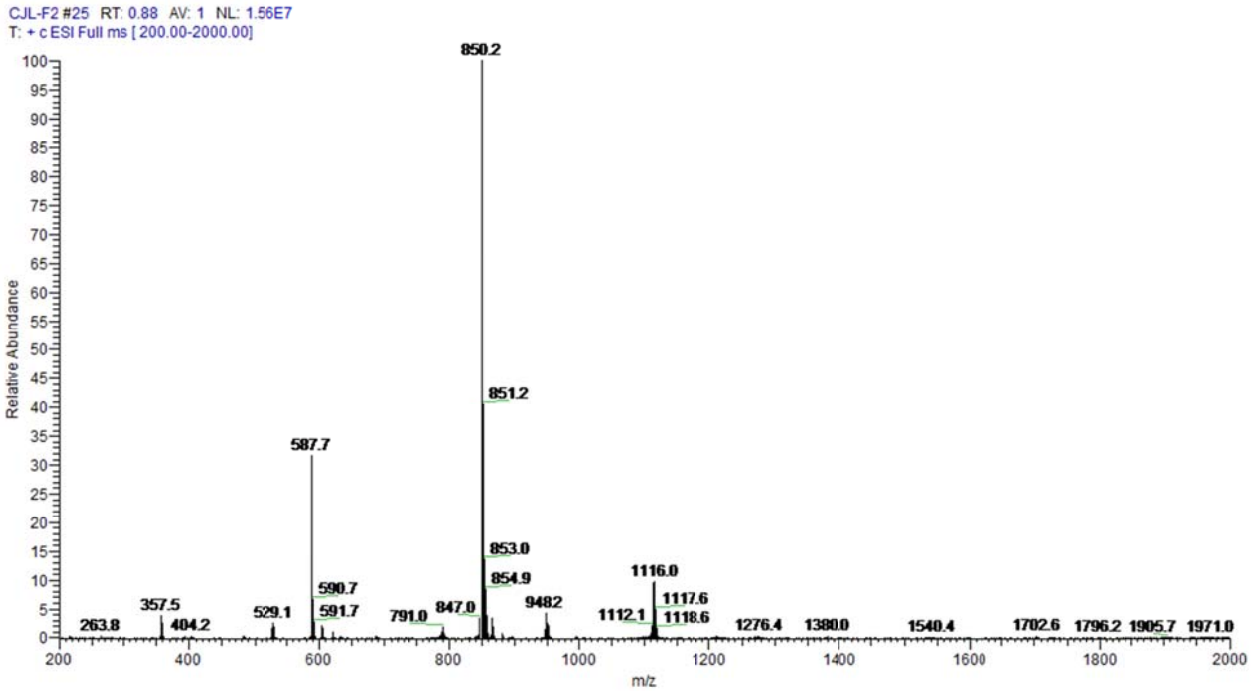


Fig. S15 ESI-MS of complex **2**.

