Supplementary Information

for

Luminescent magnesium complexes with intra- and inter-ligand charge transfer

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❖ General experimental information for the synthesis of compounds:

All reactions were performed under argon atmosphere using Schlenk techniques or inside a MBraun glove box. The solvents used were purified by an MBRAUN solvent purification system MB SPS-800. Ligand (**PyPyrH**) was prepared according to the reported literature procedure.[1] All the chemicals were purchased from Sigma–Aldrich, TCI chemicals and used without further purification. C_6D_6, $CDCl_3$ were purchased from Sigma-Aldrich, were degassed by three freeze-pump-thaw cycles and stored over molecular sieves. ^1H and $^{13}C\{^1H\}$ spectra were recorded on Bruker AV-200 MHz, AV-400 MHz and AV-500 MHz and referenced to the resonances of the solvent used. HRMS spectra were obtained using Thermo scientific Q-Exactive instrument.

X-ray intensity data measurements of compound **1** and **2** were carried out on a Bruker SMART APEX II CCD diffractometer with graphite-monochromatized (MoKα= 0.71073Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of ϕ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2006).[2] All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full-matrix least-squares refinement on F2.[3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An ORTEP III [4] views of all compounds were drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity. Powder X-ray diffraction was done in IISER, Pune for compound **2**.

❖ Synthesis, characterization and crystal data for compound 1 and 2:

1: Isopropyl magnesium chloride (1.6 mL, 3.19 mmol, 2.0 M in THF) was added to a stirring solution of ligand (**PyPyrH**) (500 mg, 2.90 mmol) in THF (20 mL) at –78 ˚C. The reaction mixture was kept in cooling bath for 2 hour and then allowed to warm slowly to room temperature and stirred further for 12 h at this temperature. The solvent was removed under vacuum and the residue was extracted with toluene (30 mL). Crystallization was performed in toluene at 4 ˚C in a freezer. Yield: 1.26 g {94.0 % (without THF molecules) and 64.2 % (with THF molecules). ^1H NMR (C_6D_6, 500 MHz, 298 K): δ 9.02 (bs, 2H, *Py*), 7.40-7.38 (d, 2H, *Py*), 7.07-7.03 (t, 2H, *Py*), 6.37-

6.33 (t, 2H, *Py*), 6.28 (s, 2H, *Pyr*), 2.93 (bs, 6H, PyrCH_3), 2.51 (s, 6H, PyrCH_3) ppm; $^{13}C\{^1H\}$ NMR (C_6D_6, 100.5 MHz, 298 K): δ 158.78, 148.63, 138.16, 131.86, 124.25, 117.67, 115.99, 115.38 (*Py* & *Pyr*), 17.93, 16.23 (CH_3) ppm. ESI-HRMS: calculated for $C_{50}H_{76}K_2N_6O_2$ $[M+H]^+$: 677.2648; found: 677.5099 (see Figure S3). Elemental analysis: calcd. C, 60.21; H, 6.84; N, 8.26; found C, 58.87; H, 5.23; N, 7.71. Due to the sensitivity of the crystals, the observed values deviate from the calculated one.

Crystal data of 1. CCDC number- 2189747, $C_{34}H_{43}Cl_2Mg_2N_4O_3$, M=675.24, green, block, 0.32 x 0.21 x 0.15 mm^3, monoclinic, space group *Cc*, *a*=8.8994(7)Å, *b*=24.393(3)Å, *c*=16.1873(14)Å, α=90°, β=105.719(3)°, γ=90°, *V*=3382.6(5)Å^3 , *Z*=4, *T*=100(2) K, 2θmax=50.00°, *Dcalc* (g cm^{-3})=1.326, *F*(*000*)=1428, μ (mm^{-1})=0.270, 10000 reflections collected, 9221 unique reflections (*R*int=0.0552), 9625 observed ($I > 2\sigma$ (*I*)) reflections, multi-scan absorption correction, *T*min=0.917, *T*max=0.960, 440 refined parameters, *S*=1.148, *R*1=0.0552, *wR2*=0.1406 (all data *R*=0.0611, *wR2*=0.1452), maximum and minimum residual electron densities; $\Delta\rho$max=0.587, $\Delta\rho$min=-0.352 (eÅ^{-3}).

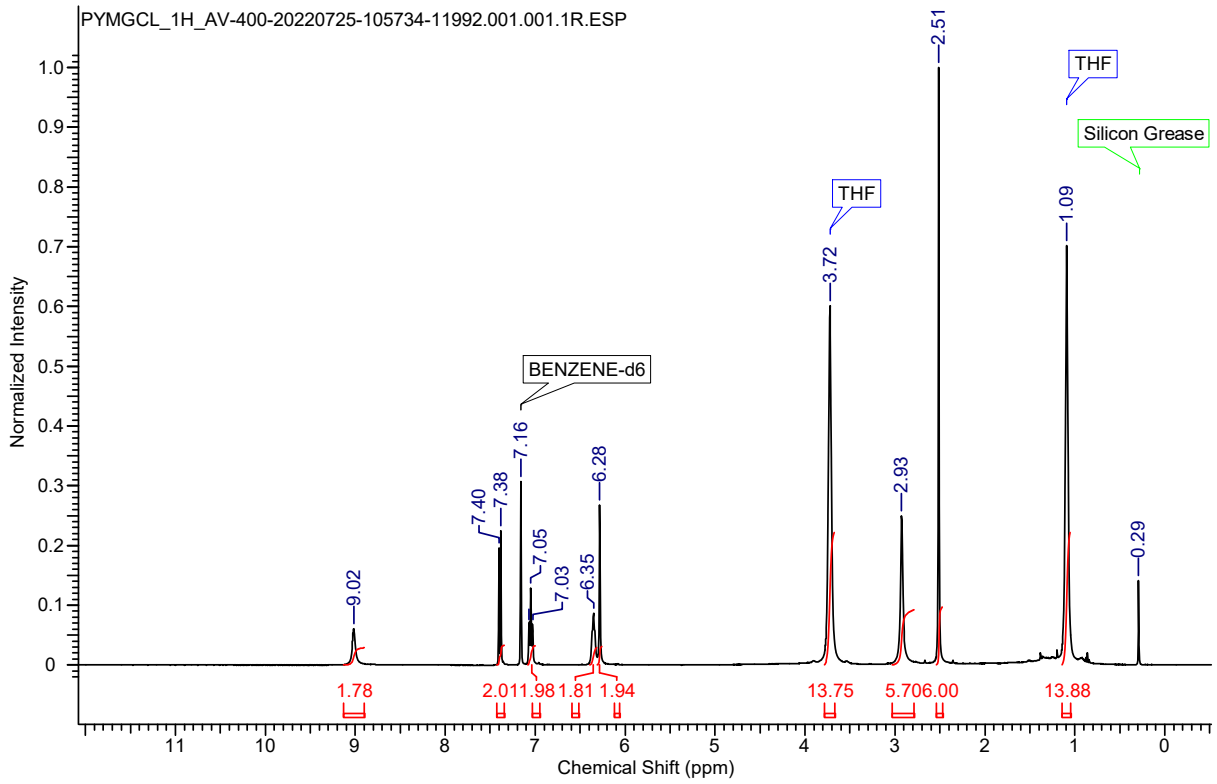

Figure S1. ^1H NMR Spectrum of **1** (C_6D_6, 500 MHz, 298 K).

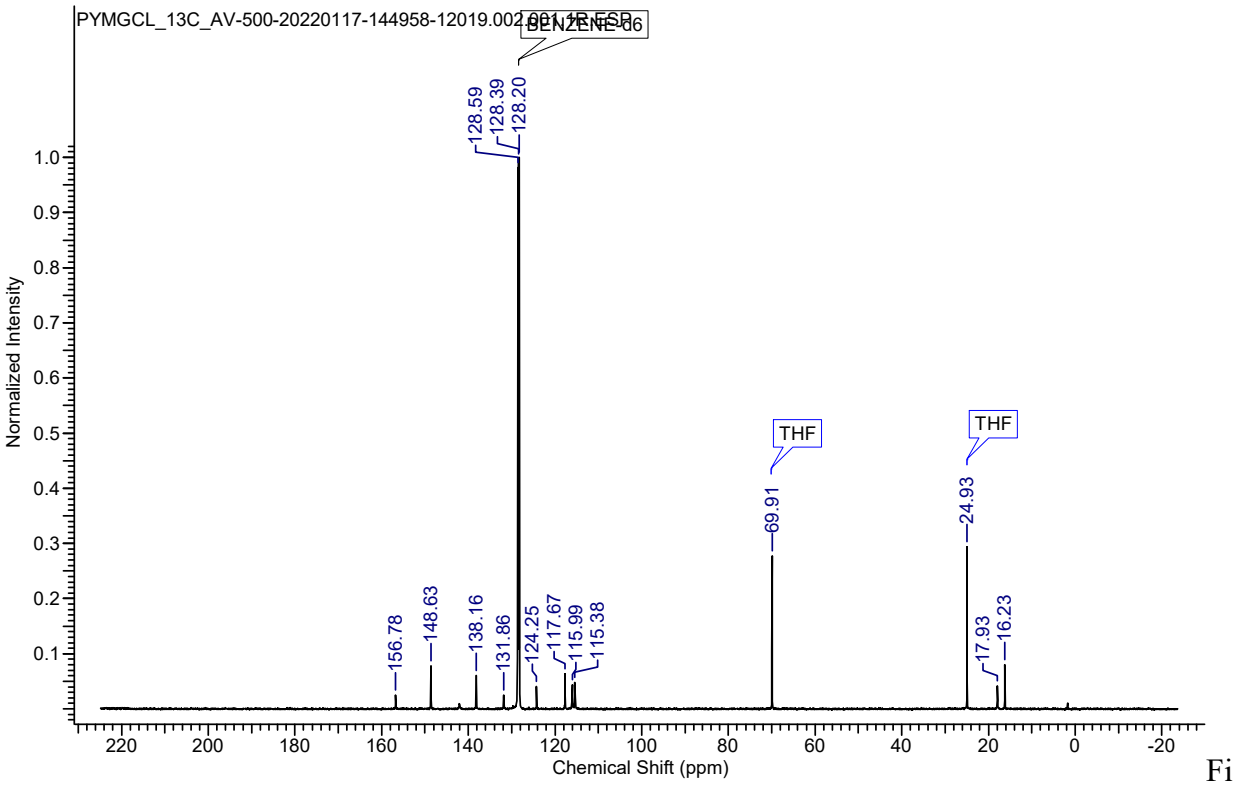

Figure S2. ^{13}C NMR Spectrum of **1** (C_6D_6, 100.28 MHz, 298 K).

