Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

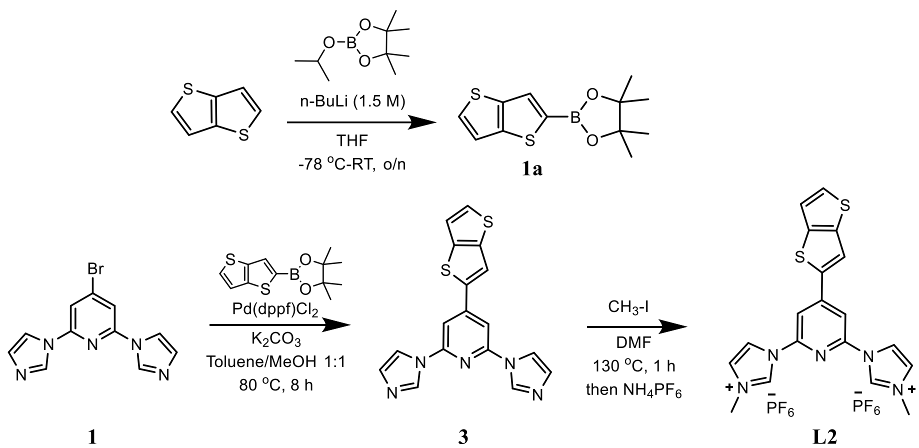
SUPPORTING INFORMATION

CONTENTS

Synthesis of ligands

Ligand **L1** was prepared according to ref 1

Synthesis of L2

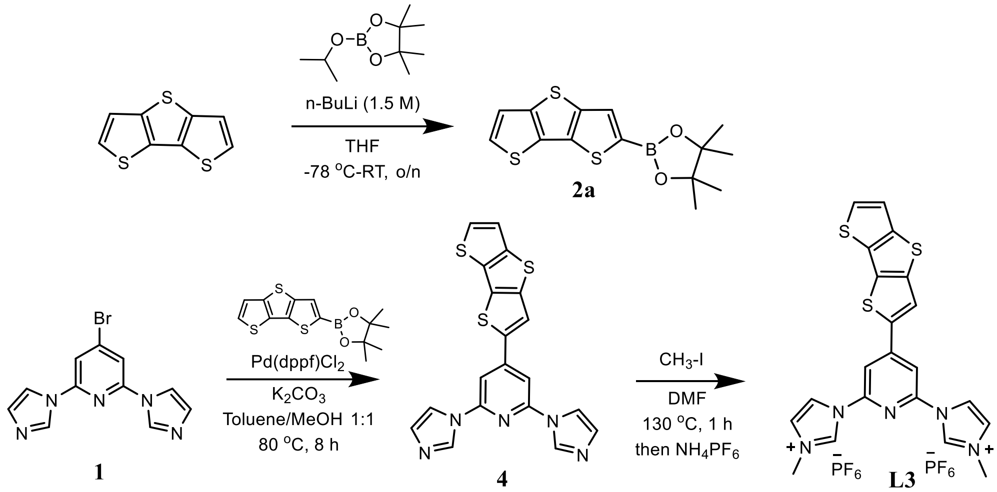


4,4,5,5-tetramethyl-2-(thieno[3,2-b]thiophen-2-yl)-1,3,2-dioxaborolane (1a) was prepared according to a literature procedure.[2]

2,6-di(1H-imidazol-1-yl)-4-(thieno[3,2-b]thiophen-2-yl)pyridine (3). To a solution of **1** (0.160 g, 0.551 mmol) in toluene (5 mL) was added a solution of compound **1a** (0.220 g, 0.827 mmol) and K_2CO_3 (0.228 g, 1.65 mmol) in methanol (5 mL). The mixture was degassed with Argon for 20 min then $PdCl_2$(dppf) (0.040 g, 0.055 mmol) was added, and the solution was refluxed at 80 °C for 12 h. After completion of reaction, the reaction mixture was filtered through celite powder and washed with dichloromethane. After evaporation of solvents, the residue was purified by column chromatography over silica gel using 3-6% methanol in dichloromethane as the eluent to give the product as a white solid (0.12 g, 62% yield). ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.82(s, 2H), 8.43(s, 1H), 8.21(s, 2H), 7.93(s, 2H), 7.86(d, *J*= 5.20 Hz, 1H), 7.56(d, *J*= 5.19 Hz, 1H), 7.18(s, 2H). ^{13}C NMR (100 MHz, CD_3CN, δ ppm): 149.0, 148.3, 141.2, 141.2, 140.0, 136.2, 131.6, 130.7, 121.4, 120.8, 117.5, 105.8. ESI-HRMS calcd for $C_{17}H_{12}N_5S_2$ m/z = 350.0529. Found: 350.0485.

1,1'-(4-(thieno[3,2-b]thiophen-2-yl)pyridine-2,6-diyl)bis(3-methyl-1H-imidazol-3-ium)hexafluorophosphate(V) (L2). Compound **3** (0.07 g, 0.200 mmol) was charged in a 10 mL round bottomed flask and dissolved in 1 mL of DMF. Then added methyl iodide (0.05 mL, 0.801 mmol) and heated the mixture at 130 °C for 1 h. Desired compound was precipitated upon addition of diethyl ether. Solid was collected by vacuum filtration and washed thrice with diethyl ether and dried under vacuum. Then the solid was dissolved in minimum amount of water (ca. 2 mL) and added saturated NH_4PF_6 solution and stirred until the product precipitated. Compound 3 was collected by vacuum filtration and washed 3 times with water and then diethyl ether and dried under vacuum (0.128 g, 95.5% yield). ^{1}H NMR (400 MHz, CD_3CN, δ ppm): 9.55(s, 2H), 8.29(s, 2H), 8.27(s, 1H), 8.06(s, 2H), 7.8(d, *J*= 5.3 Hz, 1H), 7.66(s, 2H), 7.52(d, *J*= 5.22 Hz, 1H), 4.05(s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 149.7, 146.6, 142.4, 140.2, 139.8, 136.8, 132.99, 125.4, 122.7, 121.1, 119.7, 109.6, 37.1. ESI-HRMS calcd for $C_{19}H_{17}N_5S_2$ m/z = 189.5457. Found: 189.5486 [M-2PF_6].

