Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Influence of the Protonic State of an Imidazole-Phenanthroline Ligand on the Luminescence Properties of Copper(I) Complexes: Experimental and Theoretical Research

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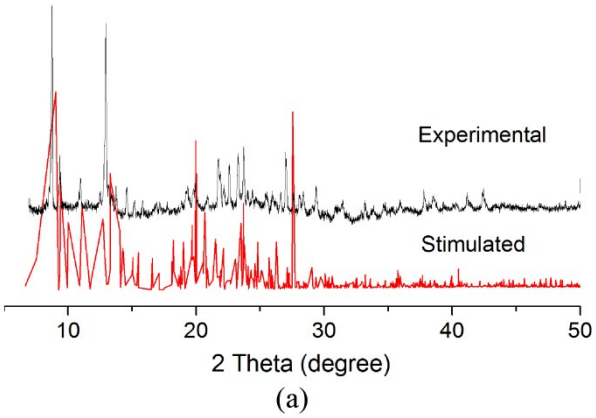
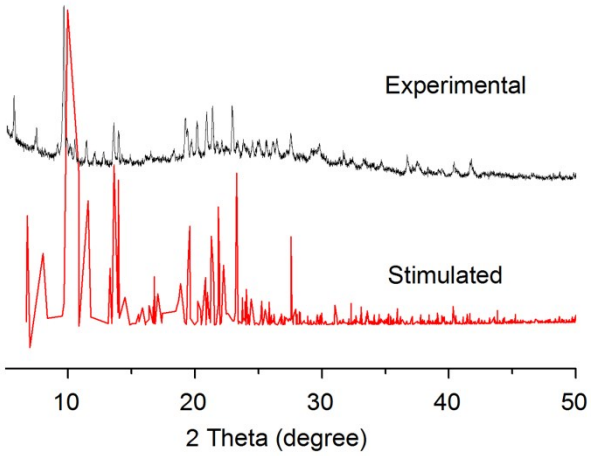
Table S1. Selected Mulliken and NBO charges of **2a** and **2b**

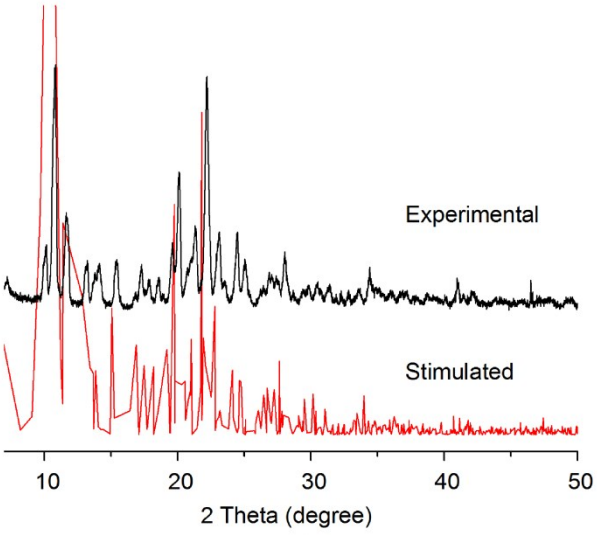
Atom	Complex **2a**		Complex **2b pph3**	
	Mulliken	NBO	Mulliken	NBO
Cu	-0.121	0.247	-0.182	0.350
P1	0.564	0.971	0.554	0.948
P2	0.541	0.972	0.537	0.949
N1	-0.482	-0.538	-0.477	-0.523
N2	-0.488	-0.538	-0.478	-0.516



(a)