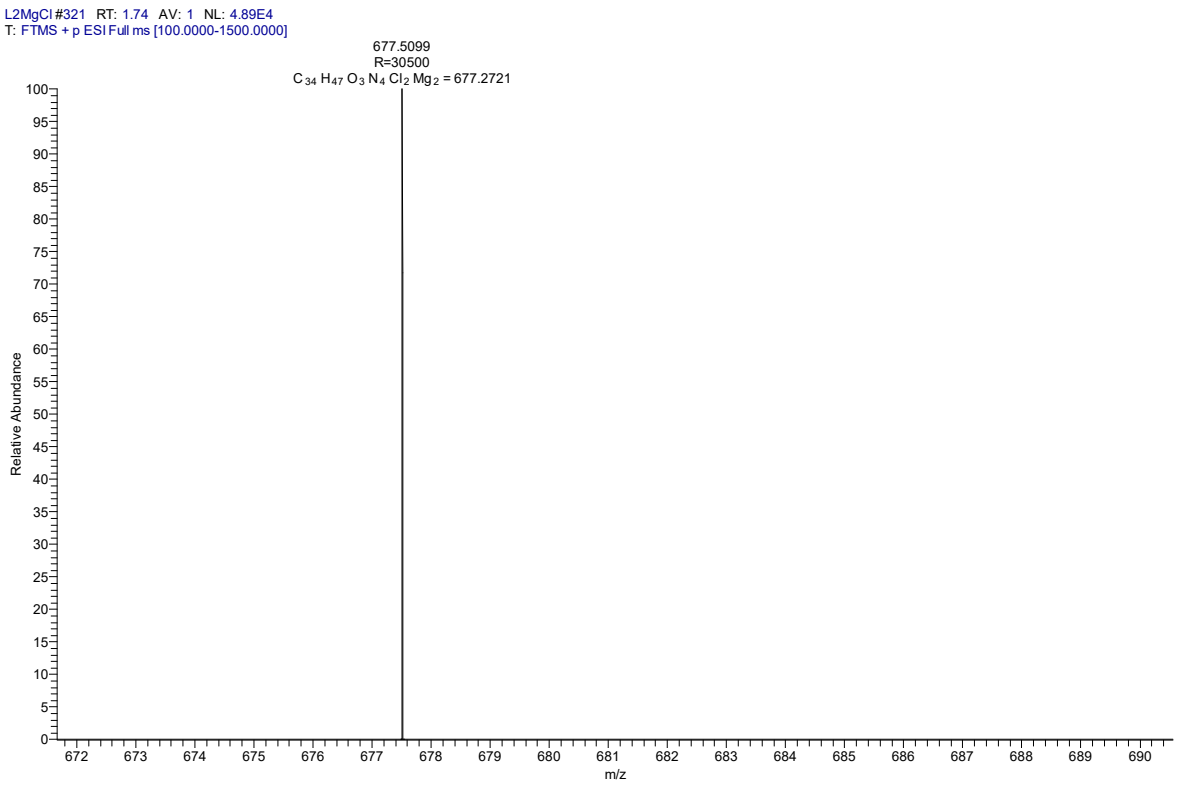

Figure S3. HRMS of compound **1**.

2: **Method (i)** *n*BuLi (1.6 mL, 3.19 mmol, 2.0 M solution in cyclohexane) was added to a stirring solution of ligand (**PyPyrH**) (500 mg, 2.90 mmol) in THF (20 mL) at –78 ˚C. The reaction mixture was kept in cooling bath for 30 min and then allowed to warm slowly to room temperature and stirred further for 4 h at this temperature. Again, reaction mixture was cooled to -78 C and isopropyl magnesium chloride (1.6 mL, 3.19 mmol, 2.0 M in THF) was added at this temperature. The reaction mixture was kept in cooling bath for 2 hours and then allowed to warm slowly to room temperature and stirred further for 4 h at this temperature. The solvent was removed under vacuum and the residue was extracted with toluene (30 mL). Crystallization was performed in toluene at 4 ˚C in a freezer. Yield: 0.920 g {86.8 % (without THF molecule) and 72.4 % (with THF molecule). ^{1}H NMR (C_6D_6, 500 MHz, 298 K): δ 8.04-8.03 (d, 2H, *Py*), 7.38-7.36 (d, 2H, *Py*), 6.95-6.93 (d, 2H, *Py*), 6.40 (s, 4H, *Py* & *Pyr*), 6.14-6.12 (t, 2H, *Pyr*), 2.60 (s, 6H, Pyr*CH*$_3$), 2.40 (s, 6H, Pyr*CH*$_3$) ppm; ^{13}C{^{1}H} NMR (C_6D_6, 100.5 MHz, 298 K): δ 157.50, 148.51, 139.64, 138.72, 132.44, 124.44, 117.92, 115.97, 115.16 (*Py* & *Pyr*), 17.16, 15.95 (*CH*$_3$) ppm. ESI-HRMS: calculated for $C_{50}H_{76}K_2N_6O_2$ $[M+H]^+$: 439.2270; found: 439.6562 (see Figure S6). Elemental analysis(**2**-THF): calcd. C, 72.05; H, 6.05; N, 15.28; found C, 71.45; H, 5.23; N, 15.11.

Method (ii) Ethyl magnesium bromide (1.6 mL, 3.19 mmol, 2.0 M in THF) was added to a stirring solution of ligand (**PyPyrH**) (500 mg, 2.90 mmol) in THF (20 mL) at –78 ˚C. The reaction mixture was kept in cooling bath for 2 hour and then allowed to warm slowly to room temperature and stirred further for 12 h at this temperature. The solvent was removed under vacuum and the residue was extracted with toluene (30 mL). Crystallization was performed in toluene at 4 ˚C in a freezer.

Method (iii) *n*BuLi (1.6 mL, 3.19 mmol, 2.0 M solution in cyclohexane) was added to a stirring solution of ligand (**PyPyrH**) (500 mg, 2.90 mmol) in THF (20 mL) at –78 ˚C. The reaction mixture was kept in cooling bath for 30 min and then allowed to warm slowly to room temperature and stirred further for 4 h at this temperature. Again, reaction mixture was cooled to -78 C and methyl magnesium bromide (1.03 mL, 3.19 mmol, 3.1 M in THF) was added at this temperature. The reaction mixture was kept in cooling bath for 2 hours and then allowed to warm slowly to room temperature and stirred further for 4 h at this temperature. The solvent was removed under vacuum and the residue was extracted with toluene (30 mL). Crystallization was performed in toluene at 4 ˚C in a freezer. The best yield for compound **2** was observed using method (i), While a little discrepancy was observed in the yield with methods (ii) and (iii).

Crystal data of 2. CCDC number- 2189748, $C_{26}H_{30}MgN_4O$, M=438.85, green, block, 0.33 x 0.25 x 0.12 mm^3, monoclinic, space group *Pc*, *a*=9.1371(8)Å, *b*=16.8002(17)Å, *c*= 8.3053(8)Å, *α*=90°, β=116.752(3)°, *γ*=90°, *V*=1138.44(19)Å^3 , *Z*=2, *T*=100(2) K, 2θmax=50.00°, *Dcalc* (g cm^{-3})=1.280, *F*(*000*)=468, μ (mm^{-1})=0.104, 4542 reflections collected, 3863 unique reflections (*R*int=0.0824), 4503 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, *T*min=0.966, *T*max=0.988, 543 refined parameters, *S*=1.141, *R*1=0.0824, *wR*2=0.1595 (all data *R*=0.0970, *wR*2=0.1662), maximum and minimum residual electron densities; *Δ*ρmax=0.464, *Δ*ρmin=-0.238 (eÅ^{-3}).

