

## Optical, Electrochemical and Photophysical Analyses of Heteroleptic Luminescent Ln(III) Complexes for Lighting Applications

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## Electronic Supporting Information

**Table S1** Energy transfer parameters of Hfodo and substituted 2,2'-bipyridine derivatives

Ligand	E <sub>S1</sub>	E <sub>T1</sub>	ΔE <sub>(S1-T1)</sub>	ΔE <sub>(T1-5D4 of Tb3+)</sub>	ΔE <sub>(T1-4G5/2 of Sm3+)</sub>
Hfodo	29,154	22,500	6,654	2,134	4,833
Bpy	29,673	22,883	6,790	2,517	5,216
DBr	31,152	23,696	7,456	3,330	6,029
MD	25,706	20,161	5,545	-205	2,494
DD	22,727	18,315	4,412	-2051	648

**Table S2** Percentage branching ratio of various transitions involved in T1-T4

Complex	Percentage branching ratio of transitions					
	Ligand	<sup>5</sup> D <sub>4</sub> → <sup>7</sup> F <sub>6</sub>	<sup>5</sup> D <sub>4</sub> → <sup>7</sup> F <sub>5</sub>	<sup>5</sup> D <sub>4</sub> → <sup>7</sup> F <sub>4</sub>	<sup>5</sup> D <sub>4</sub> → <sup>7</sup> F <sub>3</sub>	<sup>5</sup> D <sub>4</sub> → <sup>7</sup> F <sub>2,1,0</sub>
T1	-	18.06	64.09	10.94	6.26	0.64
T2	-	17.35	68.63	8.29	5.32	0.40
T3	-	21.40	59.92	12.11	6.21	0.35
T4	-	23.19	63.90	8.69	3.77	0.44

**Table S3** Percentage branching ratio of various transitions involved in S1-S4

Complex	Percentage branching ratio of transitions				
	Ligand	<sup>4</sup> G <sub>5/2</sub> → <sup>6</sup> H <sub>5/2</sub>	<sup>4</sup> G <sub>5/2</sub> → <sup>6</sup> H <sub>7/2</sub>	<sup>4</sup> G <sub>5/2</sub> → <sup>6</sup> H <sub>9/2</sub>	<sup>4</sup> G <sub>5/2</sub> → <sup>6</sup> H <sub>11/2</sub>
S1	-	6.52	24.91	65.79	2.77
S2	-	2.28	21.45	75.41	0.01
S3	66.74	1.97	7.35	21.87	2.06
S4	67.96	2.35	6.69	22.43	0.06