Synthesis of **L3**



2-(dithieno[3,2-b:2',3'-d]thiophen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2a) was prepared according to a literature procedure.[3]

4-(dithieno[3,2-b:2',3'-d]thiophen-2-yl)-2,6-di(1H-imidazol-1-yl)pyridine (4). To a solution of **1** (0.160 g, 0.551 mmol) in toluene (5 mL) was added a solution of compound **2a** (0.213 g, 0.661 mmol) and K_2CO_3 (0.228 g, 1.65 mmol) in methanol (5 mL). The mixture was degassed with Argon for 20 min then $PdCl_2$(dppf) (0.040 g, 0.055 mmol) was added, and the solution was refluxed at 80 °C for 12 h. After completion of reaction, the reaction mixture was filtered through Celite powder and washed with dichloromethane. After evaporation of solvents, the residue was purified by column chromatography over silica gel using 5-7% methanol in dichloromethane as the eluent to give the product as yellow solid (0.157 g, 70 % yield). ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.84(s, 2H), 8.54(s, 1H), 8.24(s, 2H), 8.00(s, 2H), 7.86(d, *J*= 5.23 Hz, 1H), 7.62(d, *J*= 5.22 Hz,1H), 7.19(s, 2H). ESI-HRMS calcd for $C_{19}H_{12}N_5S_3$ m/z = 406.0249. Found: 406.0248. The poor solubility prevented us from obtaining good quality ^{13}C spectra.

1,1'-(4-(dithieno[3,2-b:2',3'-d]thiophen-2-yl)pyridine-2,6-diyl)bis(3-methyl-1H-imidazol-3-ium) hexafluorophosphate(V) (L3). Compound **4** (0.100 g, 0.246 mmol) was charged in a 10 mL round bottomed flask and dissolved in 1 mL of DMF. Then added methyl iodide (0.077 mL, 1.23 mmol) and heated the mixture at 130 °C for 1 h. Desired compound was precipitated upon addition of diethyl ether. Solid was collected by vacuum filtration and washed thrice with diethyl ether and dried under vacuum. Then the solid was dissolved in minimum amount of water (ca. 3 mL) and added saturated NH_4PF_6 solution and stirred until the product precipitated. Compound 3 was collected by vacuum filtration and washed 3 times with water and then diethyl ether and dried under vacuum (0.160 g, 89.5% yield). ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.36(s, 2H), 8.83(s, 2H), 8.59(s, 1H), 8.45(s, 2H), 8.09(s, 2H), 7.92(d, 1H), 7.65(d, 1H), 4.06(s, 6H). ESI-HRMS calcd for $C_{21}H_{17}N_5S_3$ m/z = 217.5318. Found: 217.5324 [M-2PF_6]. The poor solubility prevented us from obtaining good quality ^{13}C spectra.

NMR spectra of ligands and complexes

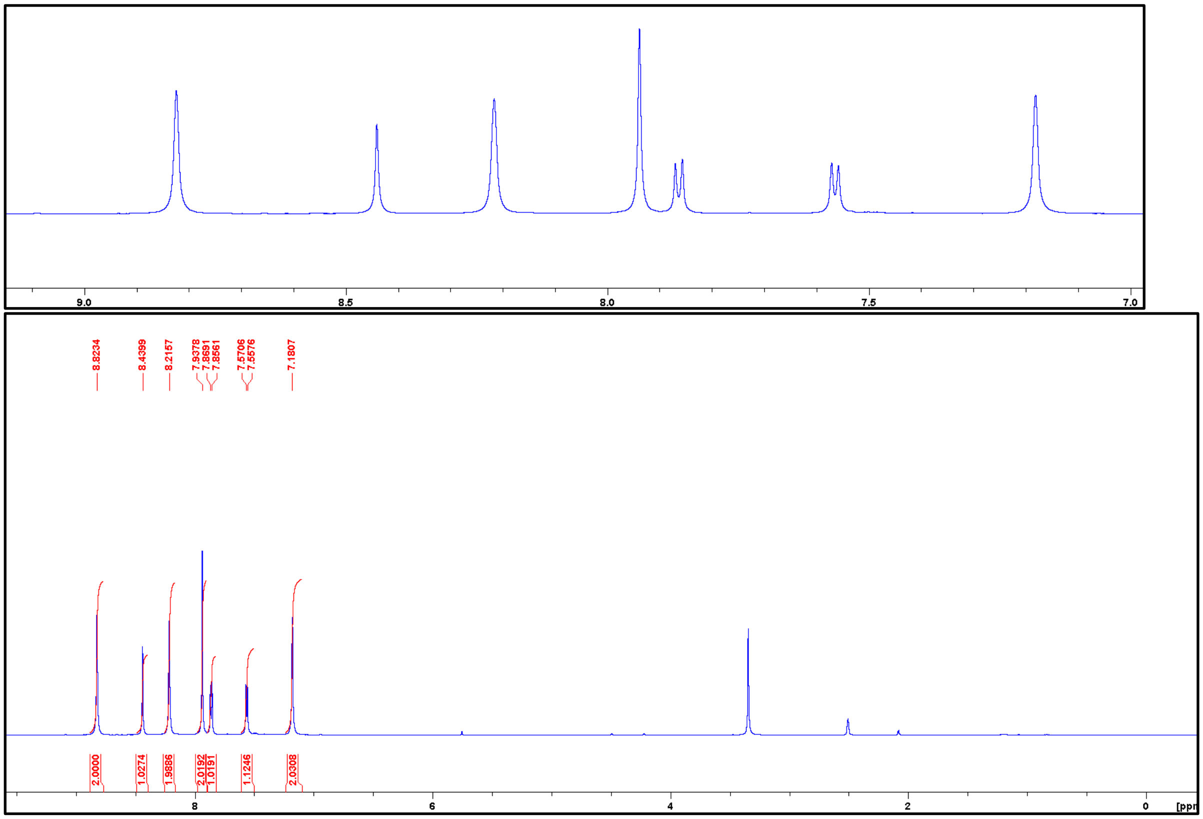


Figure S1. ^{1}H NMR spectra of compound **3**

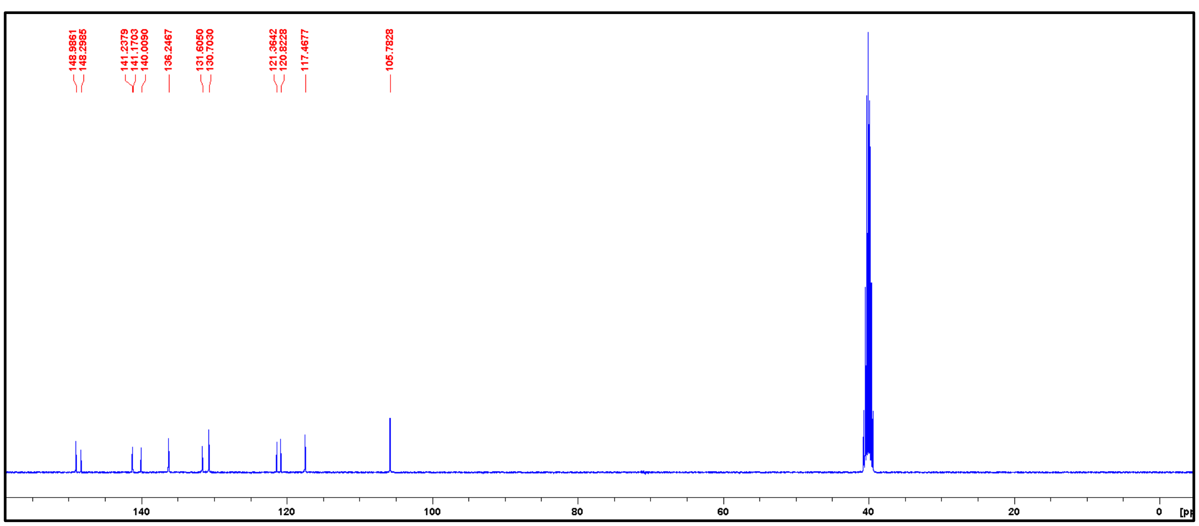


Figure S2. ^{13}C NMR spectra of compound **3**.