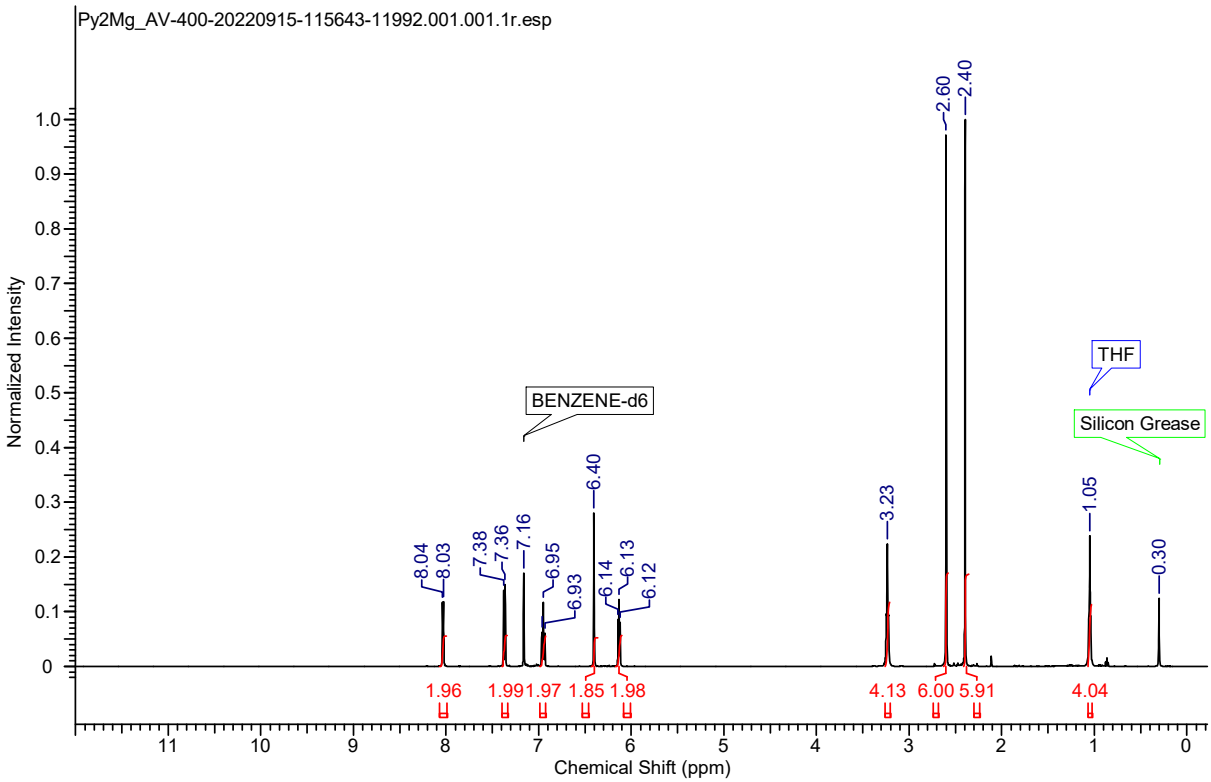

Figure S4. ^{1}H NMR Spectrum of **2** (C_6D_6, 500 MHz, 298 K).

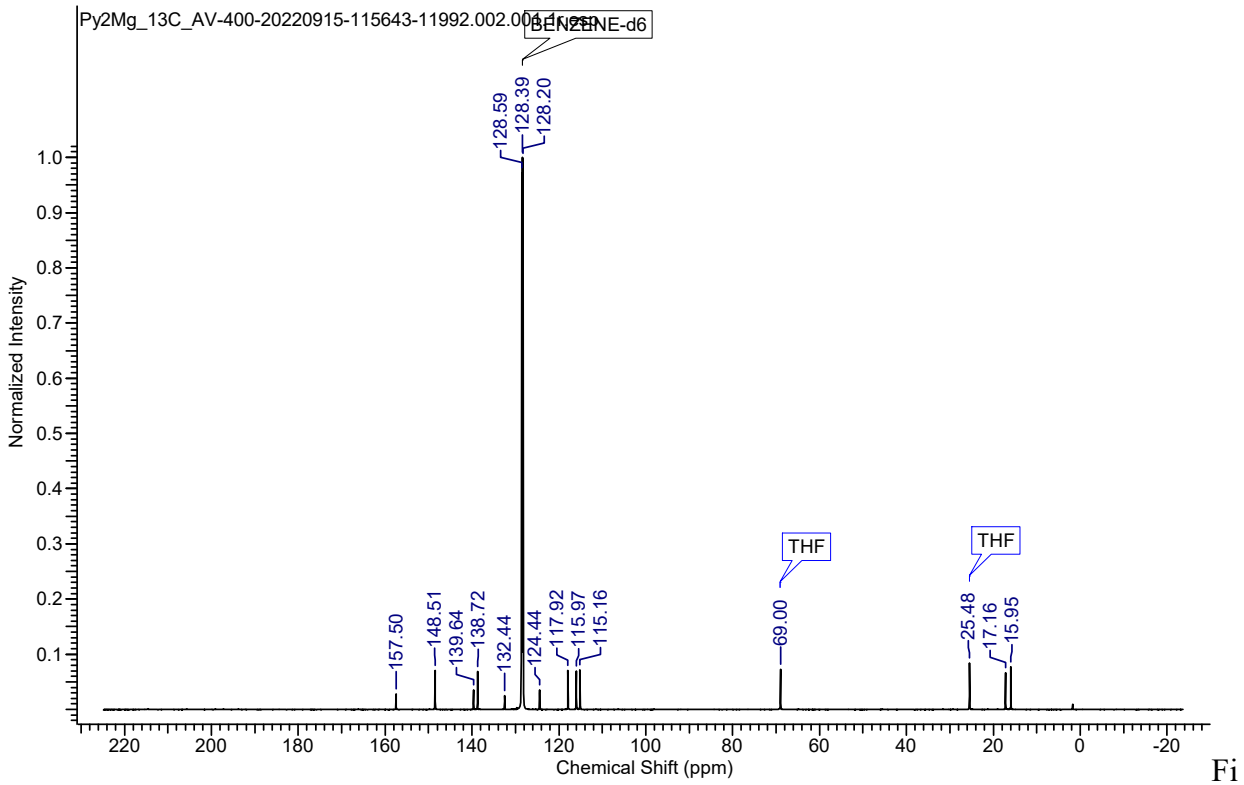

Figure S5. ^{13}C NMR Spectrum of **2** (C_6D_6, 100.28 MHz, 298 K).

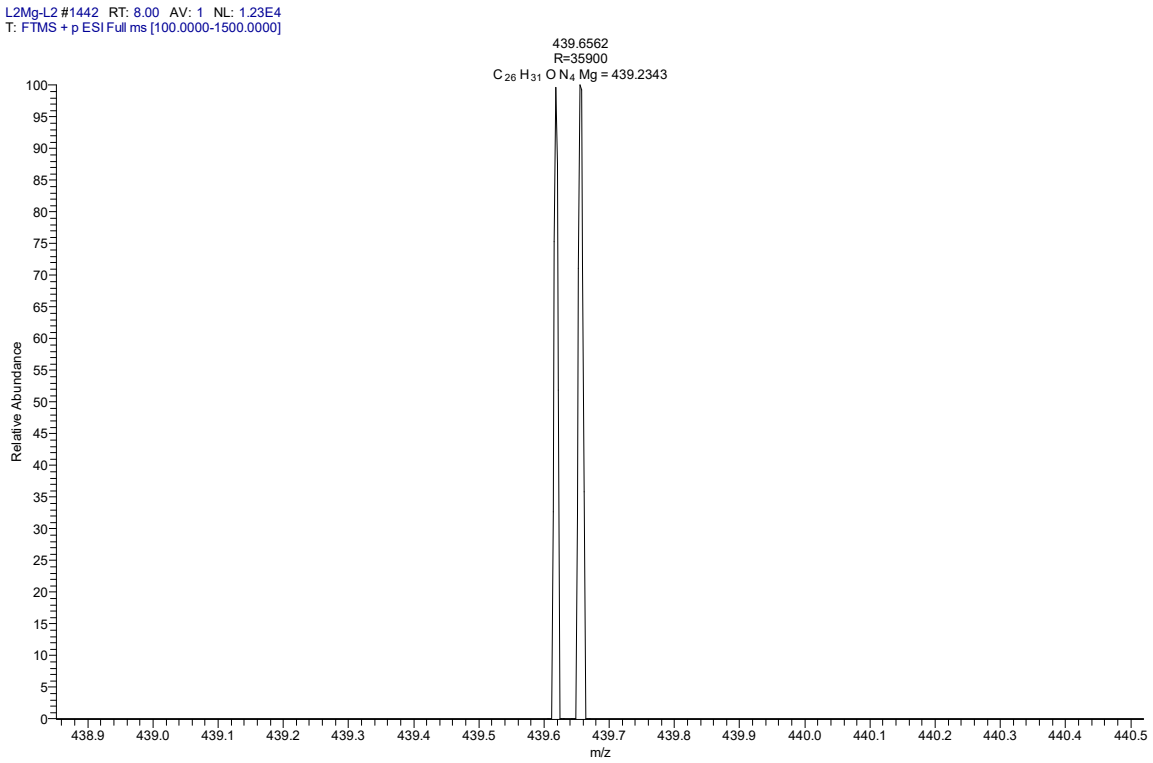

Figure S6. HRMS of compound **2**.

❖ **Photophysical investigations and quantum yield measurement:**

A Shimadzu UV−vis−IR (UV3600 Plus) spectrophotometer was used for optical absorption measurements. Absorption measurements of solid compounds were carried out with the help of an integrating sphere (ISR-603), attached to a Shimadzu UV-3600 Plus spectrophotometer. Steady-state emission spectra were collected in a Fluoromax-4 spectrofluorometer (Horiba, Jobin Yvon, USA). A spectrofluorometer FS5 (Edinburgh Instruments) was used for lifetime measurements of solid compounds using their SC-05 and SC-10 attachments (EPLED-330 picosecond pulsed diode LASER).

Photophysical studies in solid state:

Table S1. Lifetime fitting parameters of compound **1** and **2** obtained from TCSPC.

Sample	α_1	τ_1 (ns)	α_2	τ_2 (ns)	$\langle\tau\rangle$ (ns)
1	0.63	4.14	0.38	9.37	7.16
2	0.64	6.20	0.33	8.12	6.98

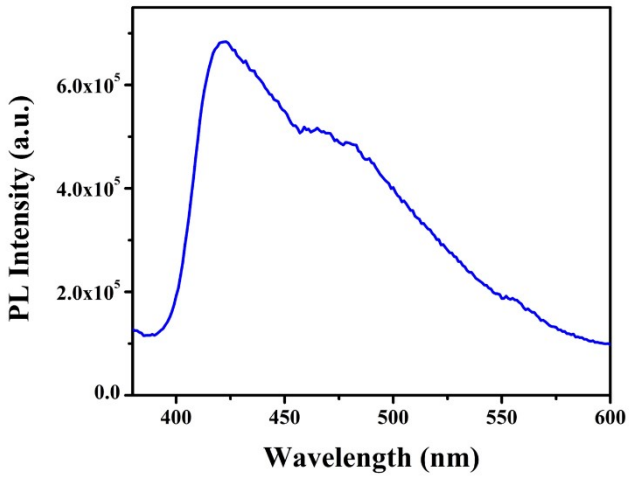

Figure S7. Solid state emission spectra of PyPyrH ligand (Excited at 340 nm).