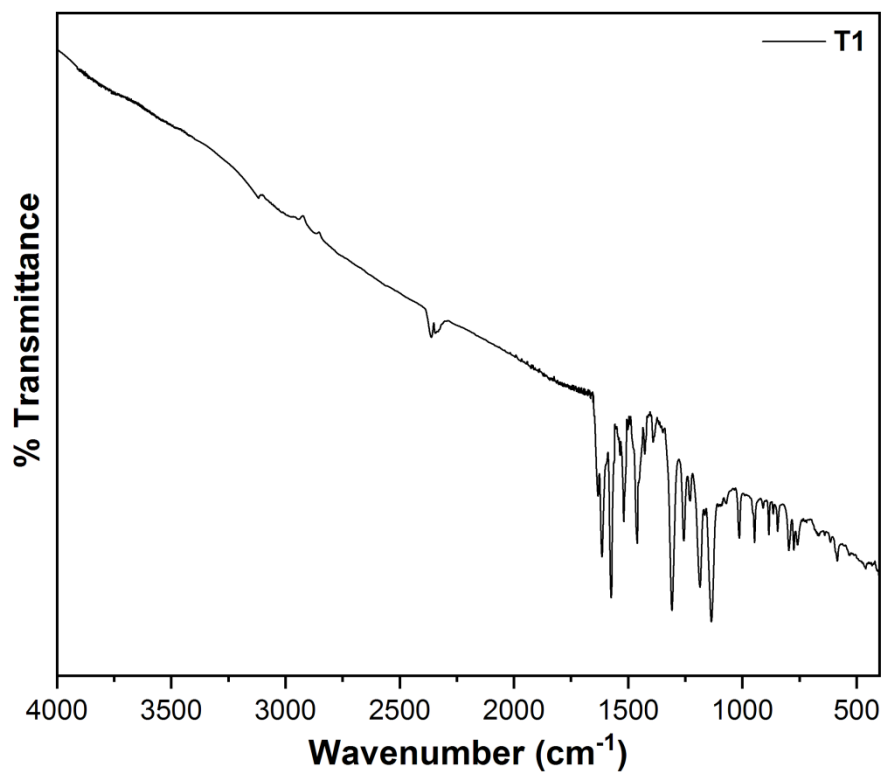


Fig. S1 IR spectrum of T1

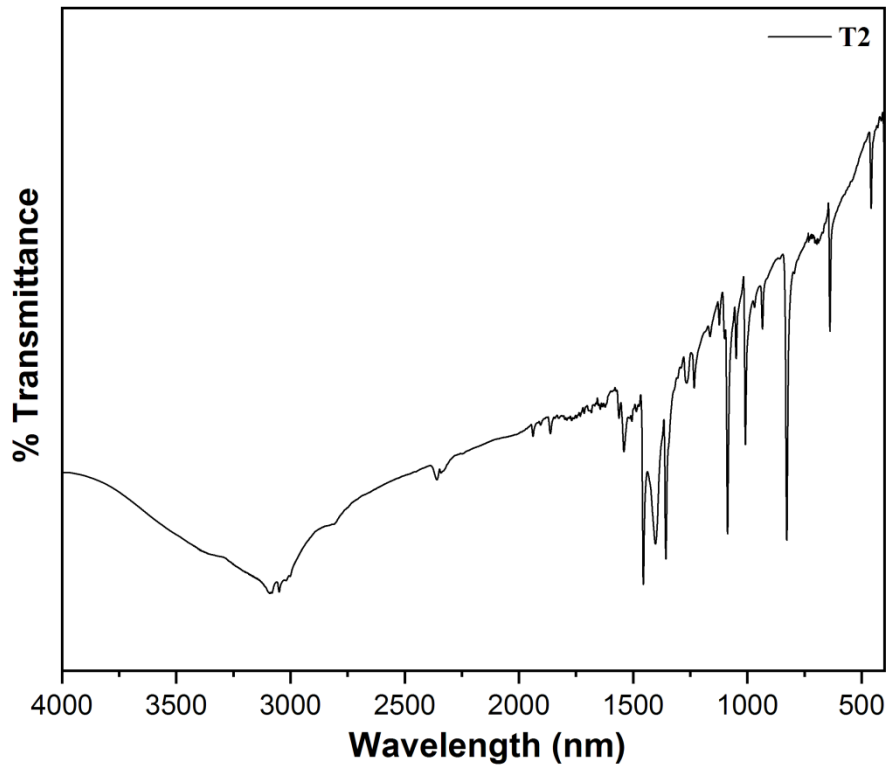
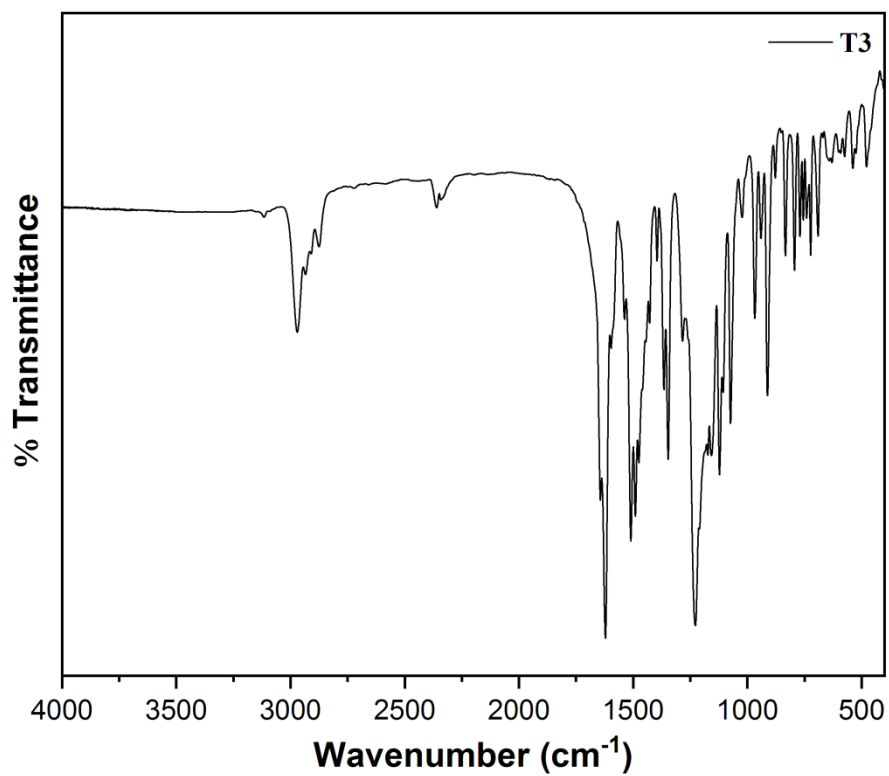
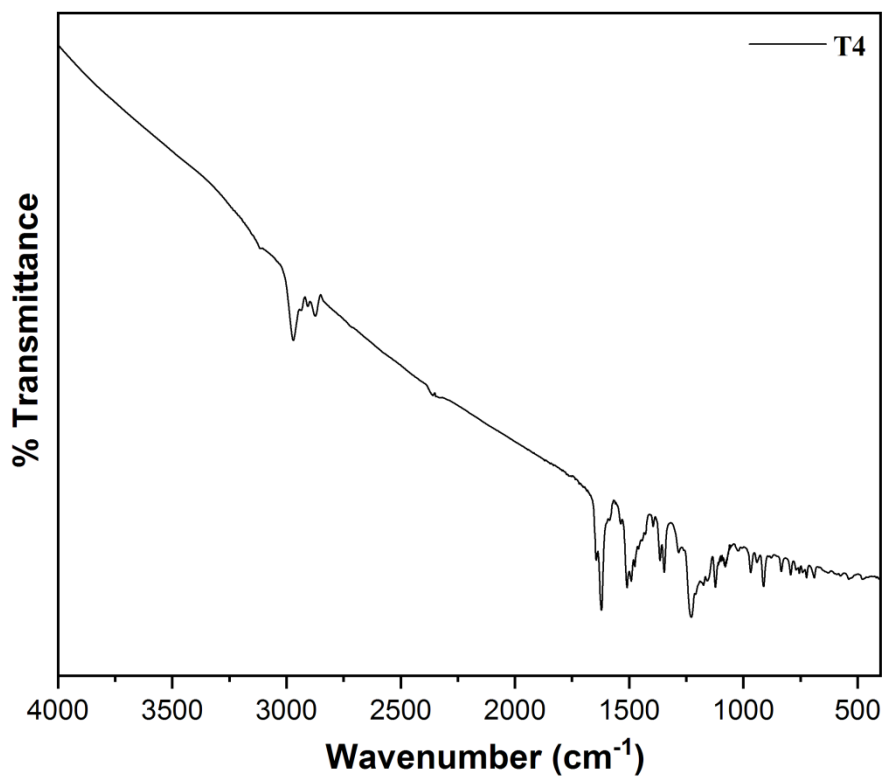