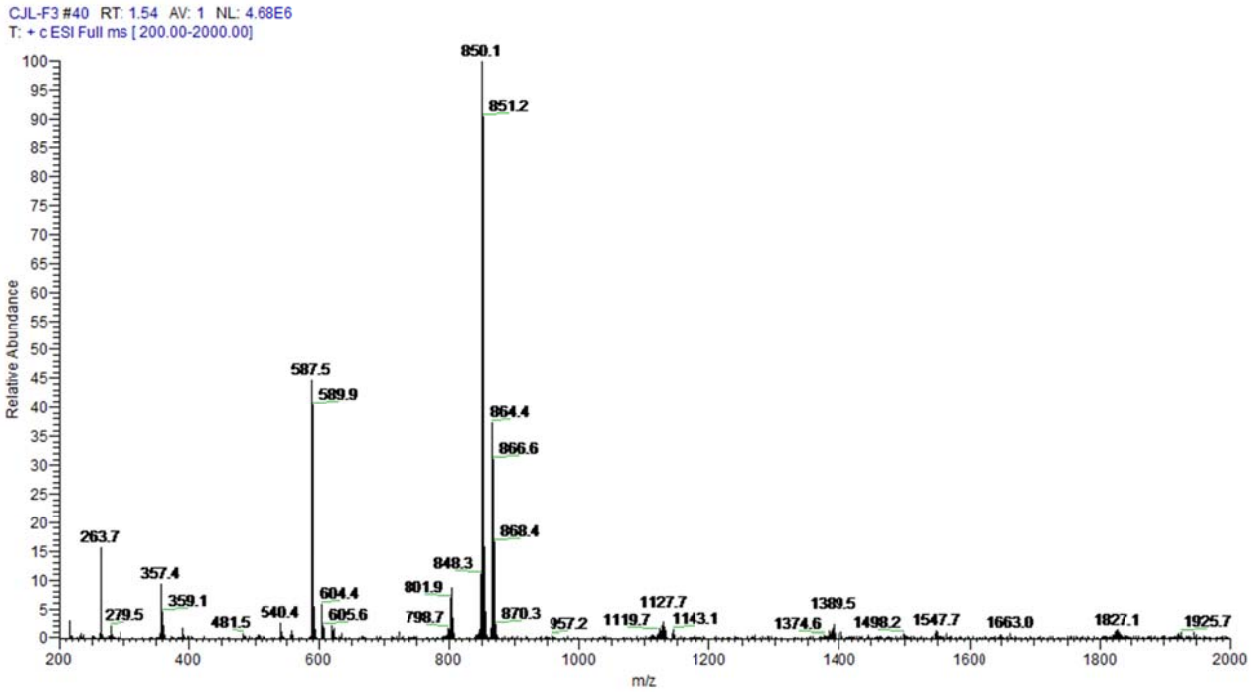


Fig. S16 ESI-MS of complex **3**

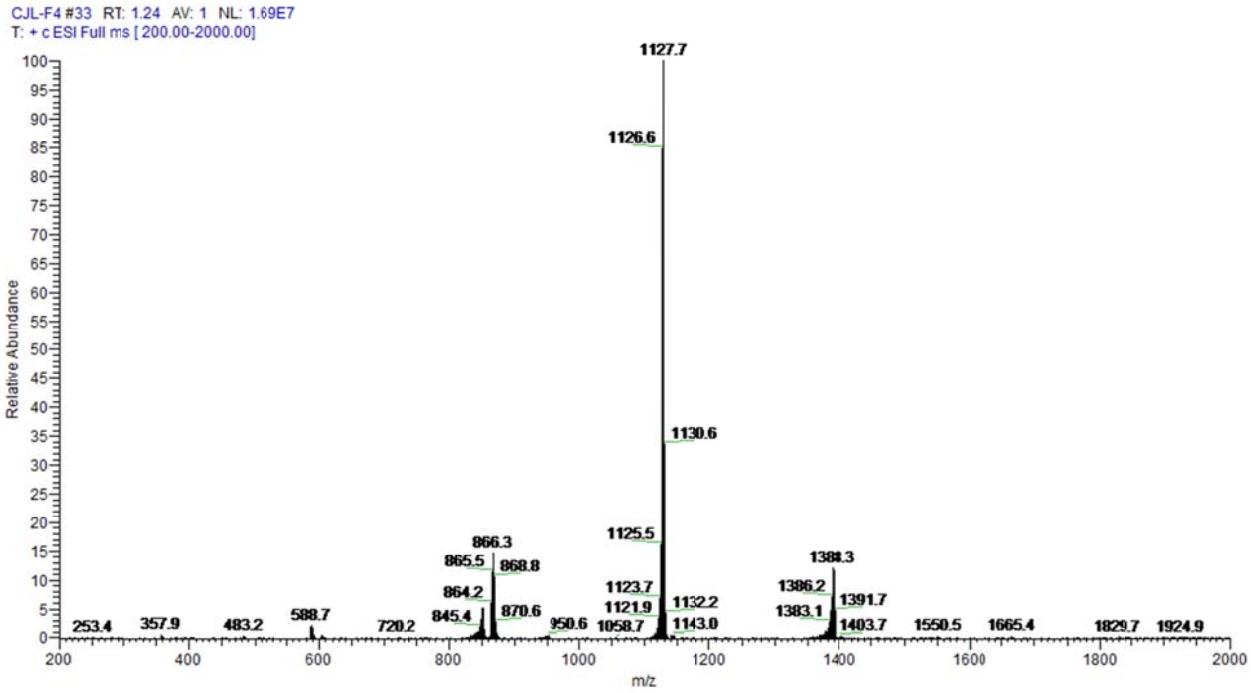


Fig. S17 ESI-MS of complex **4**

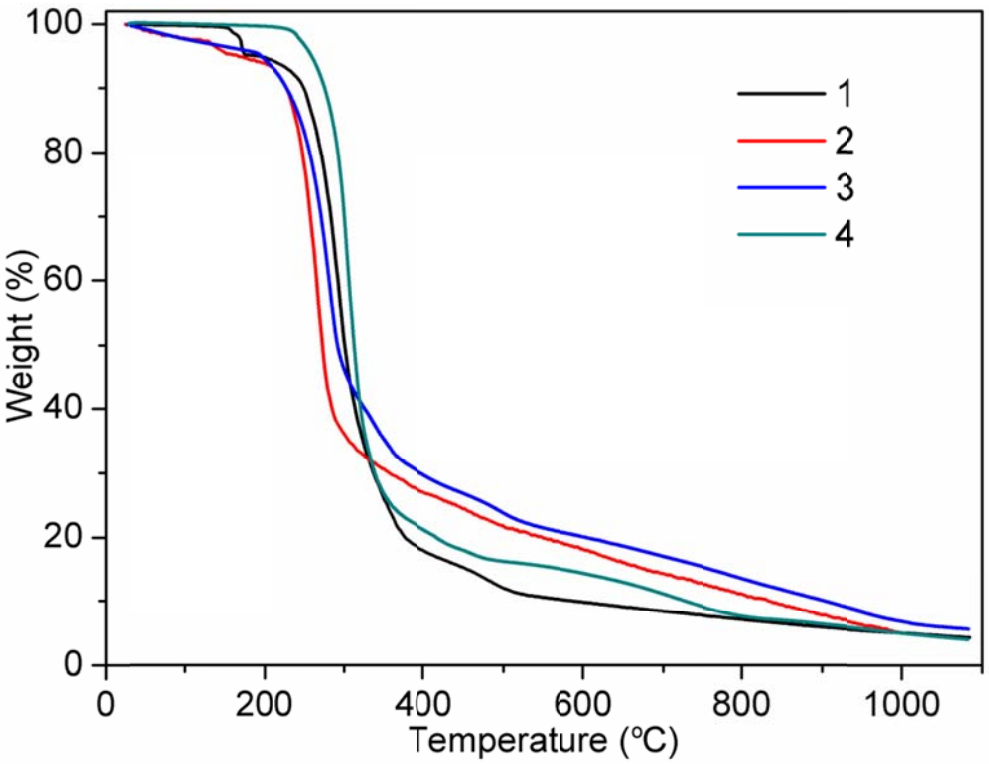


Fig. S18 TGA curves of complexes **1**–**4** in N_2.