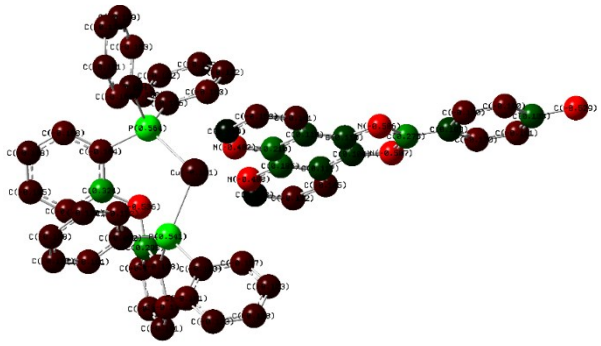


(b)

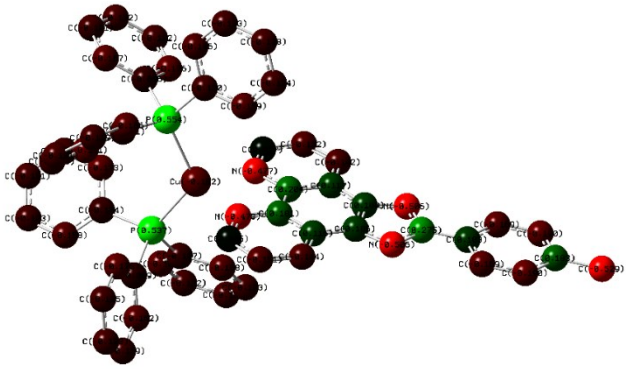


(c)

Figure S1. Comparing the X-ray powder diffraction patterns of microcrystalline powders and stimulated for **1b** (a); **2a** (b); **2b** (c).