Fig. S2 IR spectrum of T2



**Fig. S3** IR spectrum of T3



**Fig. S4** IR spectrum of T4

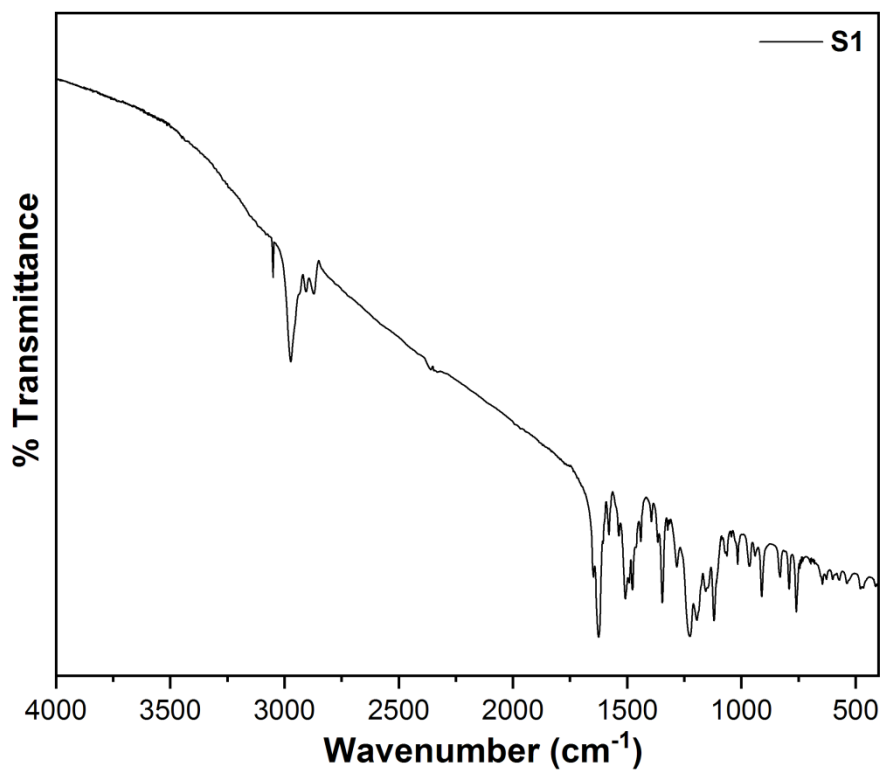