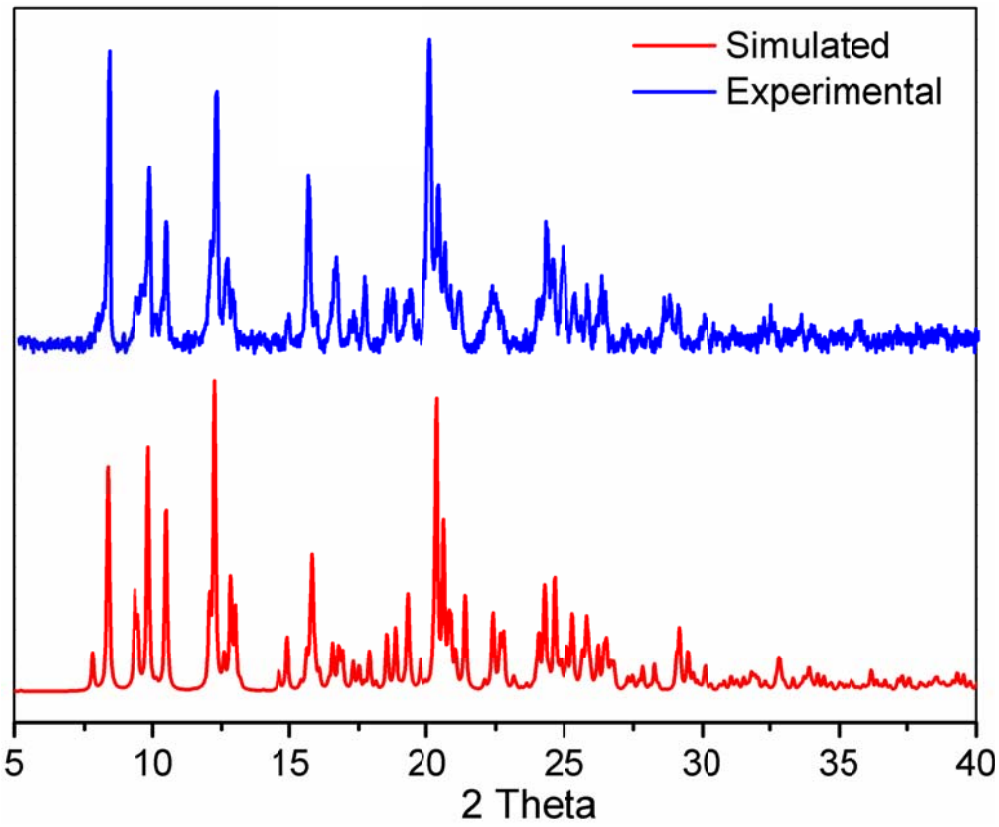


Fig. S19 The PXRD pattern of complex **1**.

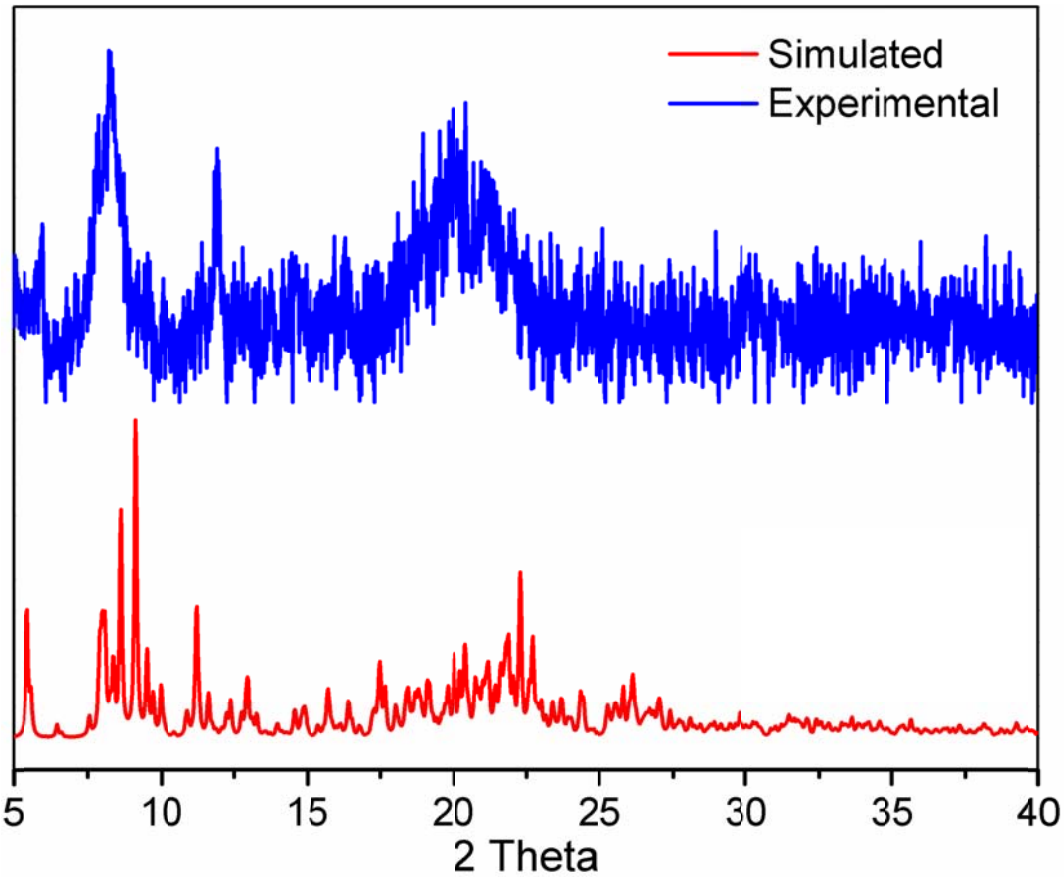


Fig. S20 The PXRD pattern of complex **2**.