2a



2b

Figure S2. Mulliken atom charges of complexes **2a** and **2b**

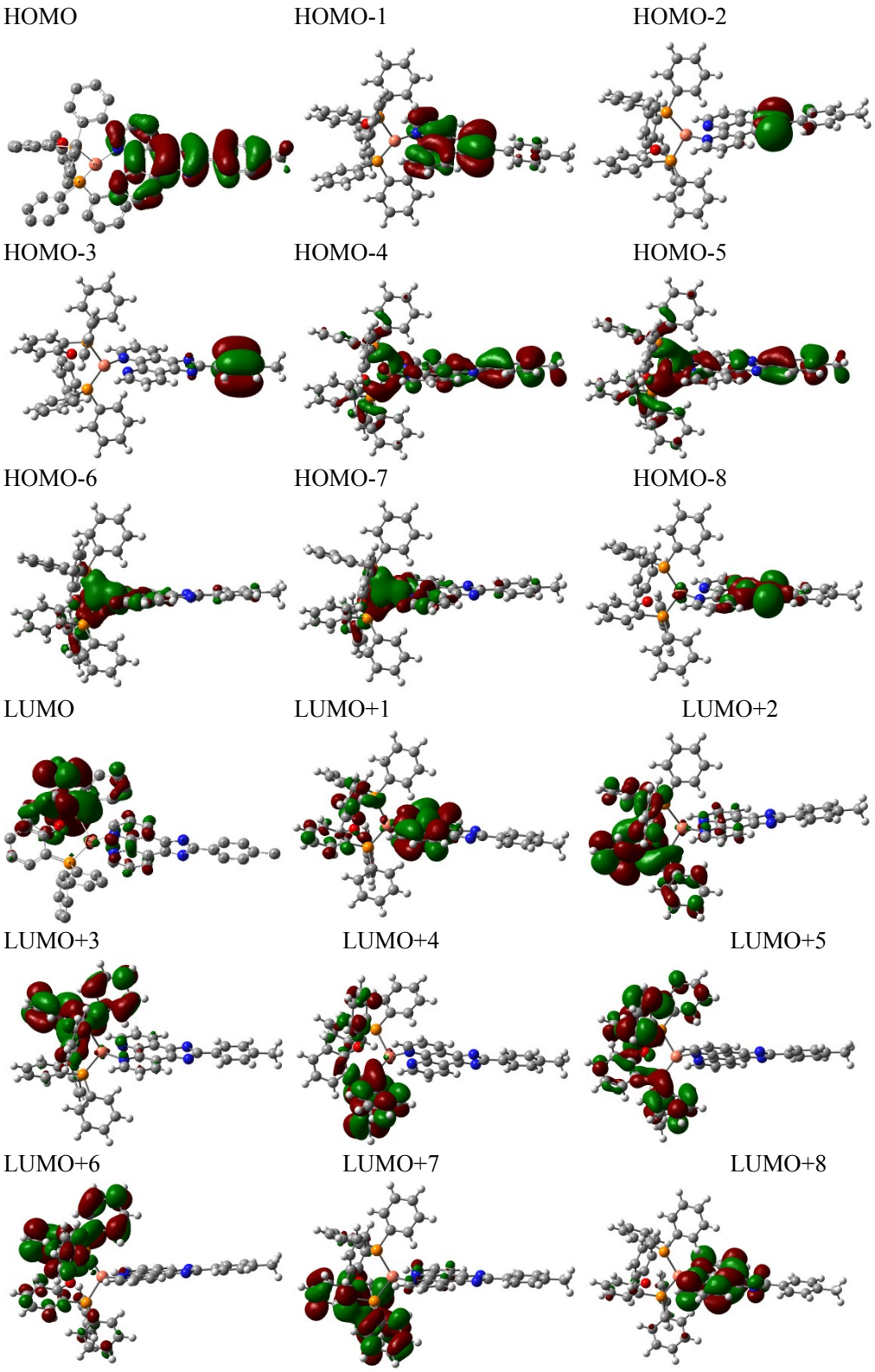