Fig. S5 IR spectrum of S1

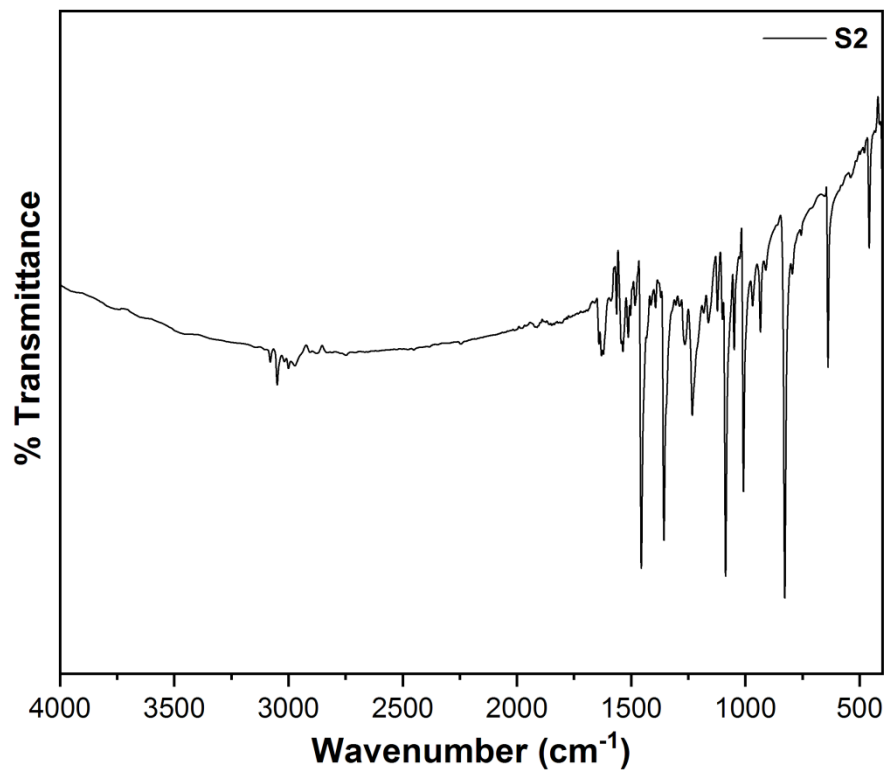
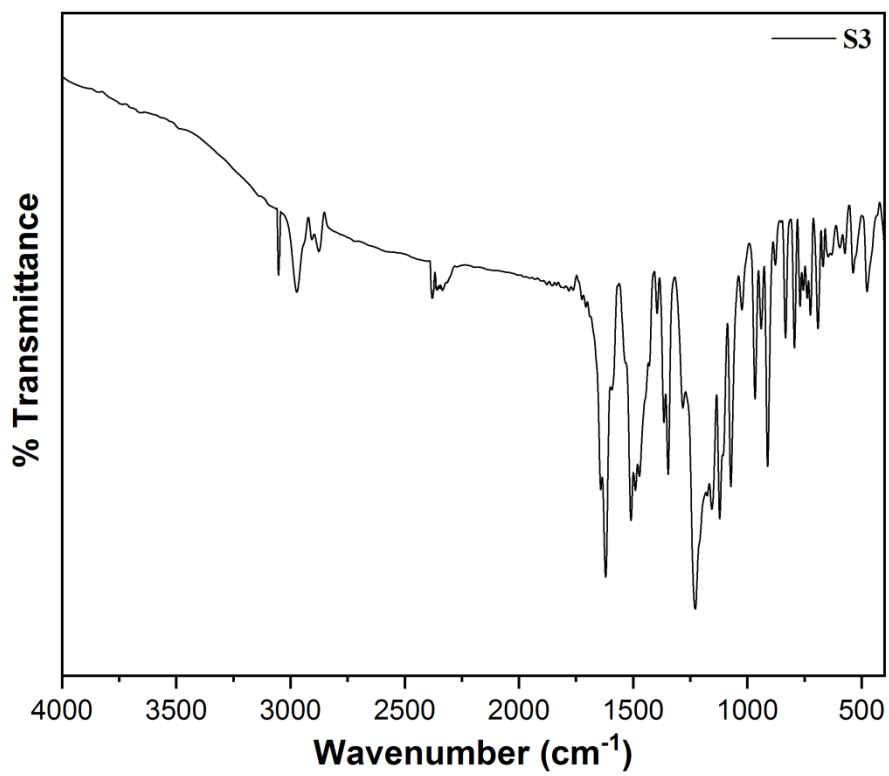
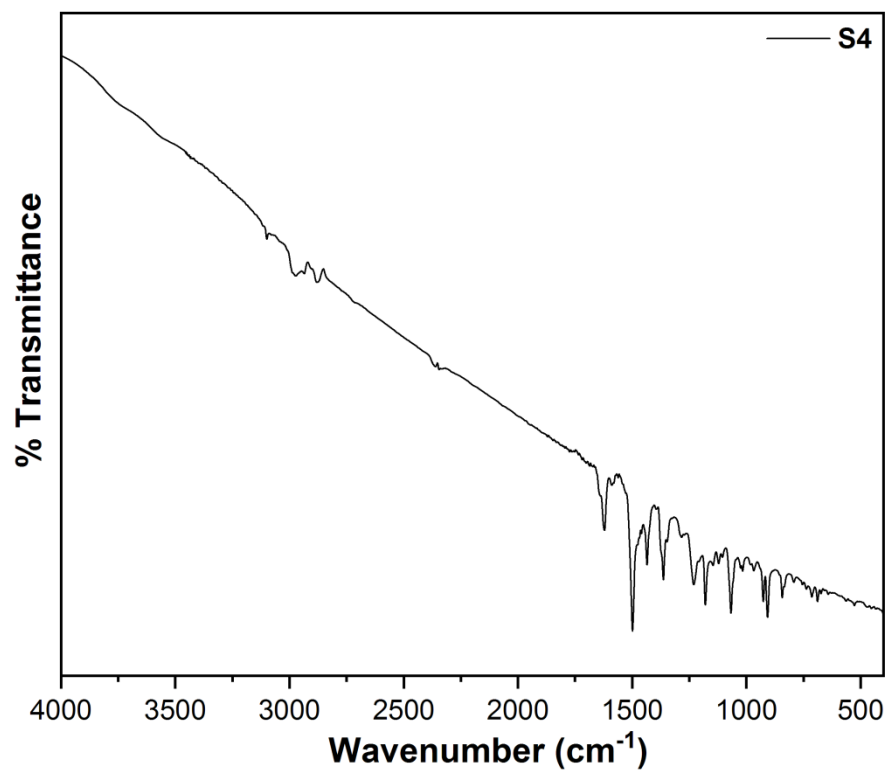