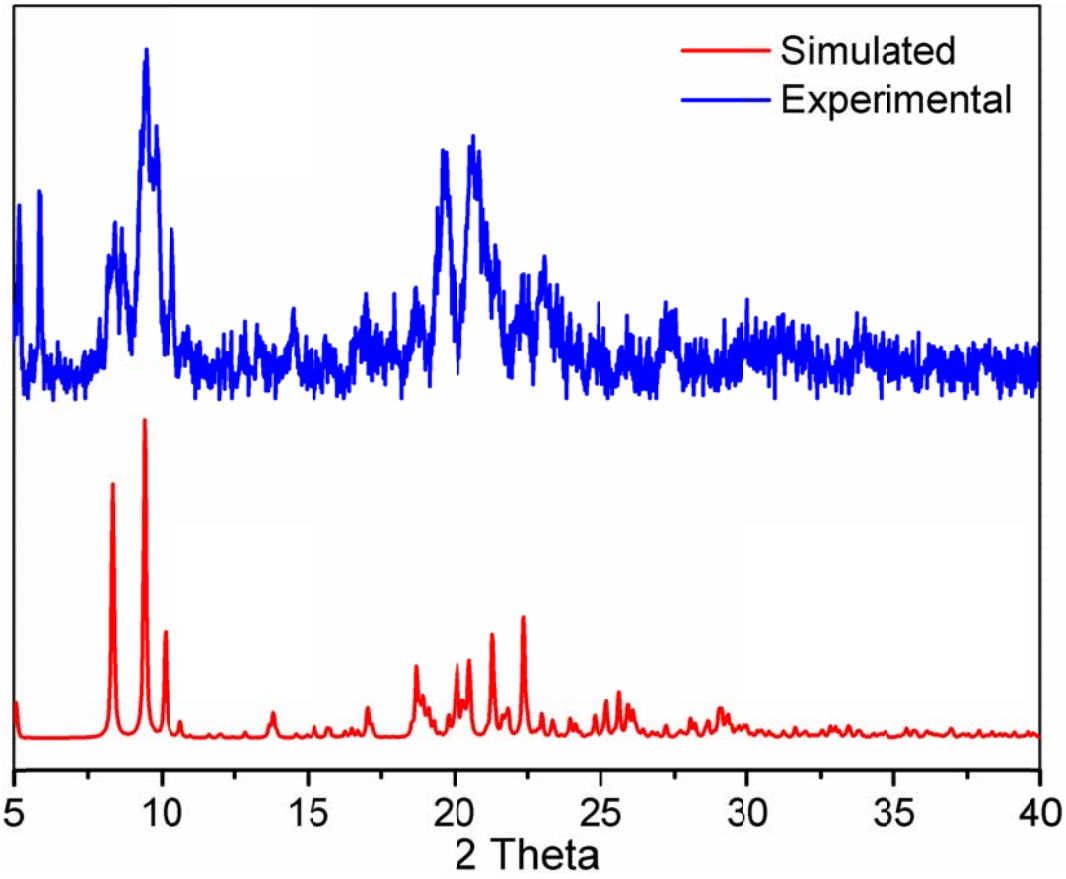


Fig. S21 The PXRD pattern of complex **3**.

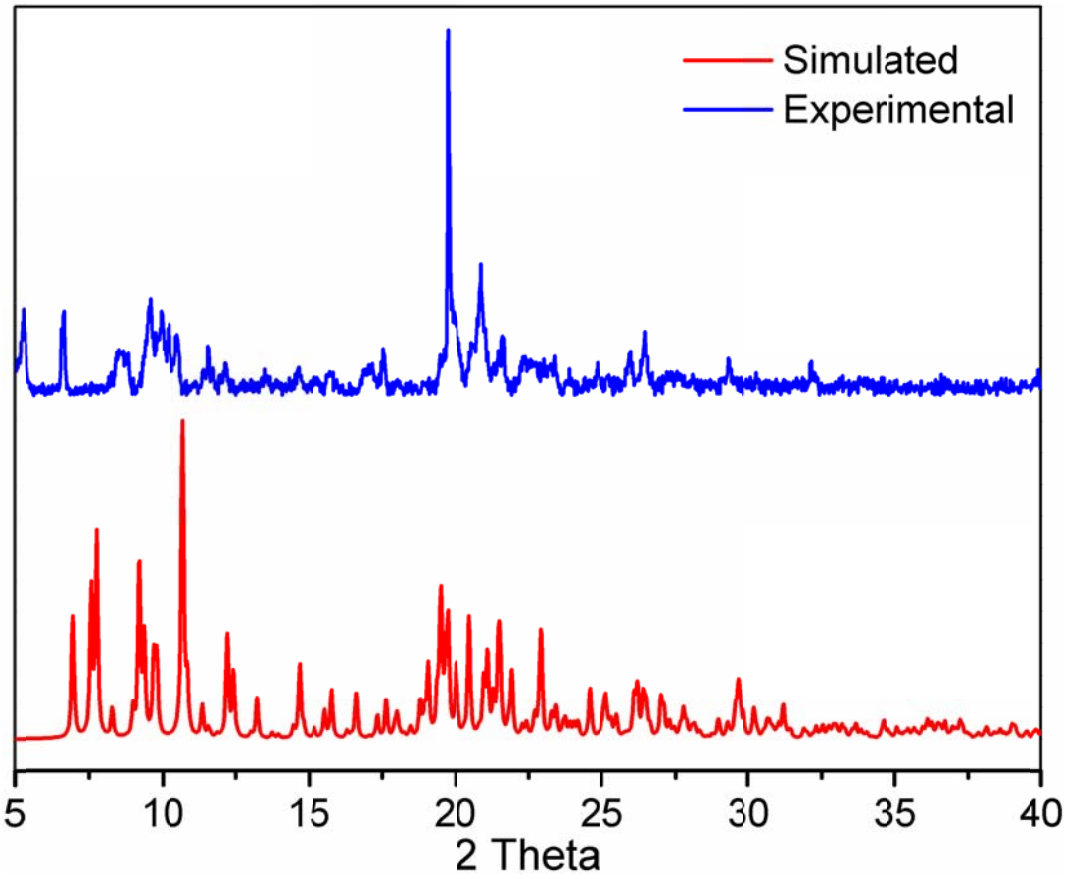


Fig. S22 The PXRD pattern of complex **4**.