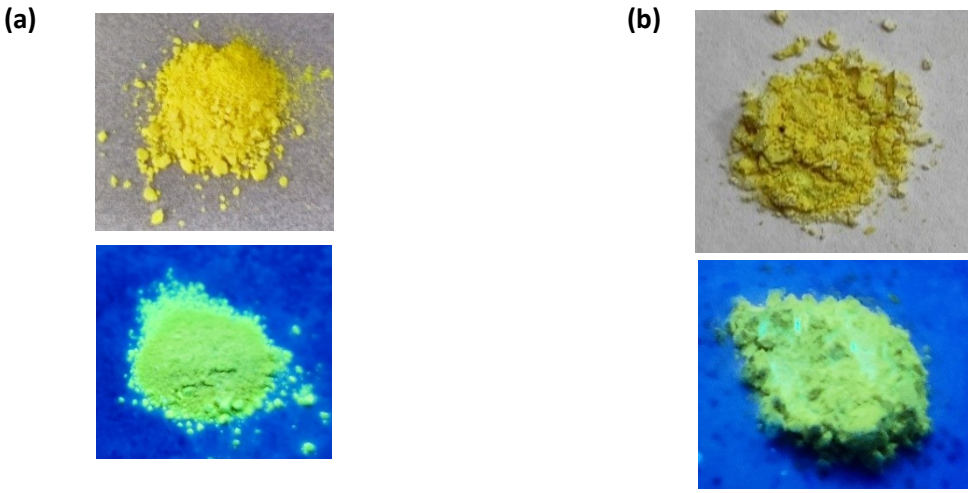

Figure S8. Daylight and UV-light images of (a) compound **1**, (b) compound **2**.

Quantum yield measurement:

Absolute quantum yield was estimated by using integrating sphere method in a Fluoromax-4 spectrofluorometer (Horiba, Jobin Yvon, USA).

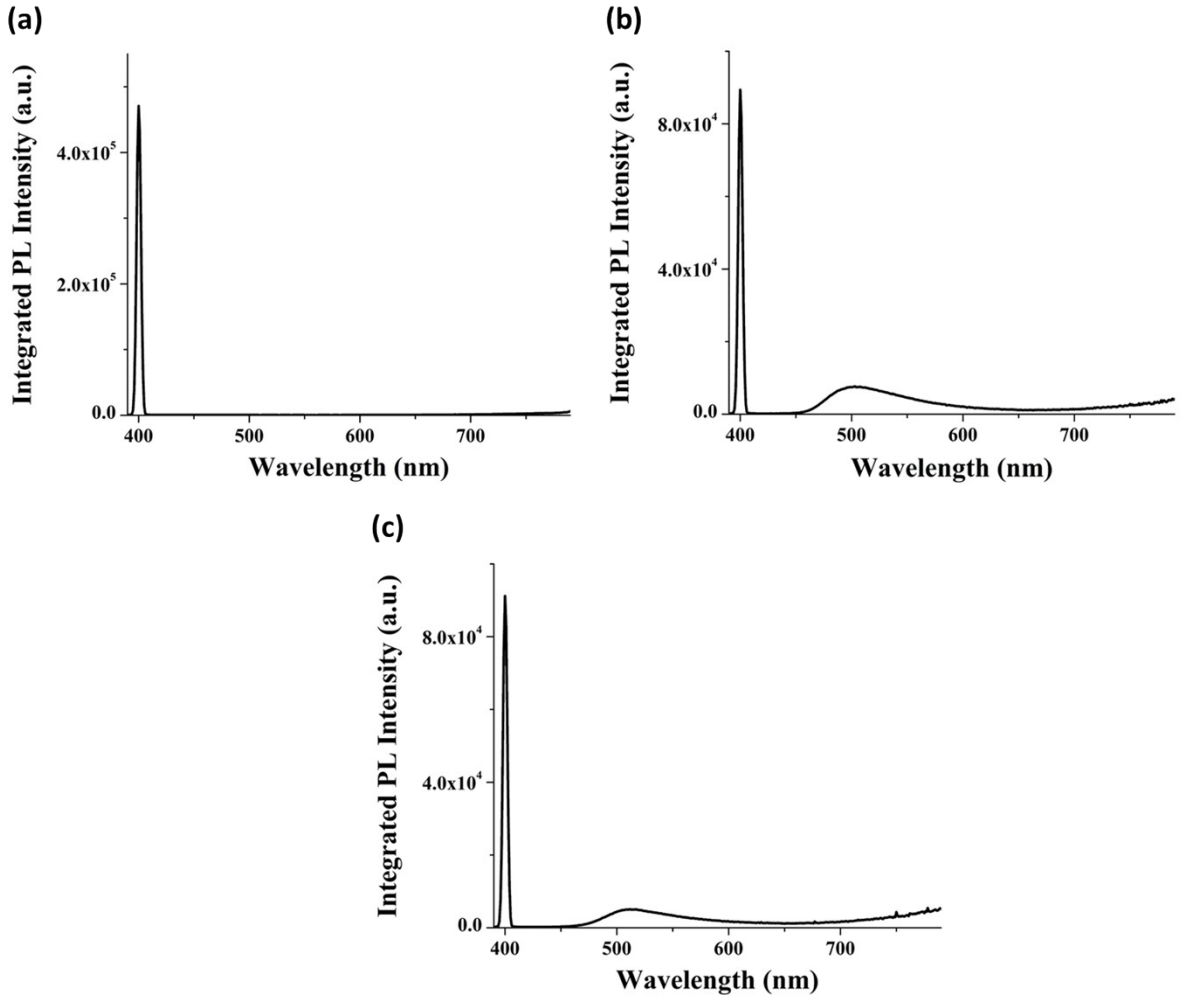

Figure S9. (a) Integrated scattering for the reference, (b) Integrated scattering and emission spectra of compound **1**, (c) Integrated scattering and emission spectra of compound **2**.

Calculated absolute quantum yield for compound **1** ~ 22.73%

Relative error = ± 0.00157

Absolute error = ± 0.036.

Calculated absolute quantum yield for compound **2** ~ 14.47%

Relative error = ± 0.00235

Absolute error = ± 0.034.

Photophysical studies in solution state:

We have done the photophysical studies in solution state and we found that both the compounds are not very stable in THF and slowly decompose to the ligand. The solution state photo luminescent studies confirmed this observation.

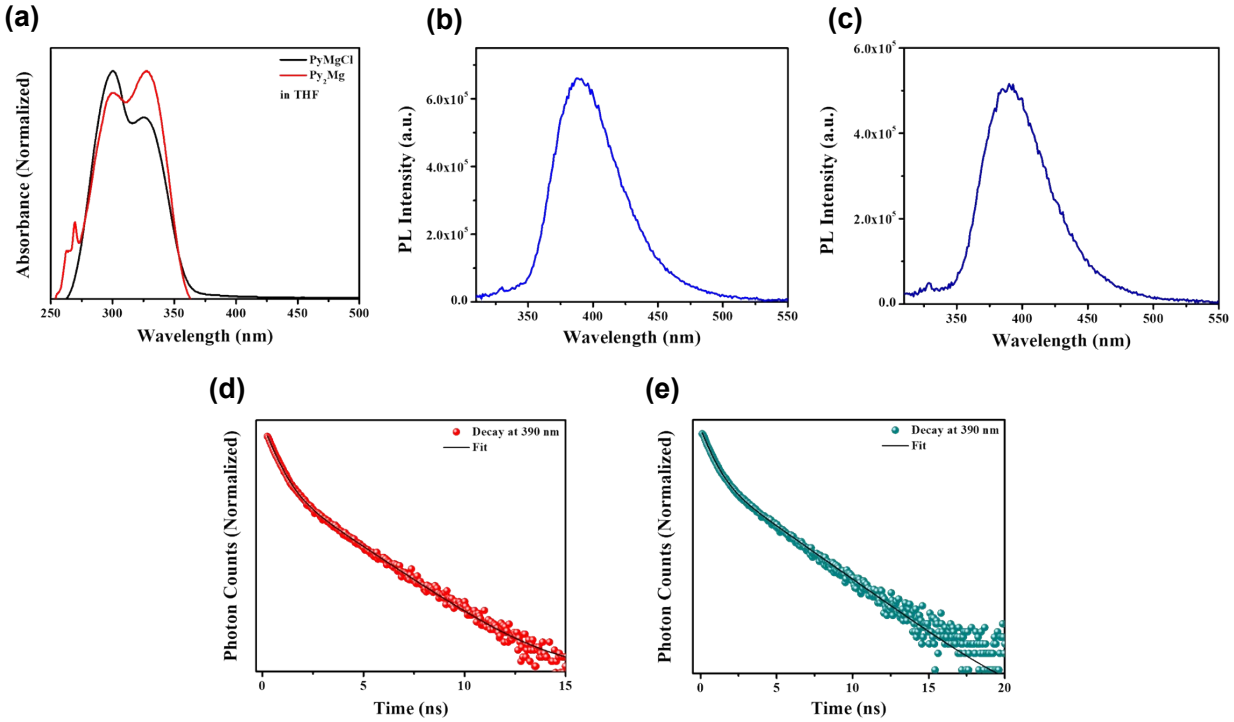

Figure S10. (a) Absorption spectra of compound 1 and 2 in THF, (b) emission spectra of 1 in THF (excited at 300 nm), (c) emission spectra of 2 in THF (excited at 300 nm), (d) fluorescent transient of 1 in THF (excited at 295 nm, collected at 390 nm), (e) fluorescent transient of 2 in THF (excited at 295 nm, collected at 390 nm).