Fig. S6 IR spectrum of S2



**Fig. S7** IR spectrum of S3



**Fig. S8** IR spectrum of S4

Feb14-2023.50.fid  
5  
1H\_8scan CDCl3 {D:\Spectra} nmr 5

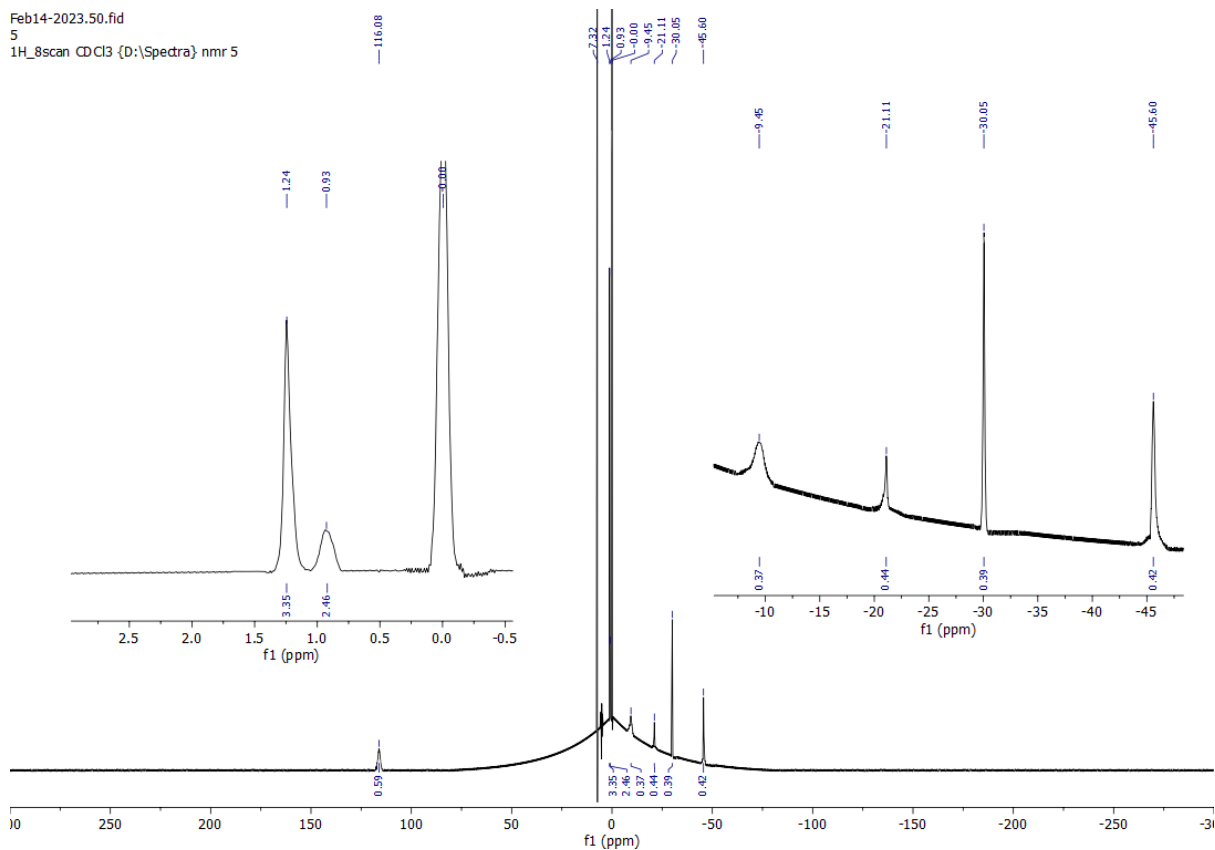