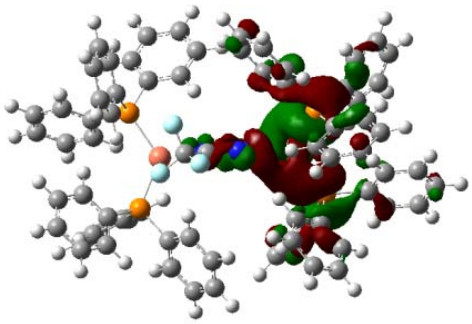
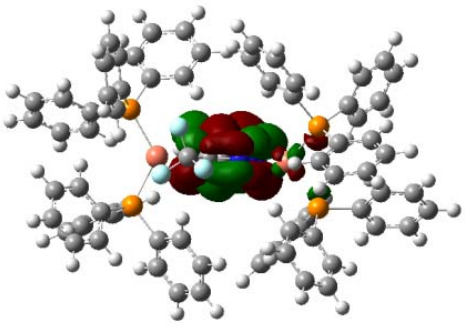
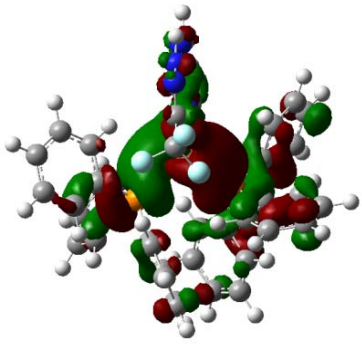
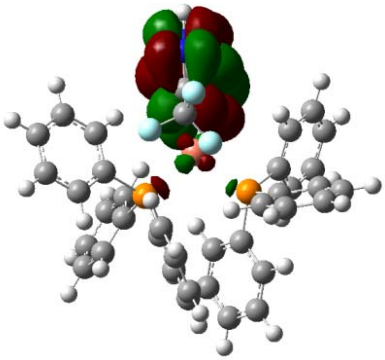
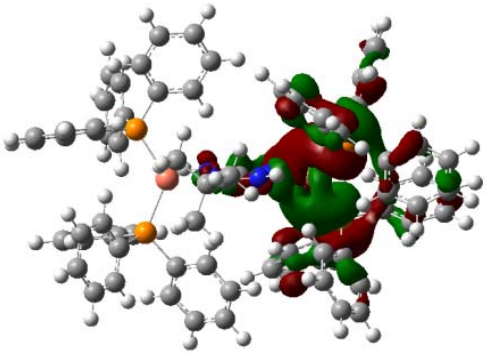
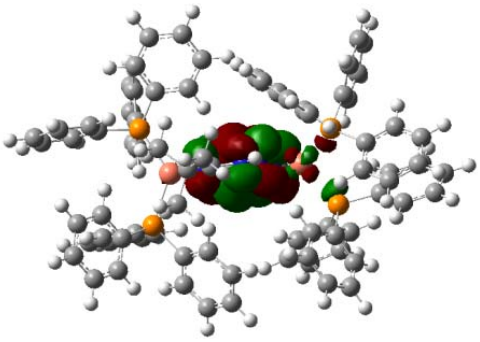
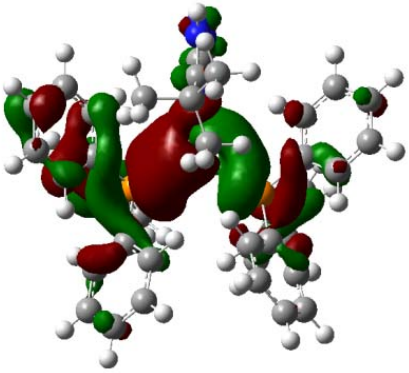
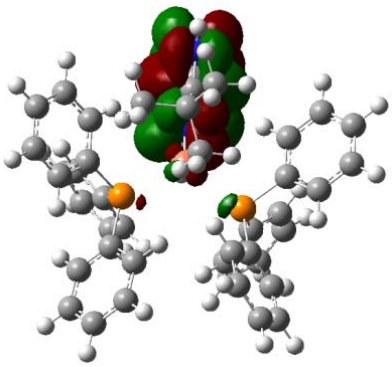
4		
3		
2		
1		
	HOMO	**LUMO**

Fig. S23 Plots of the frontier molecular orbitals involved in the lowest triplet excited state of complexes **1**–**4** based on the T_1-optimized structure in CH_2Cl_2 media calculated by TD-DFT method at the PBE1PBE level (iso_{value} = 0.02).

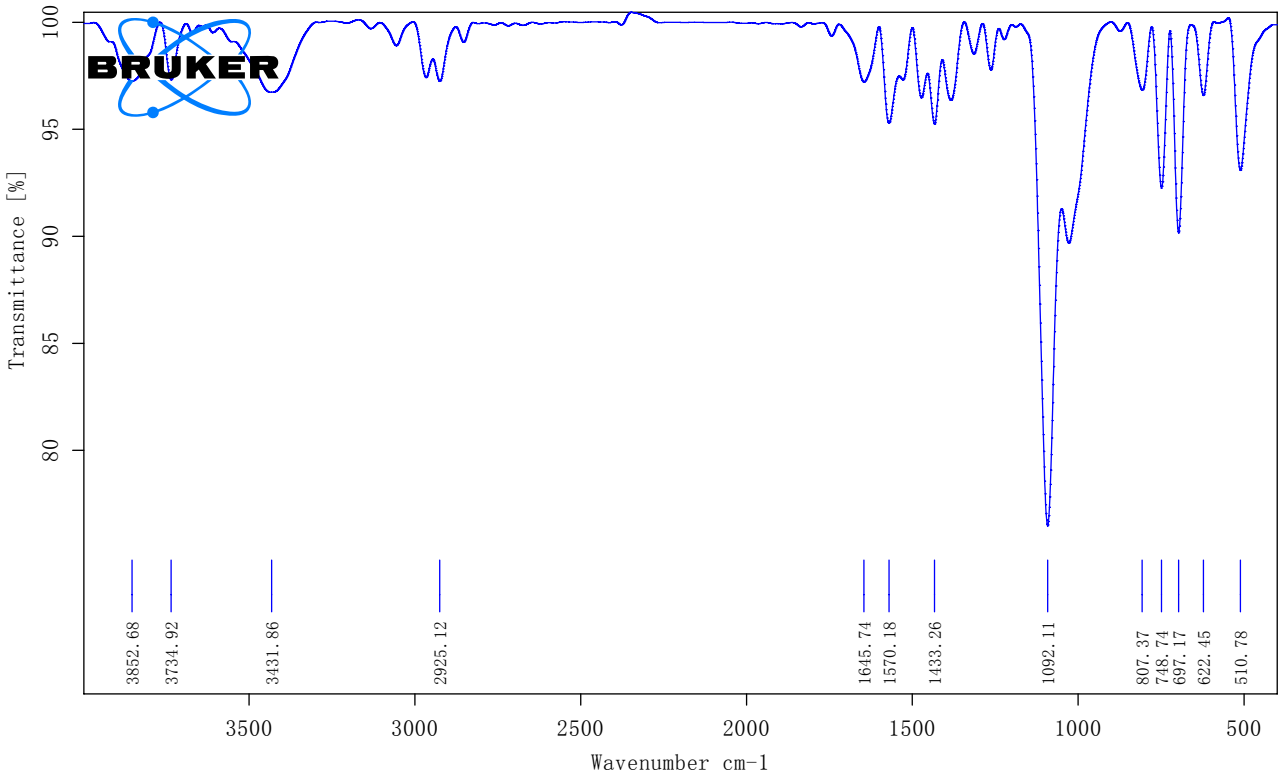


Fig. S24 IR spectrum of complex **1**.