❖ **Simulated single crystal-XRD pattern and powder-XRD pattern for compound 1 and 2:**

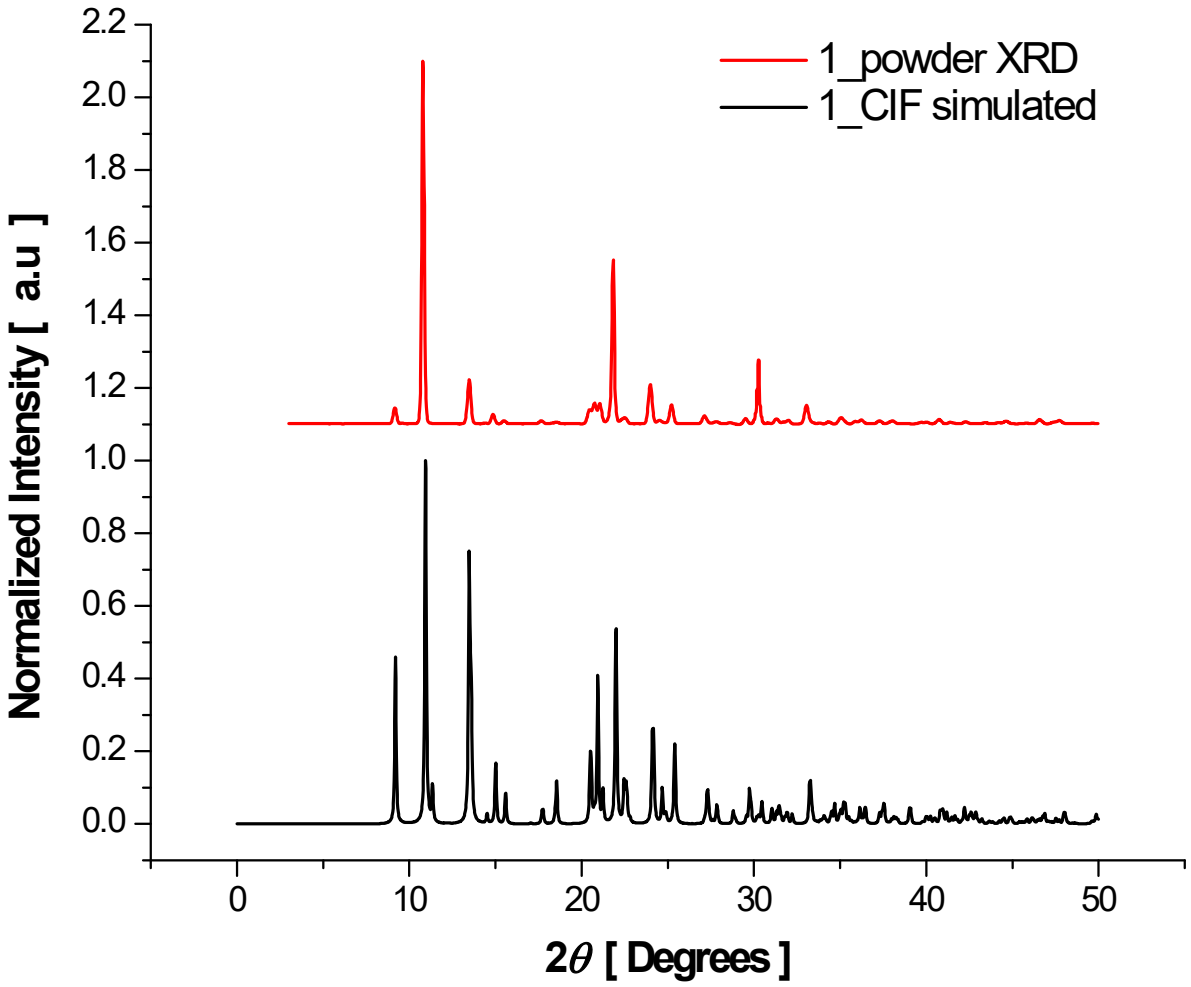

Figure S11. SC-XRD and PXRD pattern for compound **1** (1_CIF= simulated PXRD pattern for compound **1**).

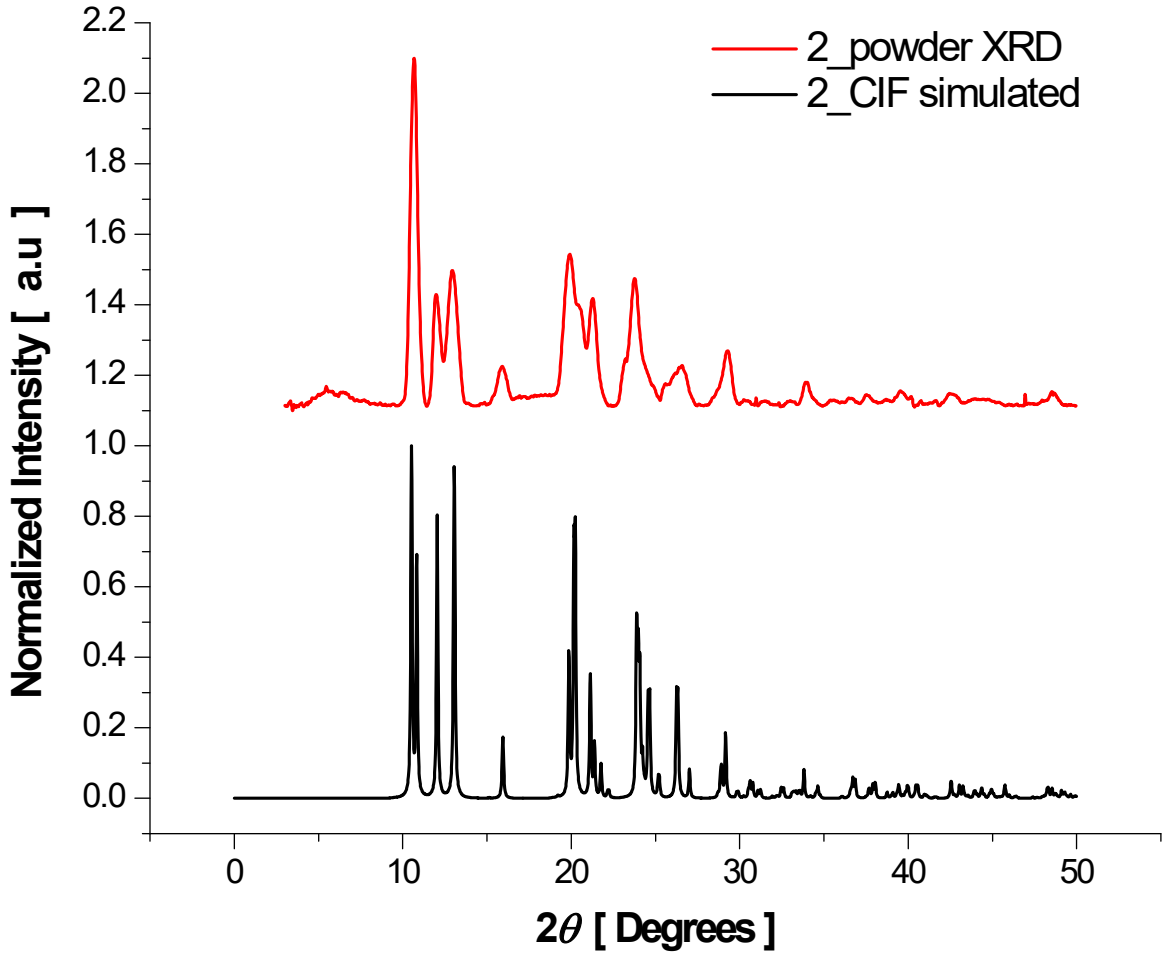

Figure S12. SC-XRD and PXRD pattern for compound **2**(2_CIF= simulated PXRD pattern for compound **2**).

❖ **Computational details:**

All the calculations were performed with Gaussian 09 program package.[5] Geometry of the ligand, **1**, and **2** were optimized by employing B3LYP-D3/def2-SVP level of theory.[6-10] The optimized geometries were confirmed to be true minima by performing harmonic vibrational frequency calculations. The B3LYP-D3/def2-SVP optimized geometries were further used to carry out single point time-dependent density functional theory (TD-DFT) calculations to obtain the absorption spectra at the triple-ζ (def2-TZVPP) level of theory along with B3LYP[6-9], BP86[11,12], cam-B3LYP[13], M06-2X[14], ωb97XD[15], PBE0[16], and B97D3[10,17] functionals (Table-S2). To obtain the emission spectra, TD-DFT calculations were performed to optimize the excited S_1 states by

employing B3LYP-D3/def2-SVP level of theory. These optimized S_1 states were further used to generate the fluorescence spectra by carrying out single point calculations at different level of theories whose absorption spectra (λ^{abs}) were close to the experimentally obtained values (Table-S3). To gain further insights, natural transition orbitals (NTOs) associated with the $S_1 \rightarrow S_0$ emission were evaluated at the M06-2X/def2-TZVPP//B3LYP-D3/def2-SVP level of theory.