Fig. S9 NMR spectrum of T1

Feb14-2023.60.fid  
6  
1H\_8scan CDCl3 {D:\Spectra} nmr 6

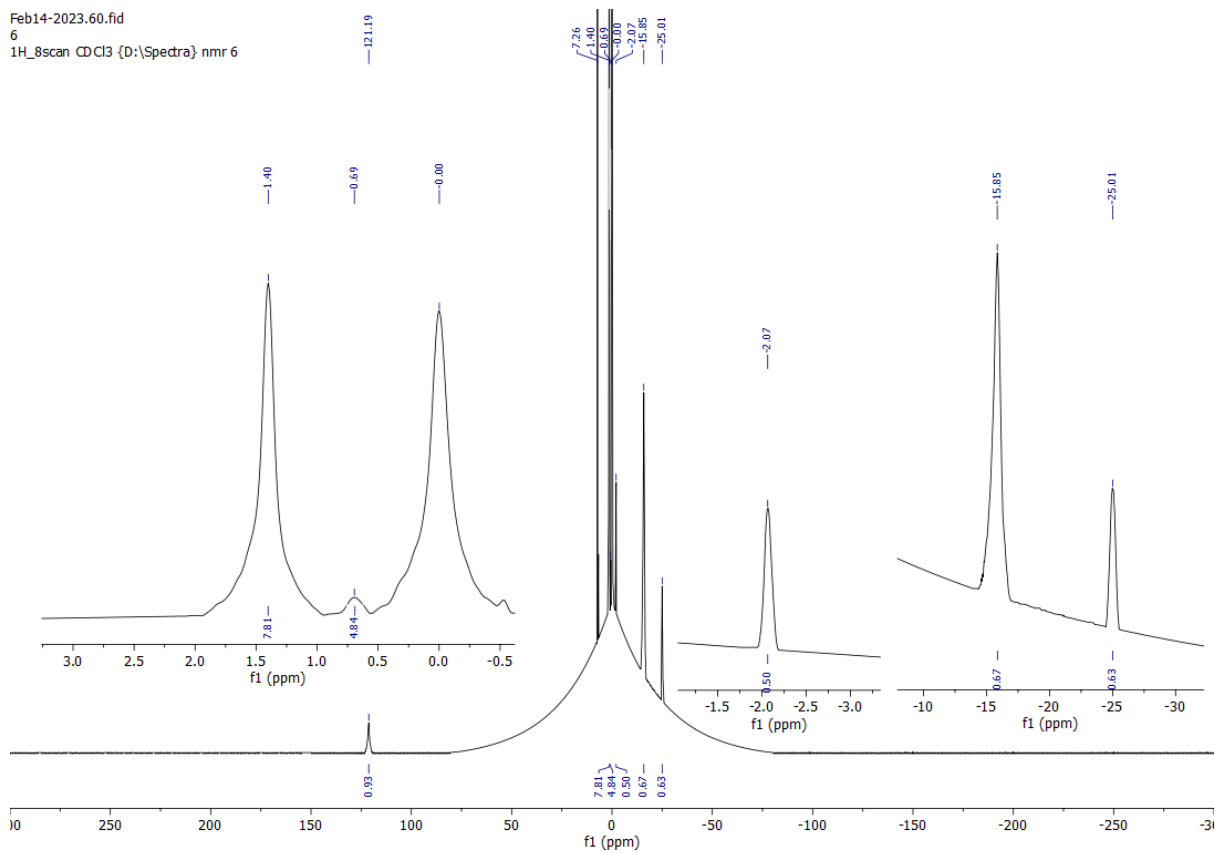


Fig. S10 NMR spectrum of T2