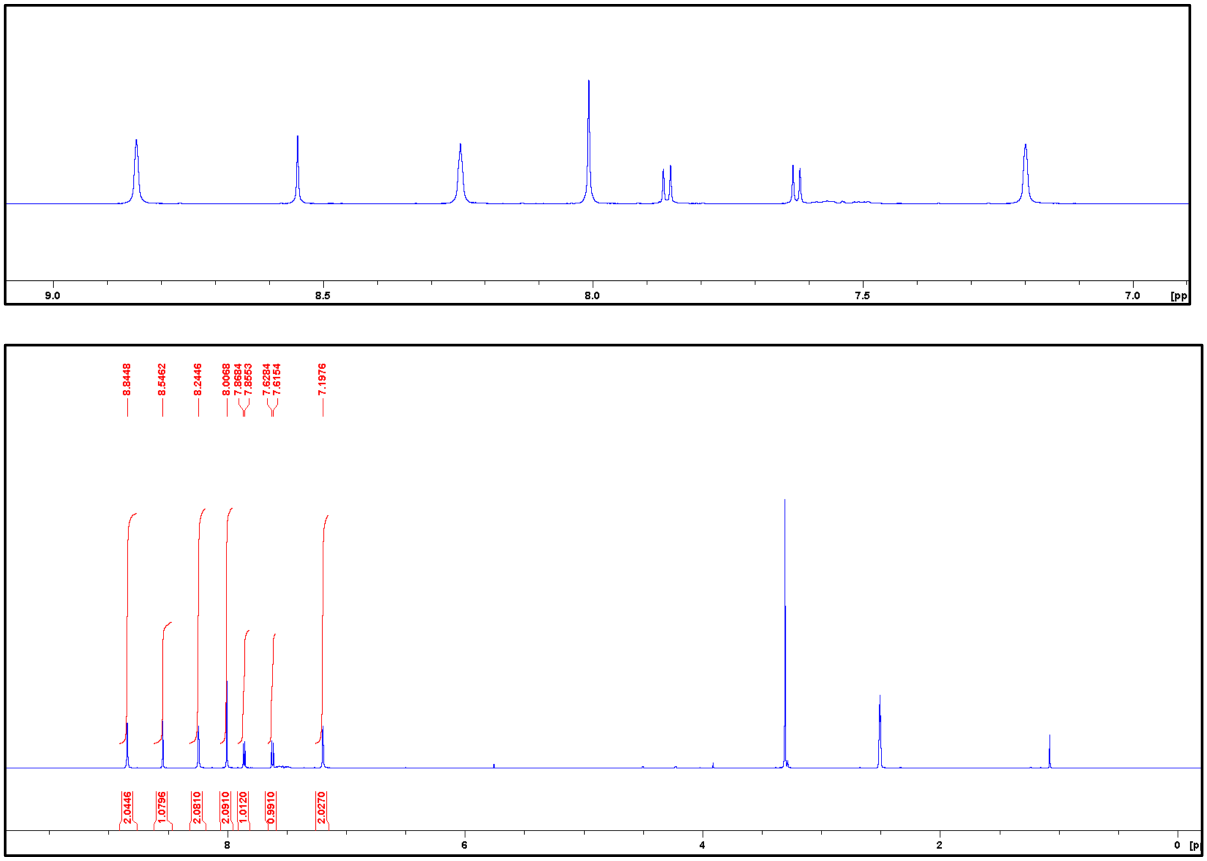
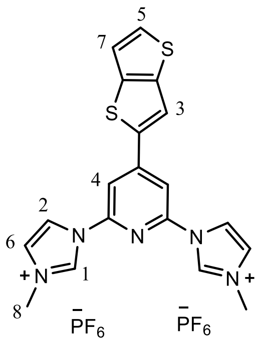


Figure S3. [1]H NMR spectra of compound **4**.



L2: ^{1}H NMR (400 MHz, CD_3CN, δ ppm): 9.55(s, 2H, H_1), 8.29(s, 2H, H_2), 8.27(s, 1H, H_3), 8.06(s, 2H, H_4), 7.8(d, *J*= 5.3 Hz, 1H, H_5), 7.66(s, 2H, H_6), 7.52(d, *J*= 5.22 Hz, 1H, H_7), 4.05(s, 6H, H_8).

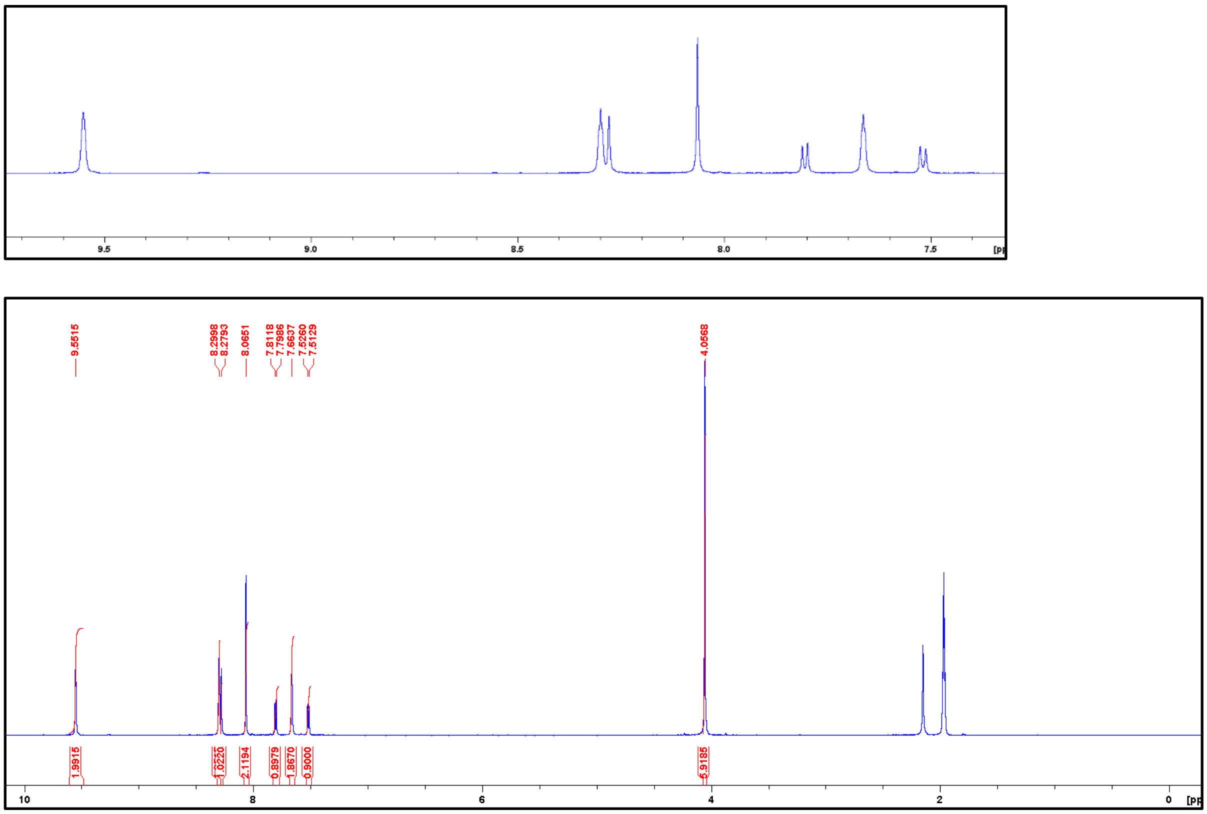
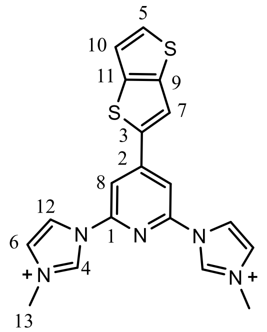