Figure S3. Frontier orbital of complex **2a**

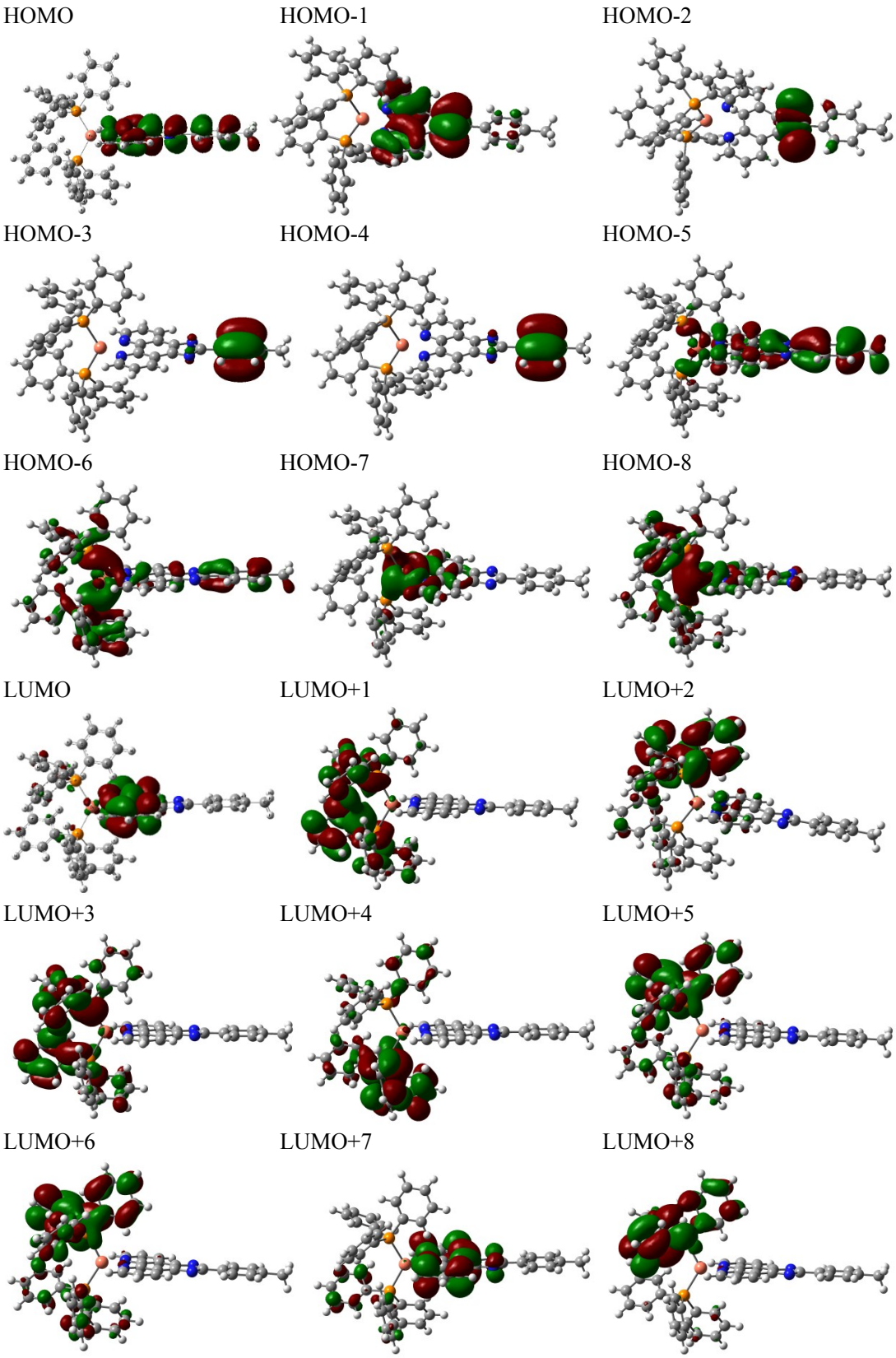
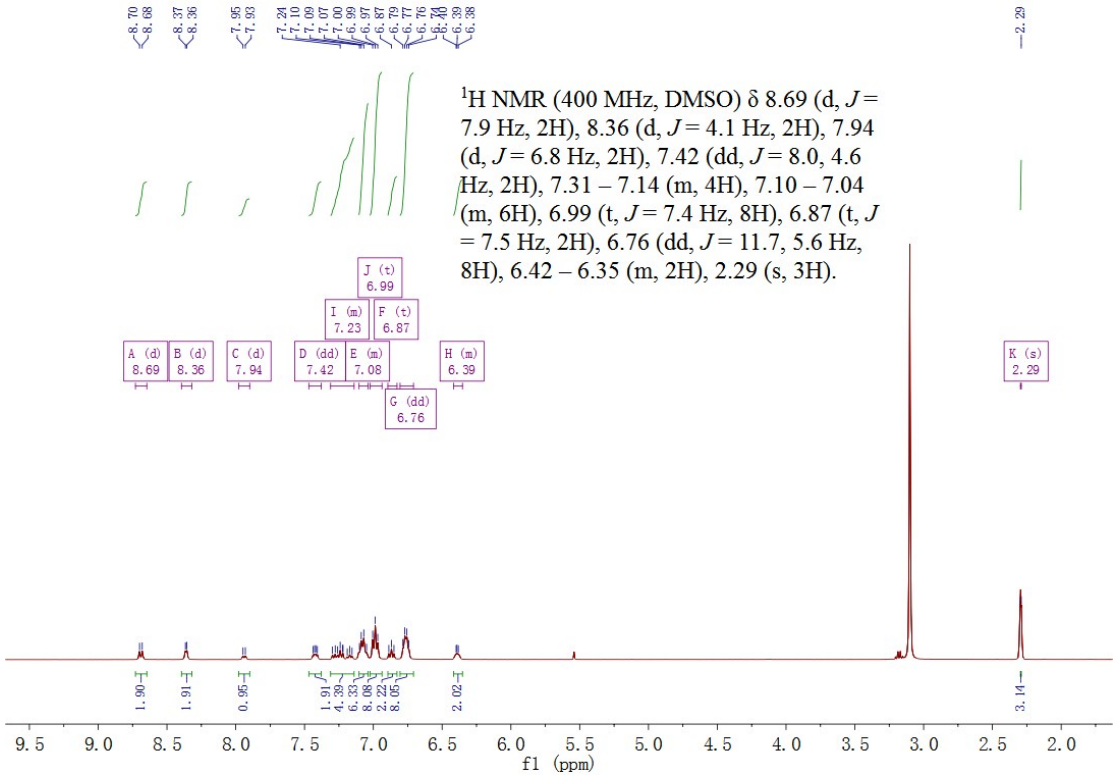