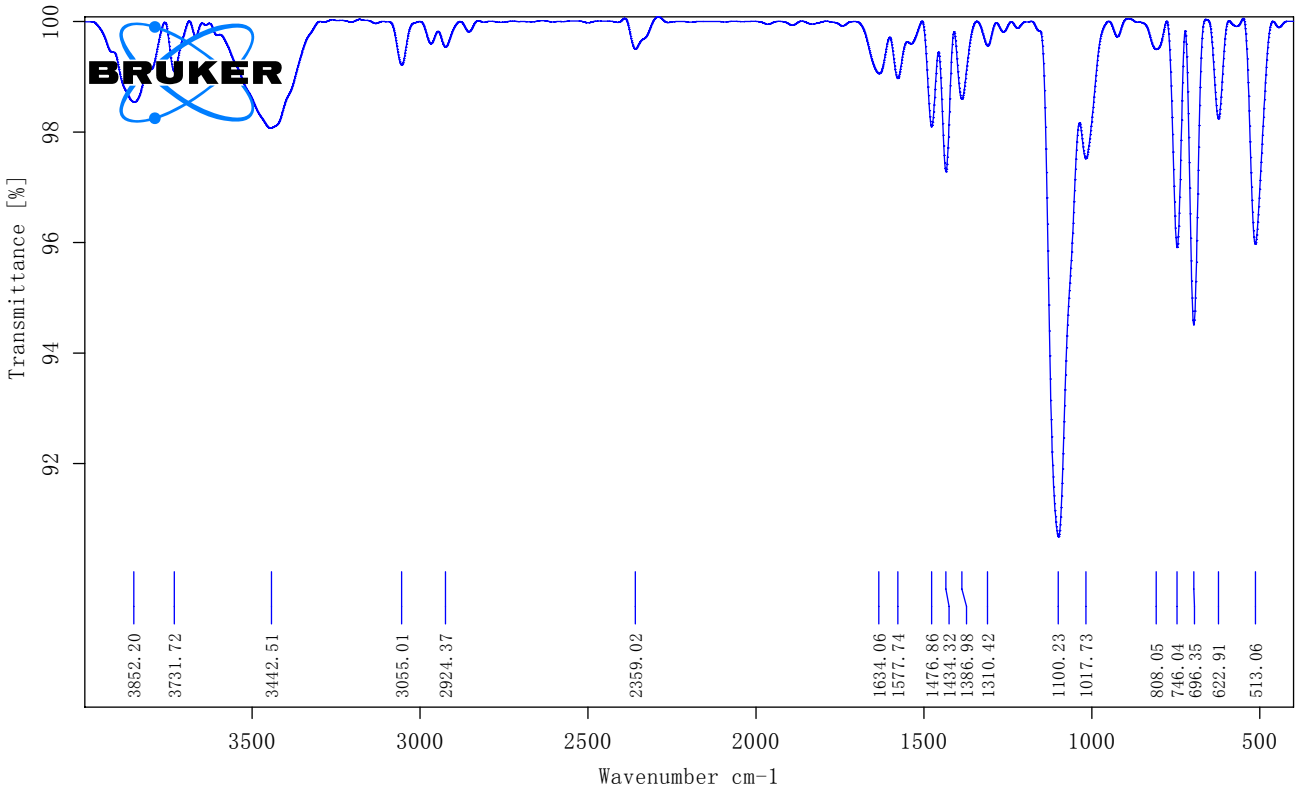


Fig. S25 IR spectrum of complex **2**.

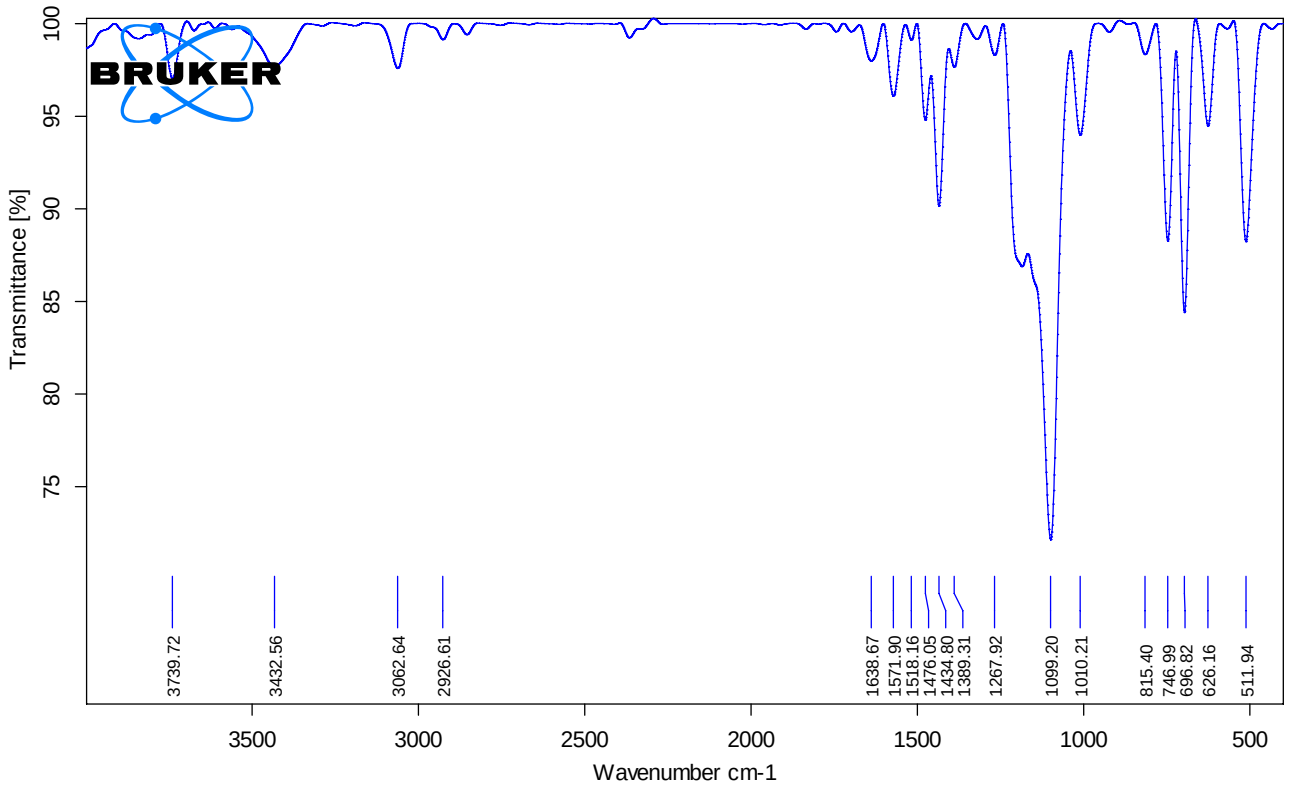


Fig. S26 IR spectrum of complex **3**.