The reorganization energies (λ^{RE}) were also calculated at the M06-2X/def2-TZVPP//B3LYP-D3/def2-SVP level of theory. The λ^{RE} consist of the external and internal reorganization energy.[18,19] The external reorganization energy caused by the polarization of the medium can be negligible.[20,21] The internal reorganization energy is caused by the geometrical deformation in the Franck–Condon vertical absorption transition and radiative process, and the value can be estimated as the following.[22,23]

$$\lambda^{RE} = \lambda_{S0} + \lambda_{S1} = [E^{S0}(S_1) - E^{S0}(S_0)] + [E^{S1}(S_0) - E^{S1}(S_1)]$$

Here, $E^{S0}(S_1)$ = energy of the S_0 state with the optimized S_1 geometry

$E^{S0}(S_0)$ = energy of the S_0 states with the optimized S_0 geometry

$E^{S1}(S_0)$ = energy of the S_1 states with the optimized S_0 geometry

$E^{S1}(S_1)$ = energy of the S_1 state with the optimized S_1 geometry

For **1**:

$E^{S0}(S_1)$ = -3088.83946521 Hartrees

$E^{S0}(S_0)$ = -3088.86816779 Hartrees

$E^{S1}(S_0)$ = -3088.73994047 Hartrees

$E^{S1}(S_1)$ = -3088.74444310 Hartrees

$\boldsymbol{\lambda^{RE}} = \lambda_{S0} + \lambda_{S1} = [E^{S0}(S_1) - E^{S0}(S_0)] + [E^{S1}(S_0) - E^{S1}(S_1)]$

= 0.03320521 Hartrees = **20.8 kcal/mol**

For **2**:

$E^{S0}(S_1)$ = -1503.21163620 Hartrees

$E^{S0}(S_0)$ = -1503.23920189 Hartrees

$E^{S1}(S_0)$ = -1503.11290525 Hartrees

$E^{S1}(S_1)$ = -1503.10978786 Hartrees

$\boldsymbol{\lambda^{RE}} = \lambda_{S0} + \lambda_{S1} = [E^{S0}(S_1) - E^{S0}(S_0)] + [E^{S1}(S_0) - E^{S1}(S_1)]$

= 0.0244483 Hartrees = **15.5 kcal/mol**

Table-S2: Absorption spectra (λ^{abs}) obtained from TD-DFT calculation at the triple-ζ (def2-TZVPP) level of theory with different functionals. (wavelength in nm, f=oscillator strength and the orbitals involved in the transition)

λ^{abs}	Exp	B3LYP	BP86	cam-B3LYP	M06-2X	ωB97XD	PBE0	B97D3
1	413 nm	402.14 nm f=0.0088 HOMO-1 to LUMO	540.29 nm f=0.0003 HOMO to LUMO+1	354.48 nm f=0.0120 HOMO-1 to LUMO	355.33 nm f=0.0115 HOMO-1 to LUMO	350.42 nm f=0.0121 HOMO-1 to LUMO	388.01 nm f=0.0092 HOMO-1 to LUMO	536.89 nm f=0.0003 HOMO to LUMO+1
2	413 nm	415.60 nm f=0.0255 HOMO to LUMO	537.23 nm f=0.0019 HOMO to LUMO	358.60 nm f=0.1053 HOMO to LUMO	360.76 nm f=0.1040 HOMO to LUMO	353.69 nm f=0.1133 HOMO to LUMO	396.05 nm f=0.0436 HOMO to LUMO	534.21 nm f=0.0018 HOMO to LUMO

Table-S3: Fluorescence spectra (λ^{em}) obtained from TD-DFT calculation at the triple-ζ (def2-TZVPP) level of theory with different functionals. (wavelength in nm, f=oscillator strength)

λ^{em}	Exp	B3LYP	cam-B3LYP	M06-2X	ωB97XD	PBE0
1	515 nm	656.23 nm f=0.0146	474.65 nm f=0.0321	479.50 nm f=0.0288	457.61 nm f=0.0348	611.82 nm f=0.0166
2	515 nm	744.81 nm f=0.0003	427.32 nm f=0.0069	447.36 nm f=0.0051	388.80 nm f=0.0352	666.70 nm f=0.0004

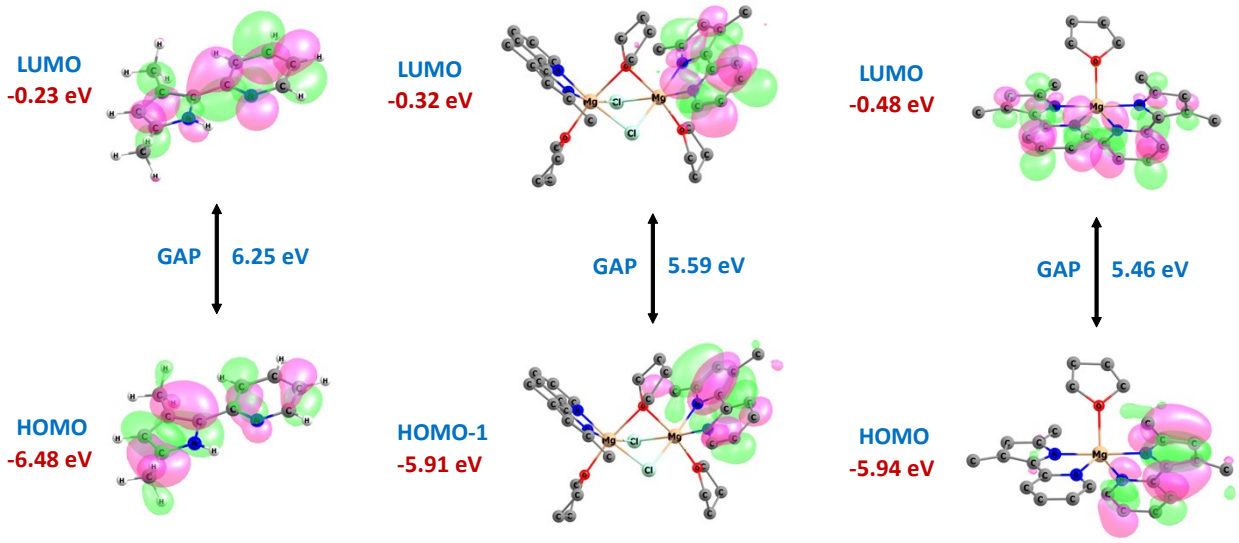

Figure S13. Frontier orbitals involved in the UV-Vis transition (and emission) as obtained from TD-DFT calculations at the M06-2X/def2-TZVPP//B3LYP-D3/def2-SVP level of theory. Left to Right: **PyPyrH**, **1**, **2**. Hydrogen atoms for **1** and **2** have been removed for clarity.

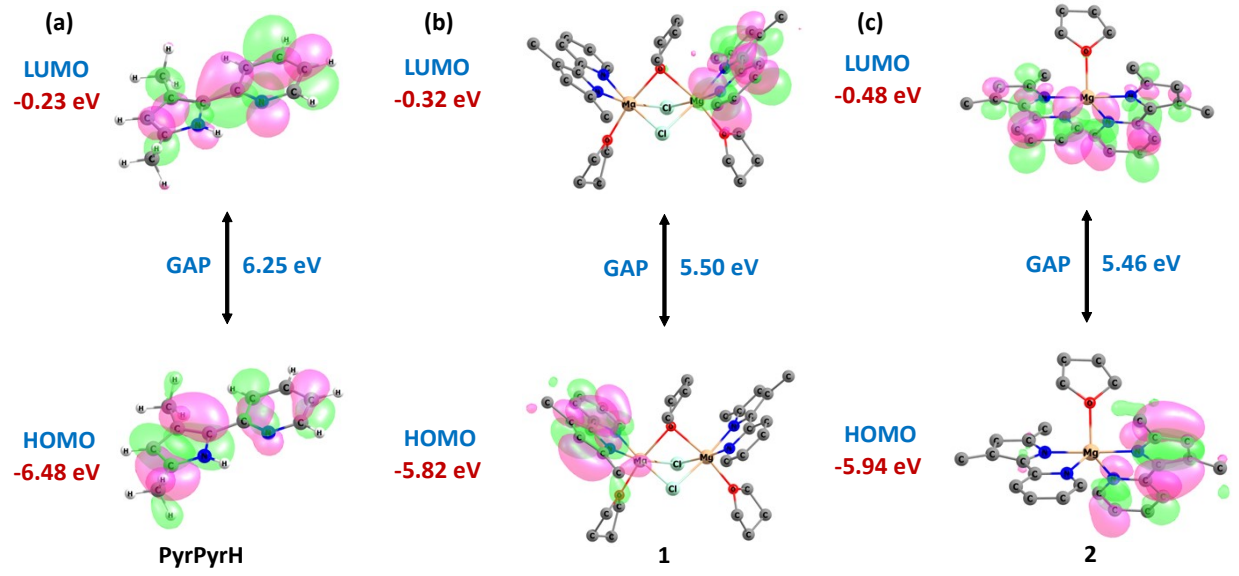

Figure S14. HOMO-LUMO diagram and associated energy values generated from the TD-DFT calculation at the M06-2X/def2-TZVPP//B3LYP-D3/def2-SVP level of theory for; (a) **PyPyrH** ligand, (b) complex **1**, and (c) complex **2**.