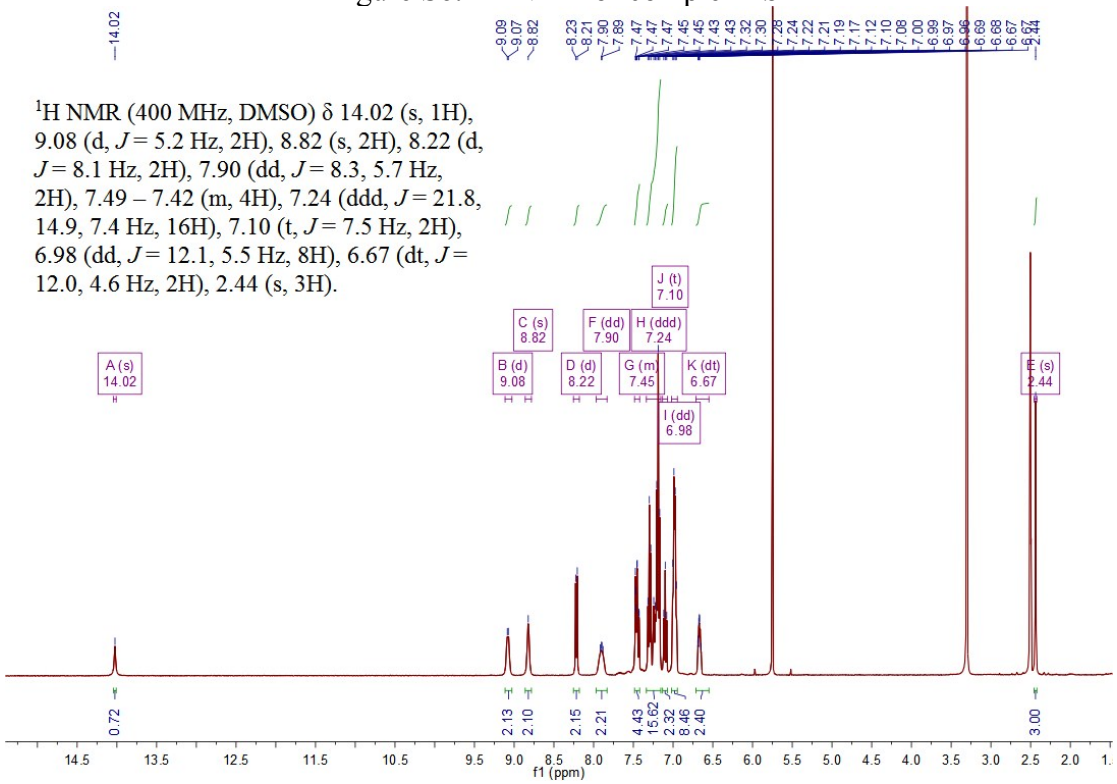
Figure S4. Frontier orbital of complex **2b**

Figure S5. ^{1}H NMR of complex **1a**



^{1}H NMR (400 MHz, DMSO) δ 8.69 (d, *J* = 7.9 Hz, 2H), 8.36 (d, *J* = 4.1 Hz, 2H), 7.94 (d, *J* = 6.8 Hz, 2H), 7.42 (dd, *J* = 8.0, 4.6 Hz, 2H), 7.31 – 7.14 (m, 4H), 7.10 – 7.04 (m, 6H), 6.99 (t, *J* = 7.4 Hz, 8H), 6.87 (t, *J* = 7.5 Hz, 2H), 6.76 (dd, *J* = 11.7, 5.6 Hz, 8H), 6.42 – 6.35 (m, 2H), 2.29 (s, 3H).