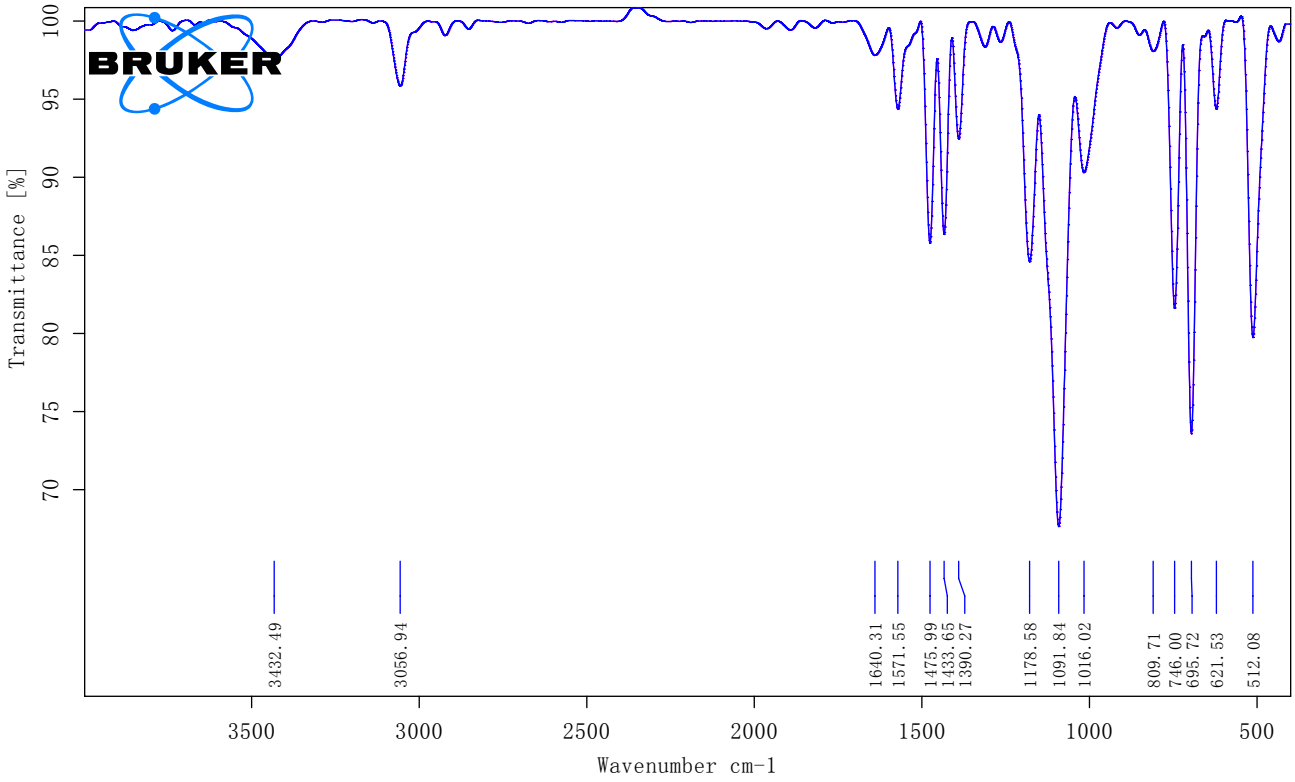


Fig. S27 IR spectrum of complex **4**.

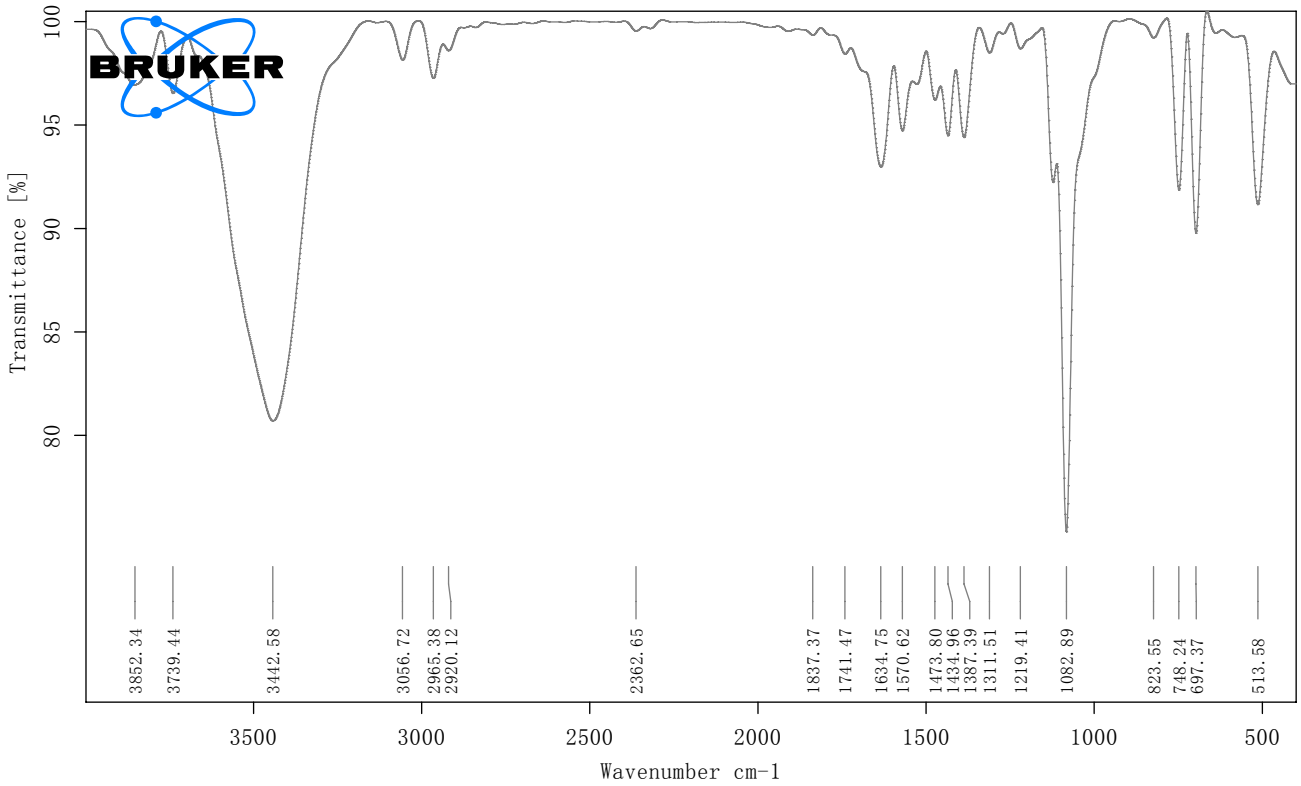


Fig. S28 IR spectrum of complex **1a**.