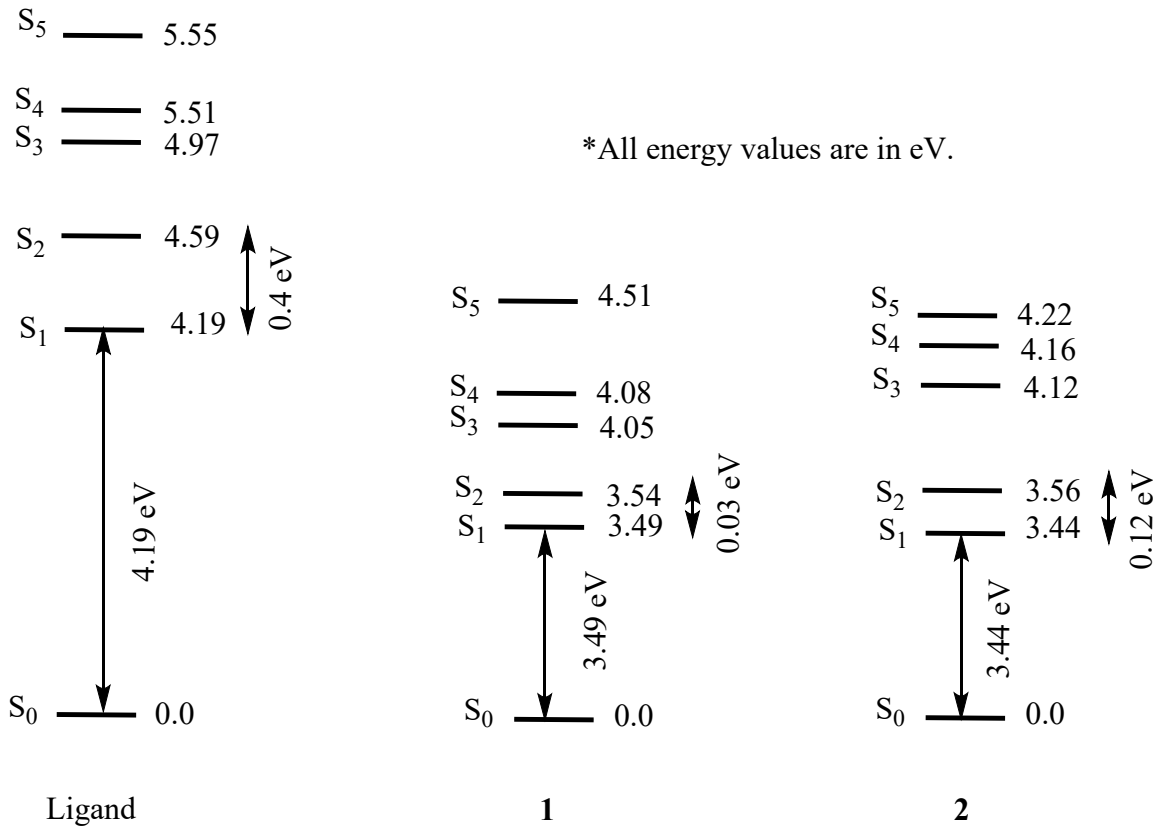

Figure S15. Franck-Condon (FC) energy levels associated with the excited states as obtained from the single point TD-DFT calculations at the M06-2X/def2-TZVPP level of theory using the optimized ground state (S0) obtained at B3LYP-D3/def2-SVP level of theory.

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❖ **Optimized cartesian coordinates:**

PyPyrH

C	2.695414235	-1.579701151	-0.000103451
H	2.980558623	-2.639101521	-0.000182107
C	3.682208226	-0.588591143	-0.000034741
H	4.740864524	-0.855740578	-0.000061737
C	3.260199916	0.744839510	0.000076948
H	3.989952128	1.559015168	0.000144467
C	1.898031948	1.031909997	0.000112080
H	1.554872113	2.064548233	0.000224091
C	0.971514045	-0.035172190	0.000022943
C	-0.474254669	0.149163281	0.000041886
C	-1.326644400	1.263359553	-0.000034414
C	-0.961476723	2.718810320	-0.000114302
H	-0.369975147	3.000319488	0.888004452
H	-1.868169682	3.342022361	-0.000297999
H	-0.369730095	3.000146119	-0.888122807
C	-2.653720630	0.752570838	-0.000004316
H	-3.567454721	1.345525746	-0.000017946
C	-2.593296758	-0.637874442	0.000078895
C	-3.682809255	-1.659936387	-0.000030725
H	-3.632888118	-2.313255994	-0.888841202
H	-4.665397557	-1.167804636	-0.000407630
H	-3.633355593	-2.312896423	0.889058694
N	1.390343159	-1.321503782	-0.000082113

N	-1.274324677	-0.975148472	0.000128762
H	-0.862401417	-1.902481387	0.000108359

Compound 1

C	3.183238245	-0.869815068	2.533304193
C	2.402792181	-0.211038016	3.629601276
H	2.417531186	0.886619065	3.540135269
H	2.811639212	-0.487055037	4.612916350
H	1.337960104	-0.494063038	3.605422273
C	4.223135321	-1.808000139	2.676181203
H	4.619108354	-2.190613166	3.617573279
C	4.660268358	-2.160853163	1.386663107
C	5.758434432	-3.139714242	1.085560082
H	5.414483402	-3.978269302	0.454976035
H	6.150980444	-3.573818274	2.017718152
H	6.610672487	-2.671584203	0.561607041
C	3.851267292	-1.405577108	0.498144038
C	3.828817291	-1.324340103	-0.941969074
C	4.719393359	-2.021986152	-1.801582140
H	5.483321425	-2.669147205	-1.379337103
C	4.616158355	-1.872522144	-3.175513242
H	5.304500420	-2.410729184	-3.833200291
C	3.629649278	-1.031115078	-3.715931284
H	3.516439267	-0.889638069	-4.791743366
C	-2.743435208	-0.176097014	2.819965213

H	-1.911324145	0.449068034	3.156227239
C	-3.634957275	-0.747020059	3.721247283
H	-3.526295267	-0.575974044	4.793168367
C	-4.665301358	-1.543490118	3.194994246
H	-5.394775413	-2.014023156	3.860115294
C	-4.761392363	-1.732456134	1.825287137
H	-5.562410404	-2.340830177	1.414245105
C	-3.816092293	-1.124857087	0.956204075
C	-3.818881289	-1.264341097	-0.479401037
C	-4.628901355	-2.044460156	-1.344961103
C	-5.753778413	-2.983645229	-1.017520075
H	-6.118848484	-3.477262264	-1.930940148
H	-6.617100509	-2.467543188	-0.561014045
H	-5.446718393	-3.779260286	-0.316659024
C	-4.155823319	-1.770074133	-2.640860204
H	-4.543874346	-2.188436167	-3.570177275
C	-3.096294238	-0.850055066	-2.523987191
C	-2.301986175	-0.249505019	-3.644427278
H	-2.278646172	0.849699067	-3.583764271
H	-2.731873209	-0.537856042	-4.615143350
H	-1.246154095	-0.566388041	-3.631517279
C	-2.843338215	3.261103248	0.964788076
H	-1.900264145	3.319166254	1.523967119
H	-3.641437278	2.905584224	1.640008127
C	-3.235819249	4.546721346	0.242730018

H	-2.333239177	5.077002390	-0.102595008
H	-3.812665293	5.230809398	0.882403068
C	-4.029290308	4.009711305	-0.956812073
H	-5.051050384	3.733787286	-0.648168051
H	-4.106465311	4.725386360	-1.788373135
C	-3.231226245	2.764383213	-1.336095103
H	-3.827227293	1.948840151	-1.767535135
H	-2.393004180	2.991394231	-2.014715156
C	0.036881003	-2.078669158	-1.087806085
H	-0.281714022	-1.502850115	-1.961289151
H	1.075031080	-2.416321185	-1.229138094
C	-0.898326070	-3.220039247	-0.683695053
H	-0.539851040	-4.177604318	-1.088719085
C	-0.888931067	-3.189812246	0.868473064
H	-1.902654148	-3.025777231	1.256595096
H	-0.507382039	-4.123047313	1.307714100
C	0.028587002	-2.015885156	1.224832094
H	1.067549080	-2.328147179	1.404234109
H	-0.307785024	-1.394082108	2.060431160
C	3.414284261	2.676869203	1.254772096
H	3.998972304	1.855168141	1.689960131
H	2.591477198	2.932640226	1.941826149
C	4.233504322	3.898585300	0.844793065
H	4.336914330	4.625586351	1.663598130
H	5.245076403	3.596087275	0.527584040

C	3.435969262	4.433370341	-0.352995027
H	4.018815308	5.094522390	-1.011095075
H	2.549333194	4.988098379	-0.004763000
C	3.006734227	3.145126238	-1.048667078
H	2.059330159	3.215268244	-1.598993123
H	3.789316289	2.759896213	-1.725773133
C	2.785657213	-0.378780029	-2.824279214
H	1.985550150	0.280044021	-3.172905245
Cl	0.061265005	1.450469109	1.697924127
Cl	0.062294005	1.387104107	-1.738040134
Mg	1.654546124	0.480438037	0.014452001
Mg	-1.551660118	0.540204043	-0.029900002
N	2.954350225	-0.628478048	1.221451091
N	2.873150220	-0.514385039	-1.493448112
N	-2.883726219	-0.551696043	-1.220816094
N	-2.820441213	-0.355264027	1.493586116
O	2.825370214	2.196784166	0.023211002
O	0.027742002	-1.163492090	0.042894003
O	-2.672569203	2.290337174	-0.088489007
H	-1.910037144	-3.041391231	-1.070080082

Compound 1 (S1 Excited State)

C	3.174746803	-0.294774074	2.715730593
C	2.349340162	0.527101332	3.658291505
H	2.433508978	1.605502950	3.443637839

H	2.668897592	0.358819326	4.697331271
H	1.276963329	0.292849744	3.577430406
C	4.256805081	-1.134658793	3.042991934
H	4.650118580	-1.314761799	4.044055343
C	4.739499660	-1.695835666	1.847598478
C	5.892330405	-2.652860034	1.748473260
H	5.605981906	-3.613360430	1.285119385
H	6.287859865	-2.880789386	2.749939876
H	6.729591156	-2.245969472	1.154005656
C	3.912313751	-1.162909005	0.823858956
C	3.916453271	-1.350706846	-0.605246865
C	4.857050977	-2.152539826	-1.307699251
H	5.638859583	-2.672252464	-0.760687136
C	4.779748643	-2.265717022	-2.686286467
H	5.506269567	-2.883050703	-3.222091868
C	3.770437377	-1.585294444	-3.388388152
H	3.677971167	-1.648315332	-4.473645831
C	-2.870373108	0.256706748	2.715989726
H	-1.941311334	0.678706870	3.095736993
C	-4.053222412	0.238860689	3.468895903
H	-4.019693789	0.627472415	4.491878744
C	-5.234189041	-0.248862304	2.944294307
H	-6.154583929	-0.287350527	3.526805098
C	-5.175297778	-0.796223177	1.581762212
H	-6.055737747	-1.230563317	1.112002191