Figure S4. ^{1}H NMR spectra of **L2**.

	**L2:** ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 149.7 (C_1), 146.6 (C_2), 142.4 (C_3), 140.2 (C_4), 139.8 (C_5), 136.8 (C_6), 132.99 (C_7), 125.4 (C_8), 122.7 (C_9), 121.1 (C_{10}), 119.7 (C_{11}), 109.6 (C_{12}), 37.1 (C_{13}).

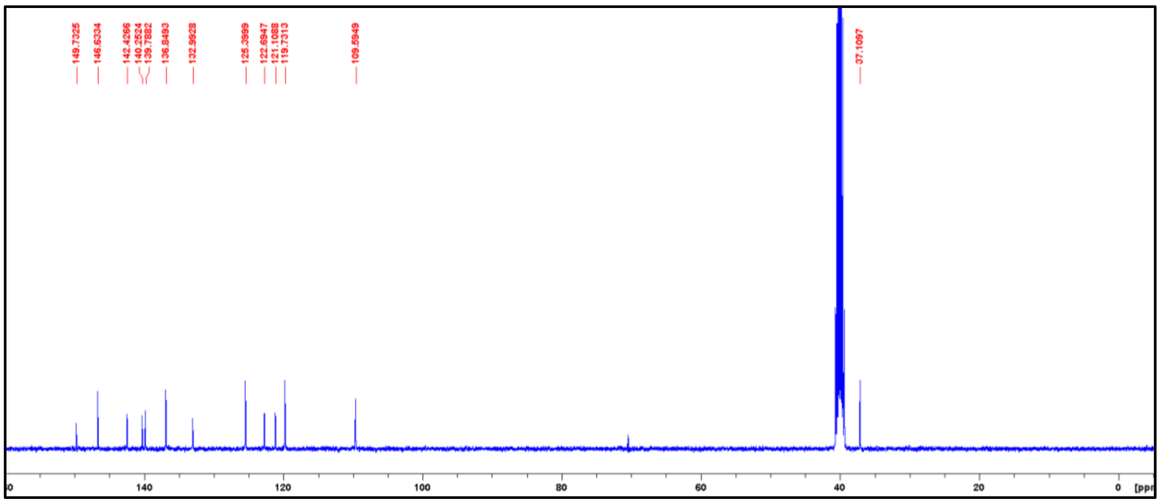
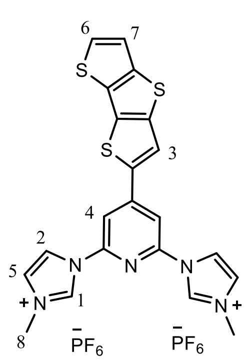
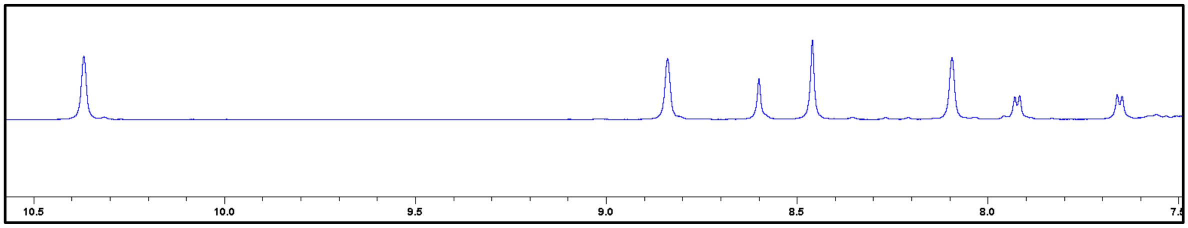


Figure S5.^{13}C NMR spectra of **L2**.



L3: ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.36(s, 2H, H_1), 8.83(s, 2H, H_2), 8.59(s, 1H, H_3), 8.45(s, 2H, H_4), 8.09(s, 2H, H_5), 7.92(d, 1H, H_6), 7.65(d, 1H, H_7), 4.06(s, 6H, H_8).



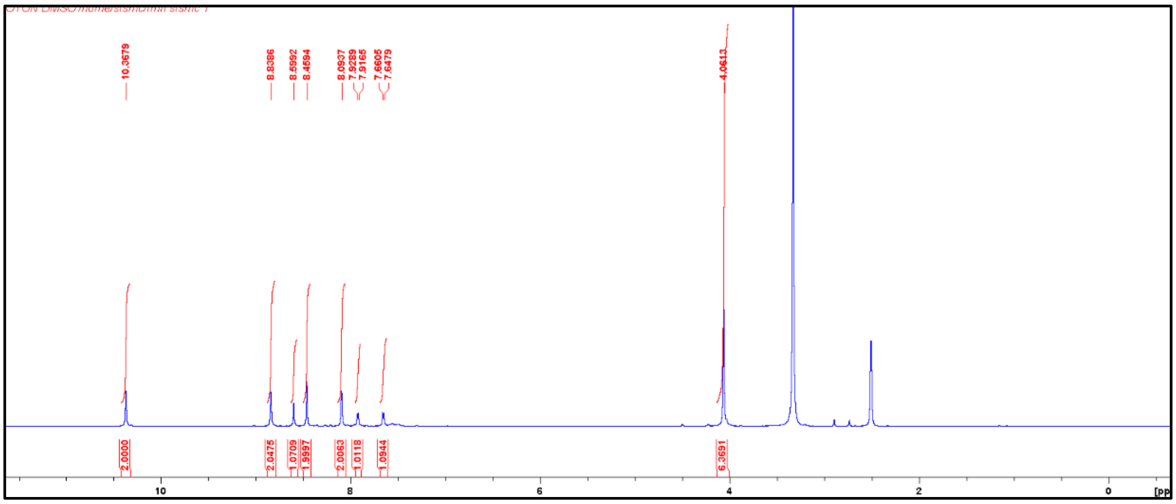
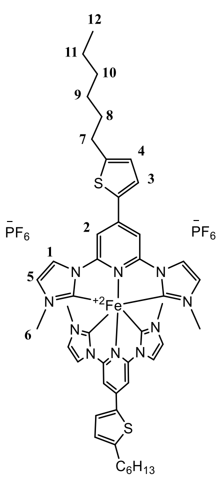


Figure S6. [1]H NMR spectra of compound **L3**.