Figure S6. ^{1}H NMR of complex **1b**



^{1}H NMR (400 MHz, DMSO) δ 14.02 (s, 1H), 9.08 (d, *J* = 5.2 Hz, 2H), 8.82 (s, 2H), 8.22 (d, *J* = 8.1 Hz, 2H), 7.90 (dd, *J* = 8.3, 5.7 Hz, 2H), 7.49 – 7.42 (m, 4H), 7.24 (ddd, *J* = 21.8, 14.9, 7.4 Hz, 16H), 7.10 (t, *J* = 7.5 Hz, 2H), 6.98 (dd, *J* = 12.1, 5.5 Hz, 8H), 6.67 (dt, *J* = 12.0, 4.6 Hz, 2H), 2.44 (s, 3H).

Figure S7. ^{1}H NMR of complex **2a**

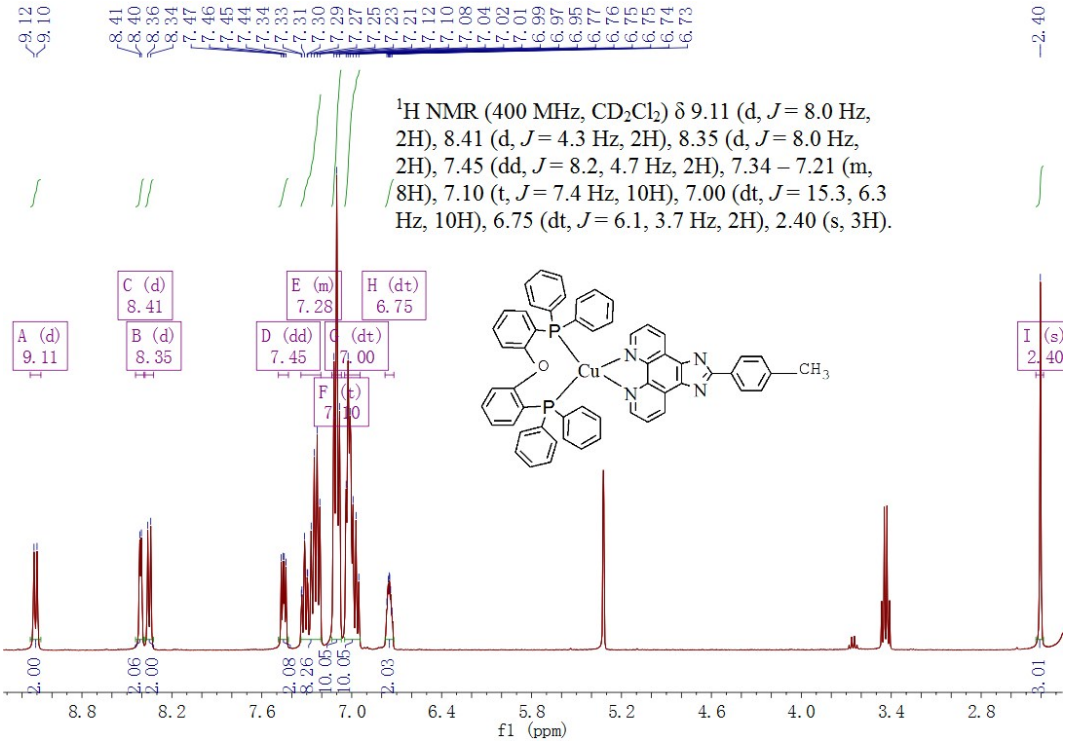


Figure S8. ^{1}H NMR of complex **2b**