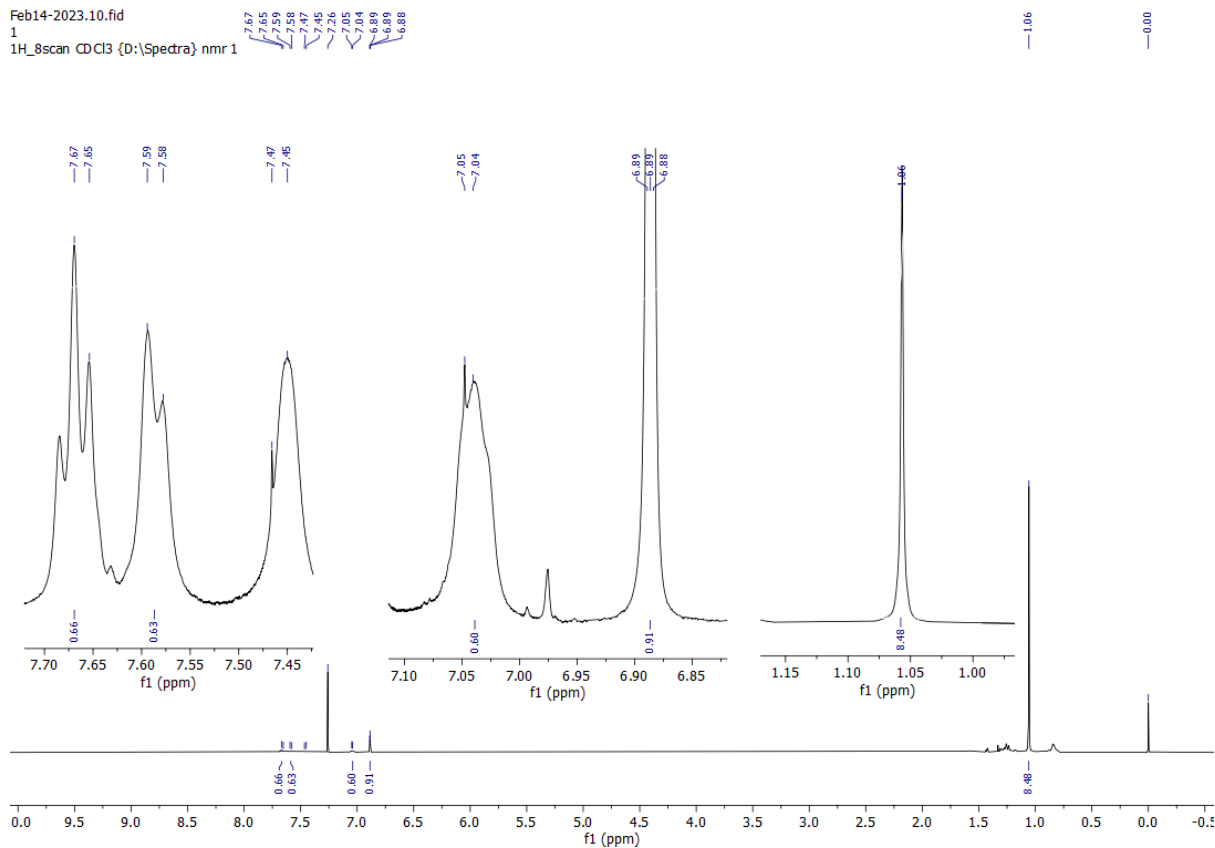


Fig. S13 NMR spectrum of S1

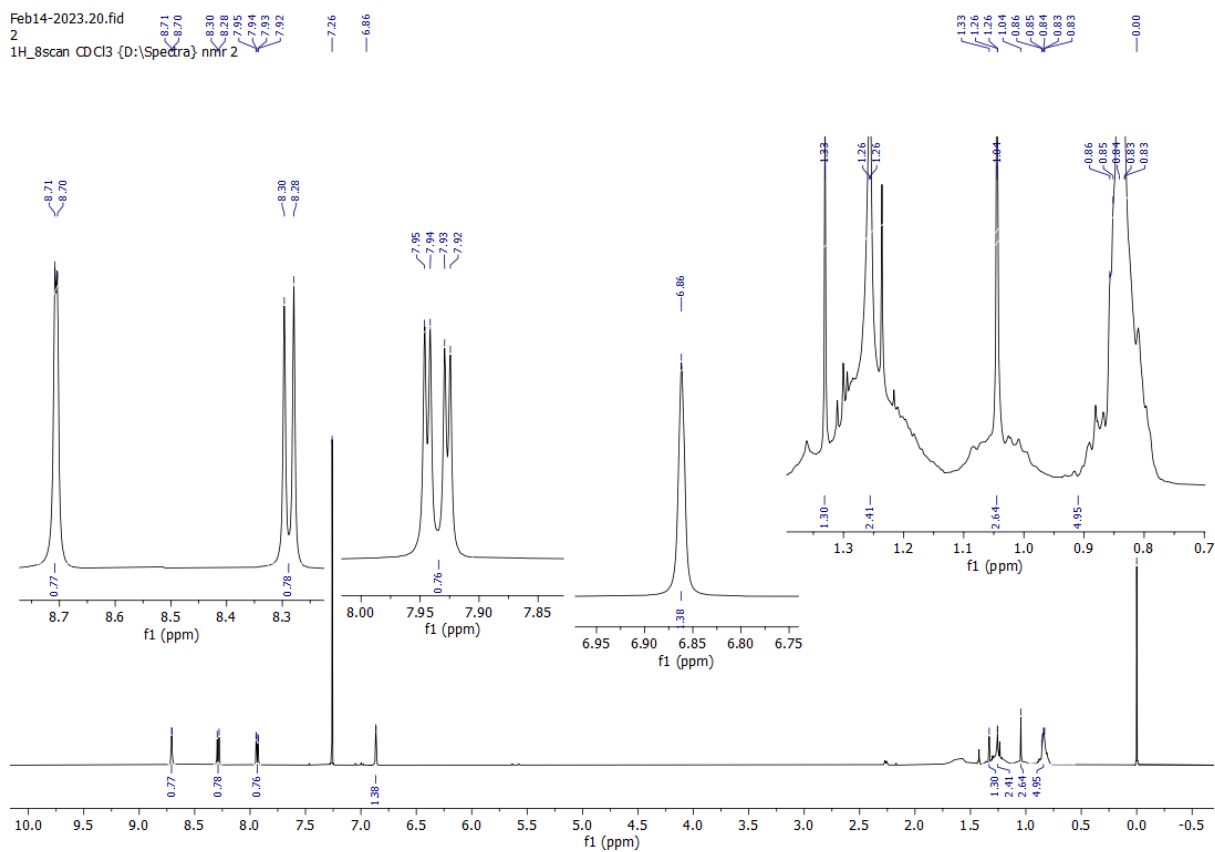


Fig. S14 NMR spectrum of S2



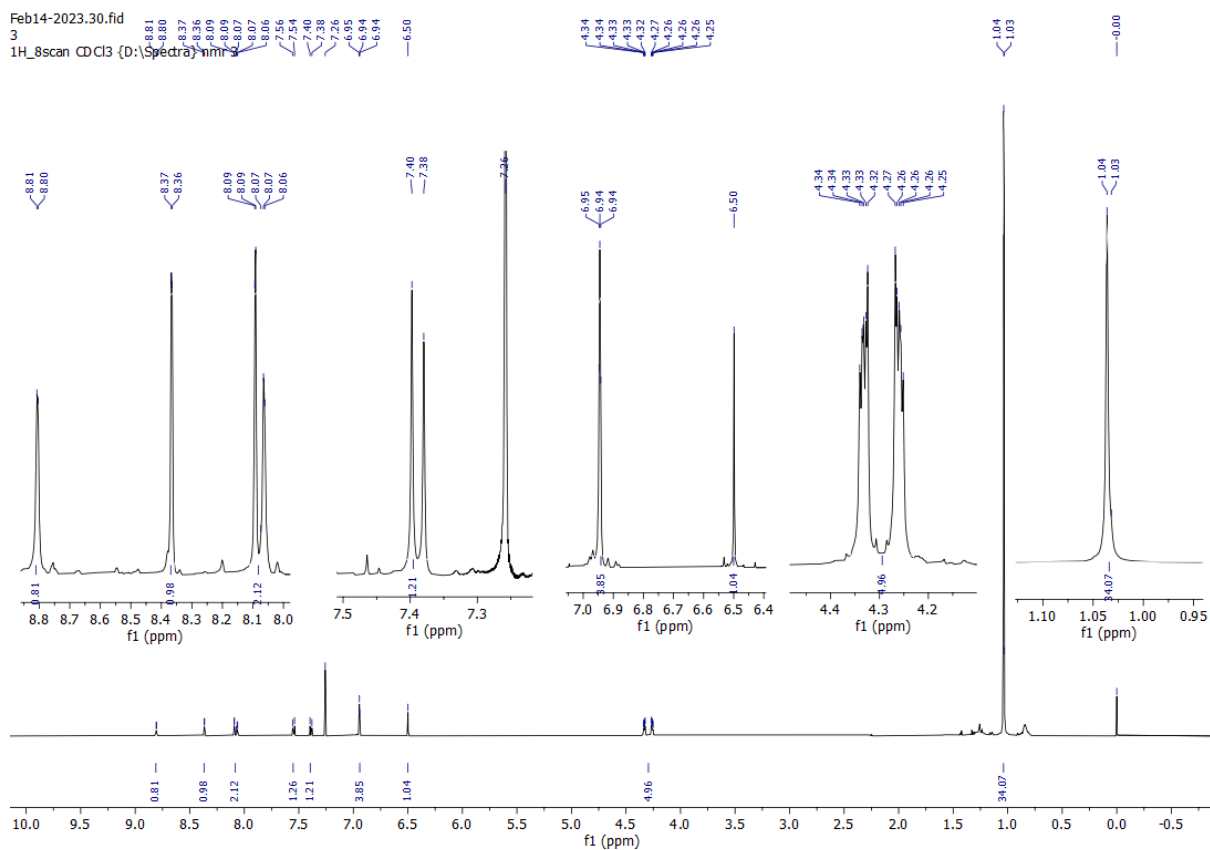


Fig. S15 NMR spectrum of S3