CTh: ^{1}H NMR (400 MHz, CD_3CN, δ ppm): 8.12 (d, *J*= 2.19 Hz, 2H, H_1), 7.95 (s, 2H, H_2), 7.84 (d, *J*= 3.72 Hz, 1H, H_3), 7.06 (s, *J*= 3.72 Hz, 1H, H_4), 7.04 (d, *J*= 2.19 Hz, 2H, H_5), 2.99 (t, *J*= 7.51 Hz, 2H, H_6), 2.62 (s, 6H, H_7), 1.79 (q, 2H, H_8), 148-1.35 (m, 6H, $H_{9,10,11}$), 0.95 (t, *J*= 7.09 Hz, 3H, H_{12}).

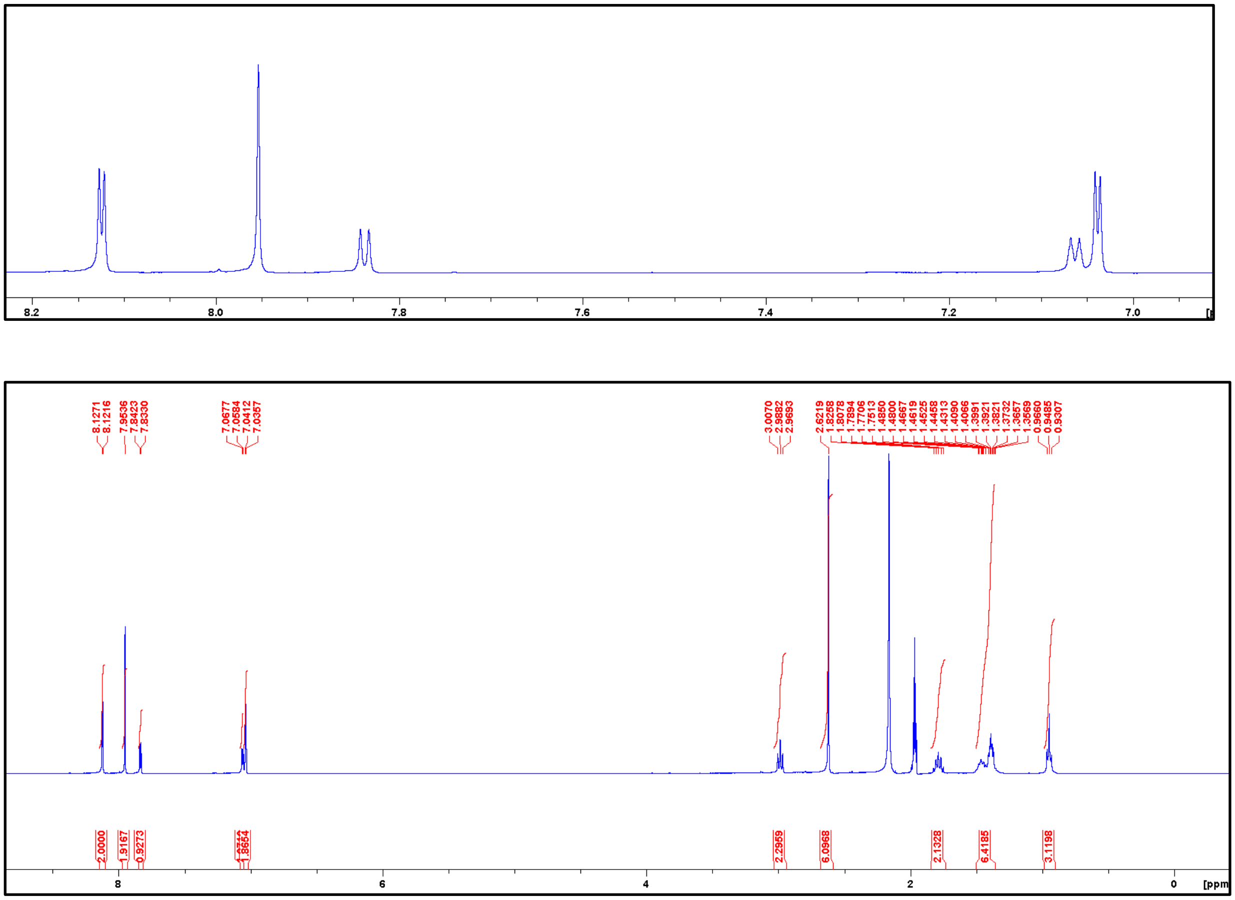
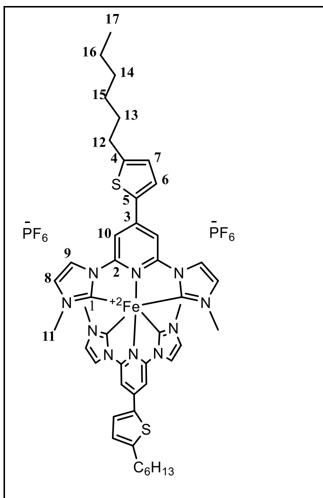


Figure S7. ^{1}H NMR spectra of **CTh**

	**CTh:** ^{13}C NMR (100 MHz, CD_3CN, δ ppm): 201.1 (C_1), 154.5 (C_2), 151.4 (C_3), 144.5 (C_4), 138.0 (C_5), 128.7 (C_6), 127.2 (C_7), 127.0 (C_8), 116.1 (C_9), 101.6 (C_{10}), 35.3 (C_{11}), 32.0 (C_{12}), 31.8 (C_{13}), 30.5 (C_{14}), 29.0 (C_{15}), 22.9 (C_{16}), 14.0 (C_{17}).