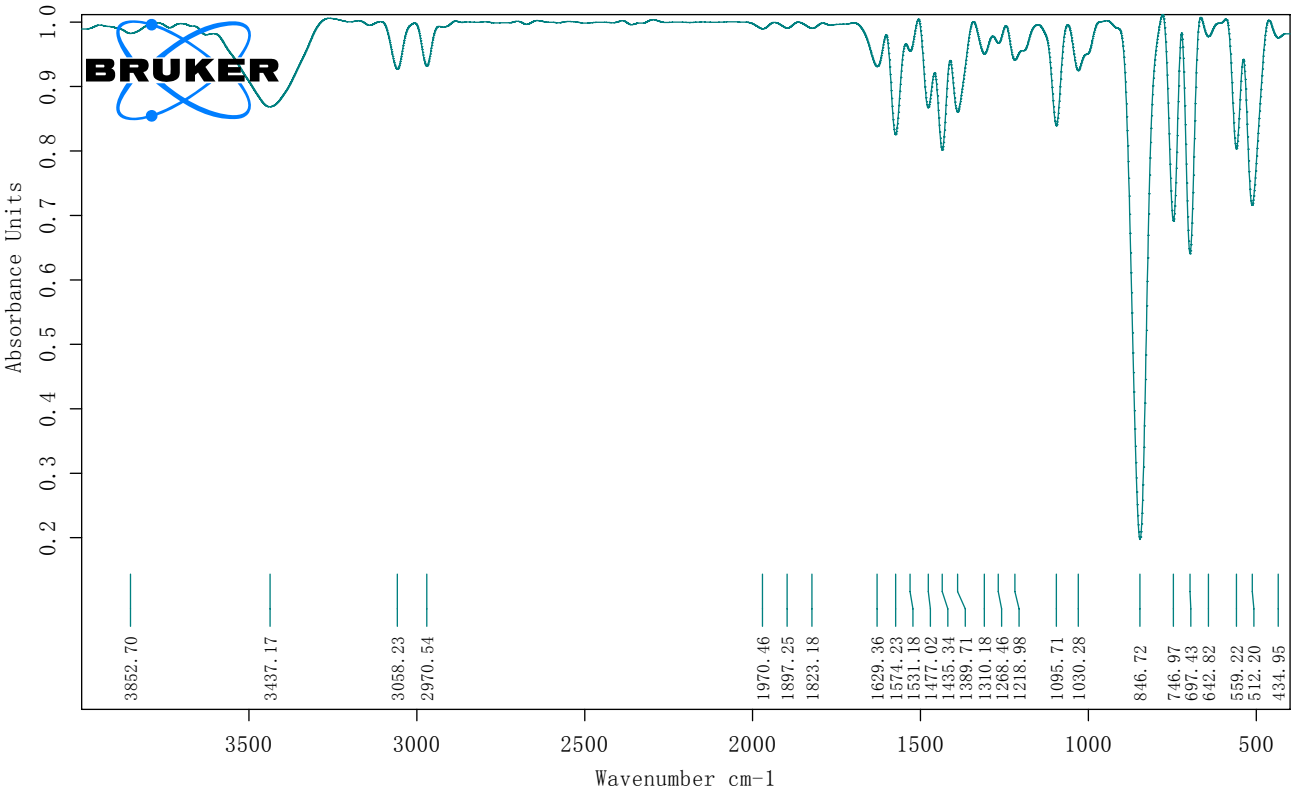


Fig. S29 IR spectrum of complex **1b**.

Table S1 Partial molecular orbital compositions (%) by SCPA approach (C-squared population analysis proposed by Ros and Schuit) for **1**–**4** based on the S_0-optimized structures in CH_2Cl_2 media calculated by TD-DFT method at the PBE1PBE level

	Orbital	Energy (eV)	HOMO-LUMO Gap (eV)	MO Contribution (%)			
				Cu	P	Ph	bpmtzH or fpmtzH
1	HOMO	-6.50	4.44	35.12	19.68	41.27	3.93
	LUMO	-2.06		0.76	0.00	1.51	97.73
2	HOMO	-6.75	3.90	31.97	18.21	45.89	3.93
	LUMO	-2.85		1.51	0.62	1.66	96.21
3	HOMO	-6.56	3.89	32.35	18.69	46.16	2.80
	LUMO	-2.67		0.96	0.23	0.87	97.94
4	HOMO	-6.30	4.27	36.80	20.22	36.67	6.31
	LUMO	-2.03		1.40	0.39	3.17	95.04

Table S2 Partial molecular orbital compositions (%) by SCPA approach (C-squared population analysis proposed by Ros and Schuit) for **1**–**4** based on the T_1-optimized structures in CH_2Cl_2 media calculated by TD-DFT method at the PBE1PBE level

	Orbital	Energy (eV)	HOMO-LUMO Gap (eV)	MO Contribution (%)			
				Cu	P	Ph	bpmtzH or fpmtzH
1	HOMO	-5.85	3.25	37.67	20.09	31.11	11.13
	LUMO	-2.60		2.20	0.32	1.64	95.84
2	HOMO	-5.98	2.62	35.64	22.45	29.6	12.31
	LUMO	-3.36		0.04	1.97	5.8	92.19
3	HOMO	-5.82	2.67	34.37	24.13	30.25	11.25
	LUMO	-3.15		2.39	1.33	1.39	94.89
4	HOMO	-5.54	3.01	41.01	21.37	22.51	15.11
	LUMO	-2.53		0.11	1.76	5.37	92.76