C	-3.972422296	-0.776237200	0.928326165
C	-3.750826904	-1.400375581	-0.430520617
C	-4.332547697	-2.599979023	-1.001850597
C	-5.293348327	-3.530087071	-0.340745230
H	-5.267383139	-4.524459674	-0.811789412
H	-6.332550366	-3.161502777	-0.407228289
H	-5.069859047	-3.631331659	0.733232388
C	-3.793481760	-2.681177409	-2.284031879
H	-3.999773303	-3.441443362	-3.036224069
C	-2.905223002	-1.586208894	-2.437570012
C	-2.121975273	-1.214910518	-3.641865912
H	-2.523030449	-0.286429300	-4.089153219
H	-2.160022683	-2.007787263	-4.401790344
H	-1.077028486	-0.977974268	-3.389669205
C	-3.322408380	2.895889654	0.571772737
H	-2.563985604	3.018410338	1.356099914
H	-4.177973726	2.339252721	0.988086141
C	-3.741922349	4.188393597	-0.119760957
H	-2.886061256	4.880101272	-0.185348805
H	-4.559624312	4.701546364	0.407105335
C	-4.134385317	3.688873219	-1.517766511
H	-5.140827331	3.240122074	-1.491434915
H	-4.132937197	4.478081966	-2.283901362
C	-3.079948339	2.614767347	-1.786571567
H	-3.442796918	1.773649984	-2.395443068

H	-2.165279720	3.016640653	-2.251589916
C	0.215319138	-2.288989100	-0.615892302
H	-0.037778694	-1.940558421	-1.622131832
H	1.270400383	-2.602093790	-0.599770441
C	-0.712718229	-3.357574902	-0.033153809
H	-0.294365532	-4.362470961	-0.190262561
C	-0.828558336	-2.983612907	1.468852255
H	-1.870518060	-2.763447559	1.734928418
H	-0.464274035	-3.781690125	2.131781684
C	0.028284548	-1.724526804	1.616744718
H	1.063391445	-1.941681610	1.917360470
H	-0.391237908	-0.957595297	2.273448482
C	3.331382967	2.958661718	0.750148137
H	3.894055569	2.258751335	1.382862630
H	2.482000977	3.358567850	1.327227913
C	4.175839951	4.055415688	0.106505677
H	4.253265335	4.950219162	0.741230432
H	5.196066937	3.688289769	-0.092463361
C	3.432248347	4.303300176	-1.214007154
H	4.048513290	4.795817153	-1.980515256
H	2.538379278	4.924207312	-1.039297820
C	3.018600498	2.889817838	-1.614762579
H	2.091434596	2.832134850	-2.200211949
H	3.820925501	2.361257784	-2.159086410
C	2.878659357	-0.820135628	-2.645653333

H	2.061936494	-0.272693932	-3.123799707
Cl	0.008683146	1.744552152	1.372165280
Cl	0.051335217	0.984211278	-1.975055120
Mg	1.653088770	0.510619574	-0.024770103
Mg	-1.541496575	0.451222802	-0.133209436
N	2.962270553	-0.314148996	1.379600670
N	2.937724270	-0.703629059	-1.311552296
N	-2.883476548	-0.829271481	-1.280124502
N	-2.832371324	-0.230990039	1.410925693
O	2.792467856	2.209355364	-0.364433793
O	0.082713580	-1.150054057	0.273965340
O	-2.732464093	2.104131543	-0.484664497
H	-1.695217142	-3.324651827	-0.520551586

Compound 2

C	0.853893215	2.963175219	-0.857634001
H	-0.210336859	3.162094270	-0.696779987
C	1.738229315	3.967562268	-1.235235031
H	1.389186324	4.990648357	-1.381349040
C	3.083691406	3.607655200	-1.420320044
H	3.817951488	4.360562230	-1.719999068
C	3.485099395	2.292775083	-1.233436029
H	4.522235468	2.007833031	-1.393790045
C	2.533520293	1.313458038	-0.850014002
C	2.819028268	-0.087383076	-0.636712982
C	4.034777336	-0.815695169	-0.579002981

C	5.442011467	-0.329098179	-0.771064995
H	5.627250493	0.024529843	-1.800950075
H	6.160766466	-1.138829266	-0.573444979
H	5.693409502	0.505685877	-0.094015943
C	3.661616267	-2.140432261	-0.277456957
H	4.338651291	-2.986484344	-0.154005948
C	2.257732156	-2.170116215	-0.170913949
C	1.372067054	-3.346652276	0.115216073
H	1.883187066	-4.088425352	0.748677120
H	1.060050014	-3.869584307	-0.806542996
H	0.449569993	-3.030784222	0.628225112
C	-0.976863080	-1.930278094	-2.229956108
H	0.096426994	-2.141298143	-2.255458106
C	-1.874275171	-2.596656118	-3.056889171
H	-1.526445171	-3.356984186	-3.757509222
C	-3.231558261	-2.247839044	-2.951841163
H	-3.976943338	-2.743415062	-3.580123209
C	-3.630441261	-1.265207958	-2.057859094
H	-4.677303330	-0.979727903	-1.986597090
C	-2.664261168	-0.617266941	-1.245697029
C	-2.942809155	0.434252149	-0.296949959
C	-4.152434230	1.010557230	0.167697077
C	-5.565938323	0.696610254	-0.229077953
H	-5.764437366	0.926068277	-1.291121033
H	-6.275508392	1.289116319	0.368246092

H	-5.818667398	-0.367446820	-0.077559942
C	-3.764349166	1.968662294	1.124684151
H	-4.432868199	2.611606365	1.698386194
C	-2.358657063	1.944032247	1.202745157
C	-1.458331968	2.781792282	2.061430220
H	-0.572846919	2.206412207	2.376119245
H	-1.983395996	3.136529325	2.961565292
H	-1.086448910	3.675610338	1.528656179
C	1.374647142	-0.497161061	2.767290275
H	1.497129180	0.347909000	3.468654329
H	2.202156209	-0.500057087	2.048332220
C	1.169407085	-1.828143155	3.510407334
H	1.666807097	-2.646972233	2.973061292
H	1.594149119	-1.786669168	4.523990410
C	-0.371560038	-2.025251123	3.517955333
H	-0.780293074	-2.176690121	4.527595409
H	-0.651264087	-2.899737180	2.912008288
C	-0.914953036	-0.742045005	2.876010286
H	-1.806360113	-0.867934986	2.248901235
H	-1.126460028	0.040321061	3.626812343
Mg	-0.037585944	0.090244030	-0.033487938
N	1.232212206	1.693058110	-0.663727989
N	1.751293161	-0.935838106	-0.384699965
N	-1.351375081	-0.990040012	-1.352281037
N	-1.864681055	1.021523158	0.347815091

O	0.156726058	-0.294447006	2.030235221

Compound 2 (S1 Excited State)

C	-0.769228575	2.119440159	2.275063557
H	0.238055461	2.540261683	2.207760223
C	-1.683449156	2.632652146	3.162630326
H	-1.396712156	3.476542139	3.796206632
C	-2.977478330	2.055098990	3.253501861
H	-3.725442563	2.426931443	3.952780475
C	-3.252234100	0.946855894	2.398704546
H	-4.222334332	0.457932591	2.456491231
C	-2.309733113	0.464831513	1.509173646
C	-2.536780247	-0.657799743	0.575027261
C	-3.704486615	-1.350536065	0.209899998
C	-5.110138665	-1.161113422	0.701585493
H	-5.237614252	-1.456772176	1.759333602
H	-5.813416160	-1.767854414	0.108820135
H	-5.438017978	-0.108647268	0.631562950
C	-3.303766788	-2.295413233	-0.780455224
H	-3.955539028	-3.010926364	-1.284930569
C	-1.935489511	-2.140303475	-0.977318570
C	-1.027854870	-2.915853581	-1.887803894
H	-1.610666022	-3.491141964	-2.623963892
H	-0.387120650	-3.641994375	-1.351958408
H	-0.341909415	-2.260021874	-2.454695087

C	1.156217501	-2.644435865	0.947867972
H	0.071776273	-2.783933370	0.950791972
C	2.057038991	-3.646314985	1.343940384
H	1.681875695	-4.614711420	1.677663656
C	3.420176221	-3.371267971	1.296267461
H	4.151318317	-4.126939280	1.592205747
C	3.851988380	-2.110654372	0.869516258
H	4.912918950	-1.876517877	0.833389512
C	2.889514767	-1.158659262	0.499774087
C	3.179053125	0.206767782	0.069579386
C	4.444195984	0.922268890	-0.099421098
C	5.836520832	0.414796627	0.099884127
H	6.008733525	0.094428397	1.140855348
H	6.568186962	1.201224275	-0.131080402
H	6.054586151	-0.447952441	-0.551131464
C	4.074190034	2.190002474	-0.484681691
H	4.734740991	3.026838094	-0.703536168
C	2.631747354	2.222292568	-0.540482264
C	1.767204097	3.381927755	-0.873638602
H	1.084140570	3.110720033	-1.691644370
H	2.357627856	4.265836226	-1.146521376
H	1.124118371	3.624873226	-0.012995834
C	-1.735005006	1.948991358	-1.722620999
H	-1.609868059	2.934048361	-2.210859810
H	-1.991112628	2.088955650	-0.666200892

C	-2.684872553	1.036447258	-2.493927415
H	-3.115053688	0.290456822	-1.812616274
H	-3.505570792	1.604144177	-2.956089869
C	-1.773500354	0.343075523	-3.536603857
H	-1.946239440	0.710900950	-4.559497161
H	-1.945977058	-0.740632662	-3.529324389
C	-0.340834633	0.684736252	-3.079055734
H	0.322098946	-0.189132987	-2.997811865
H	0.138823644	1.423426241	-3.746768485
Mg	0.090295490	0.174292957	-0.004983383
N	-1.029045535	1.053550892	1.424332536
N	-1.462649282	-1.144687560	-0.162117824
N	1.568648771	-1.450015699	0.538591333
N	2.123825430	1.017587053	-0.213398185
O	-0.459172224	1.263262571	-1.768341458