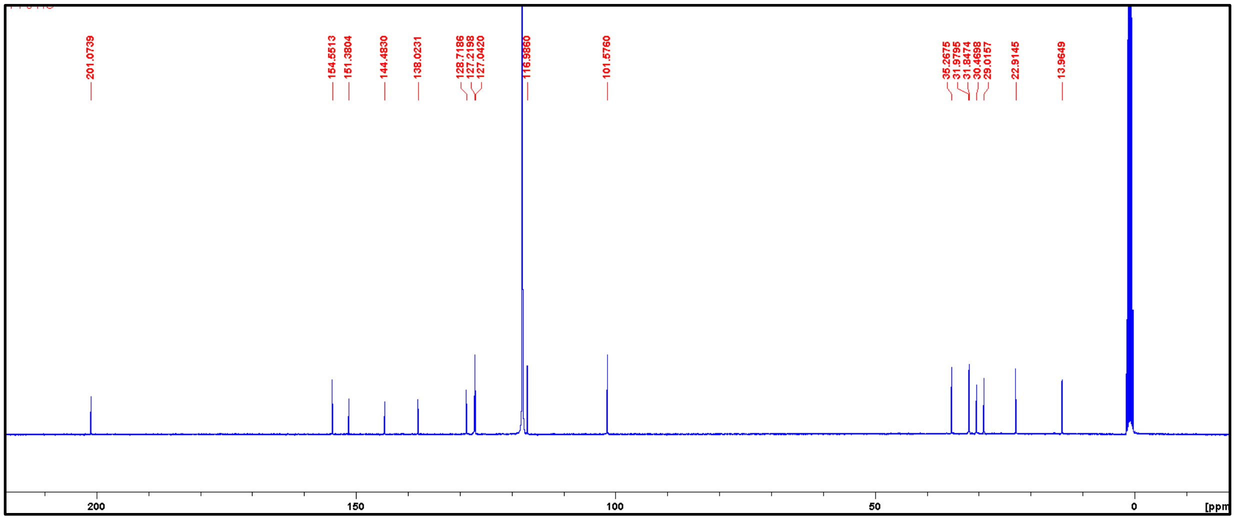
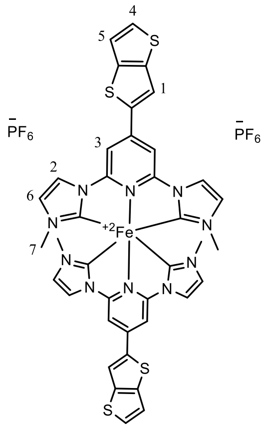
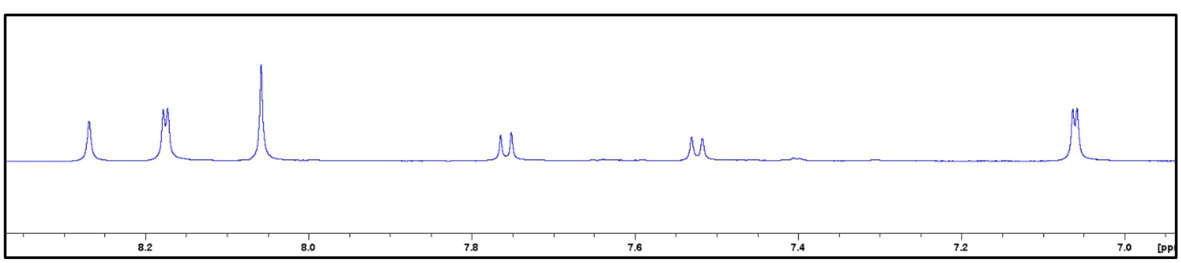


Figure S8. ^{13}C NMR spectra of **CTh**



CTh2: ^{1}H NMR (400 MHz, CD_3CN, δ ppm): 8.26 (s, 1H, H_1), 8.17(d, *J*= 2.10 Hz, 2H, H_2), 8.05(s, 2H, H_3), 7.76(d, *J*= 5.30 Hz, 1H, H_4), 7.52(d, *J*= 5.28 Hz, 1H, H_5), 7.05(d, *J*= 2.10 Hz, 2H, H_6), 2.64(s, 6H, H_7).



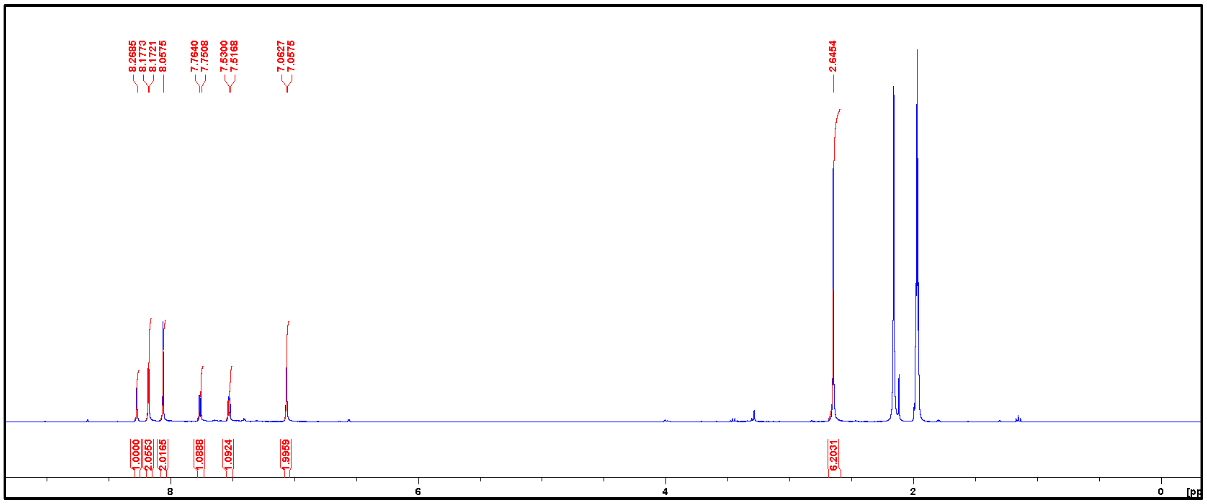
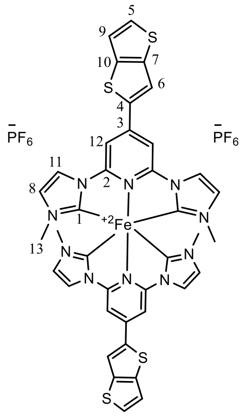


Figure S9. ^{1}H NMR spectra of **CTh2**



CTh2: ^{13}C NMR (100 MHz, CD_3CN, δ ppm): 200.8 (C_1), 154.6 (C_2), 144.6 (C_3), 142.2 (C_4), 141.7 (C_5), 141.0 (C_6), 131.7 (C_7), 127.1 (C_8), 120.9 (C_9), 120.7 (C_{10}), 117.1 (C_{11}), 101.9 (C_{12}), 35.3 (C_{13}).