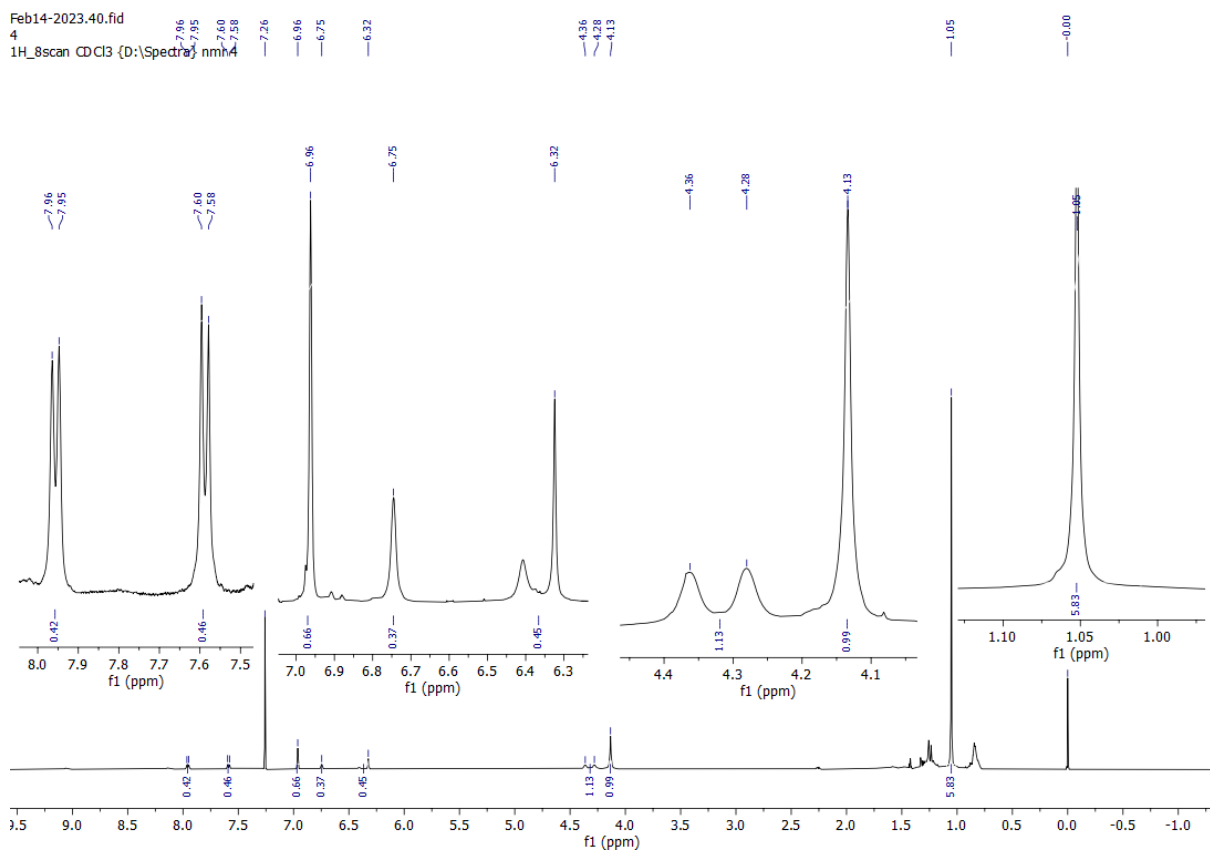
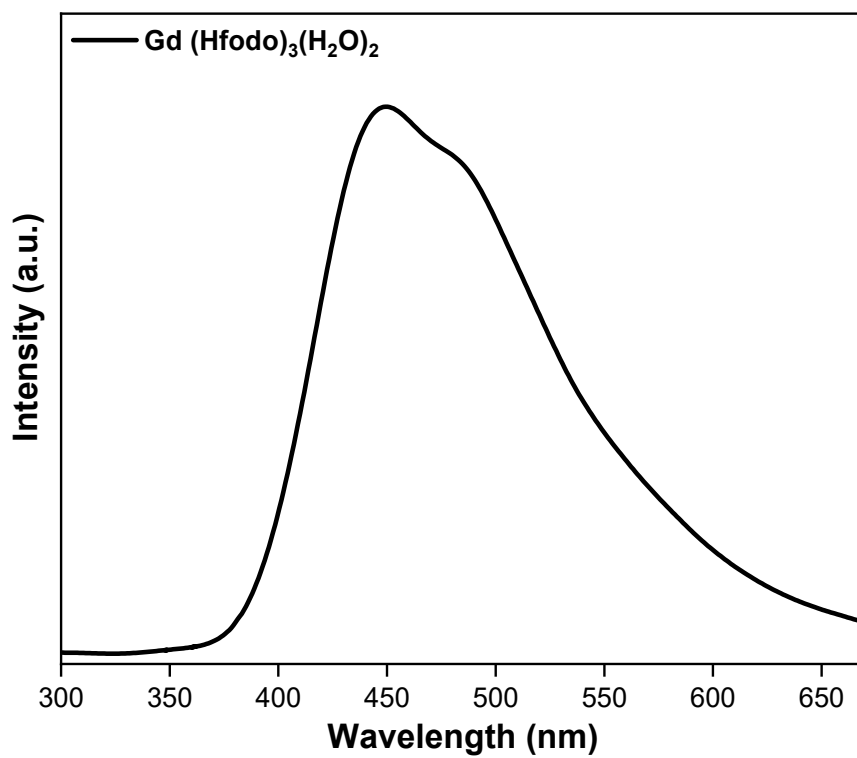


Fig. S16 NMR spectrum of S4



**Fig. S17** Phosphorescence spectrum of  $[Gd(Hfodo)_3(H_2O)_2]$