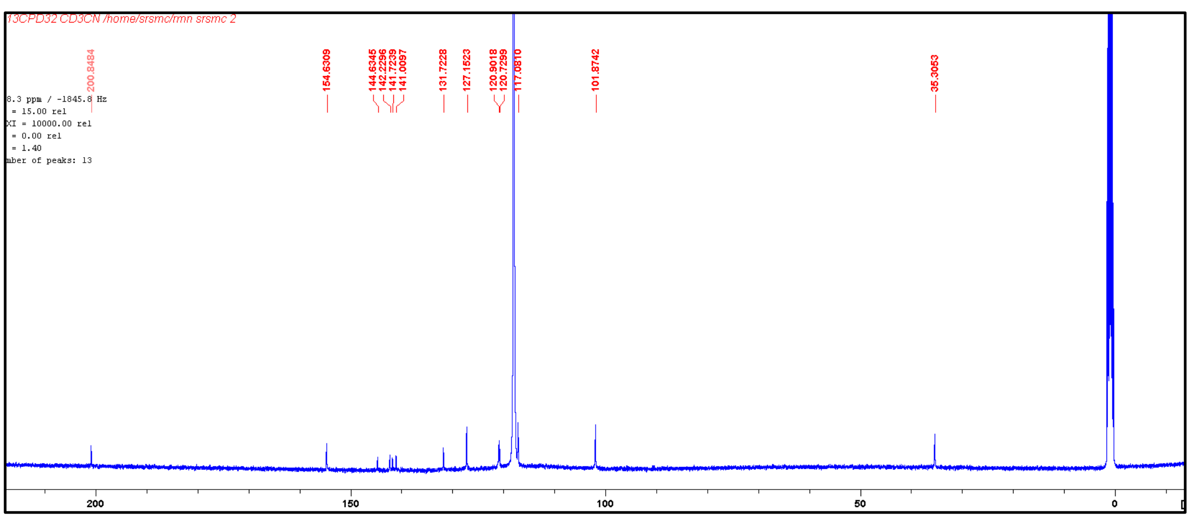
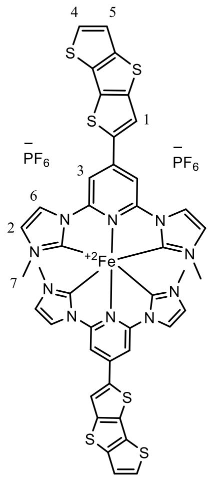
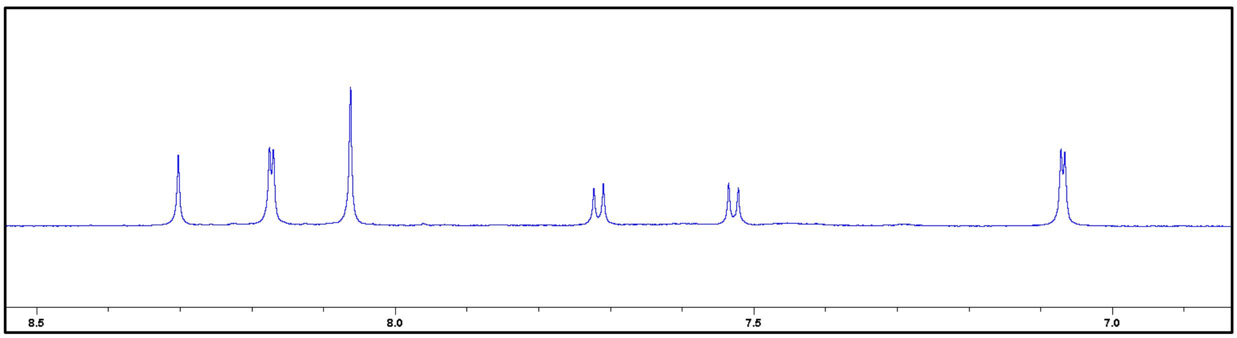


Figure S10. ^{13}C NMR spectra of **CTh2**



CTh3: ^{1}H NMR (400 MHz, CD_3CN, δ ppm): 8.30 (s, 1H, H_1), 8.17 (d, *J*= 2.12 Hz, 2H, H_2), 8.06 (s, 2H, H_3), 7.71 (d, *J*= 5.29 Hz, 1H, H_4), 7.53 (d, *J*= 5.30 Hz, 1H, H_5), 7.06 (d, *J*= 2.09 Hz, 2H, H_6), 2.65 (s, 6H, H_7).



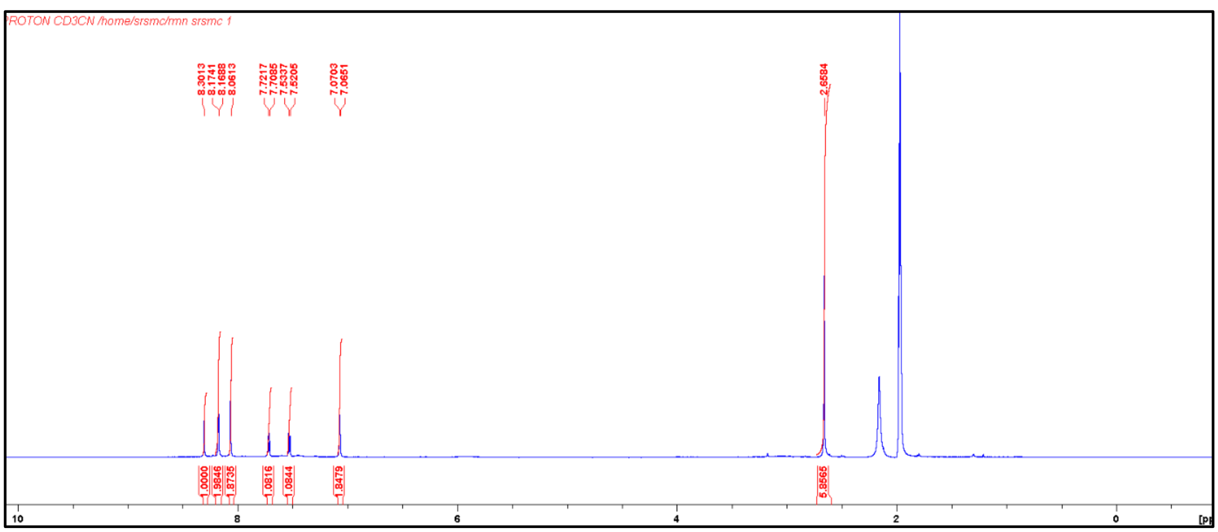
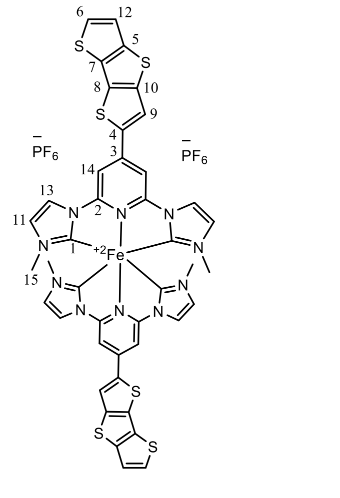


Figure S11. ^{1}H NMR spectra of **CTh3**

	**CTh3:** ^{13}C NMR (100 MHz, CD_3CN, δ ppm): 200.8 (C_1), 154.6 (C_2), 144.5 (C_3), 144.2 (C_4), 143.3 (C_5), 140.8 (C_6), 133.1 (C_7), 131.2 (C_8), 129.7 (C_9), 127.2 (C_{10}), 122.4 (C_{11}), 122.0 (C_{12}), 117.1 (C_{13}), 101.8 (C_{14}), 35.3 (C_{15}).

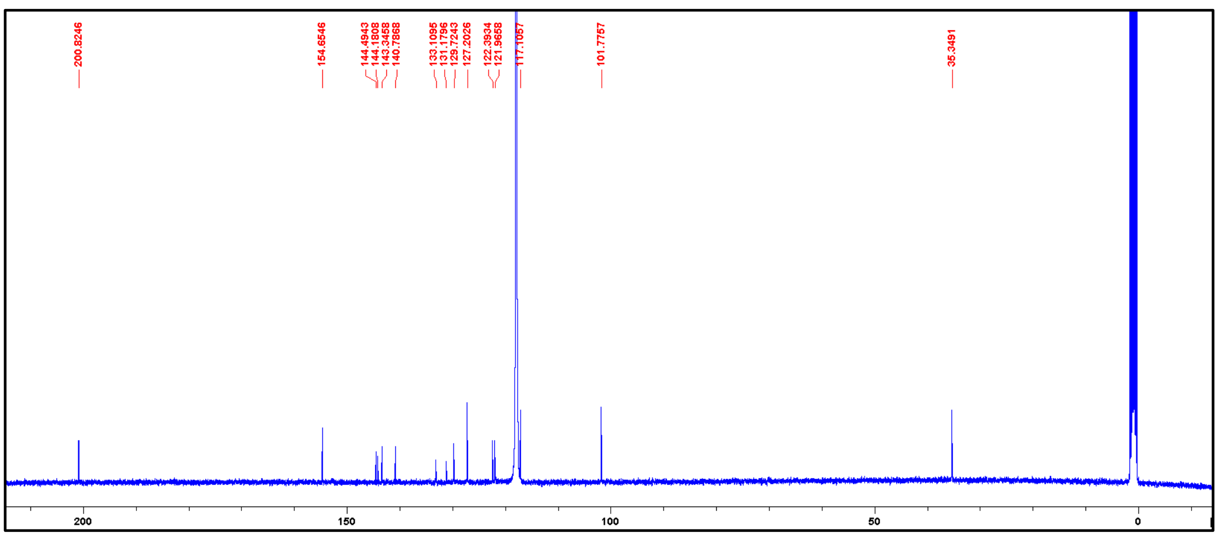


Figure S12.^{13}C NMR spectra of **CTh3**.

Cyclic Voltammograms

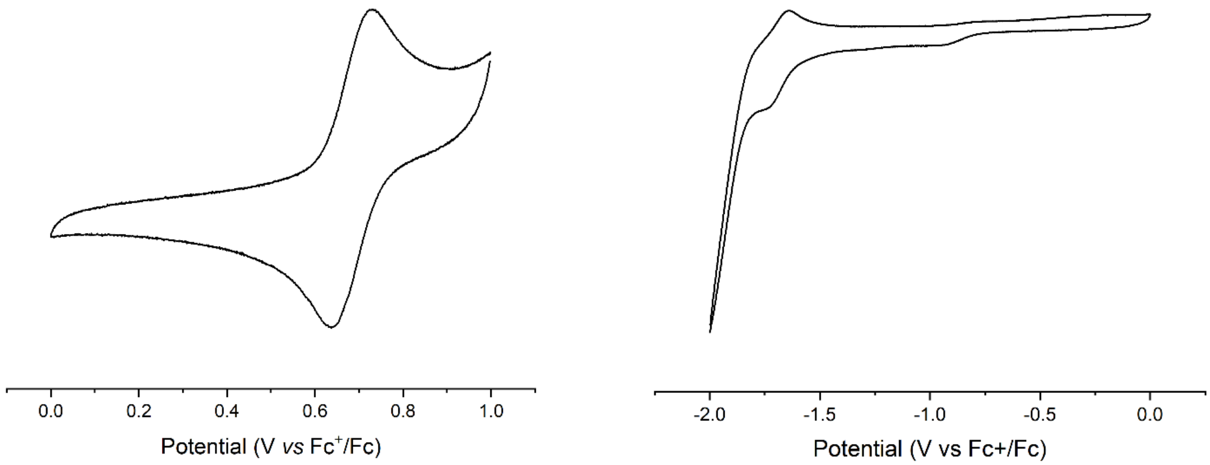


Figure S13. Cyclic Voltammetry of complex CTh

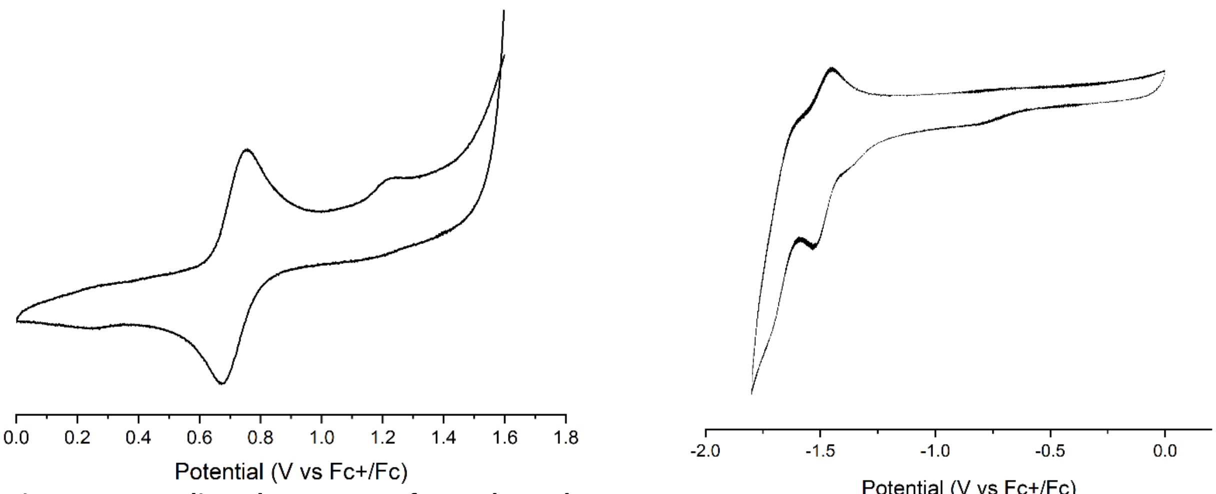


Figure S14. Cyclic Voltammetry of complex CTh2

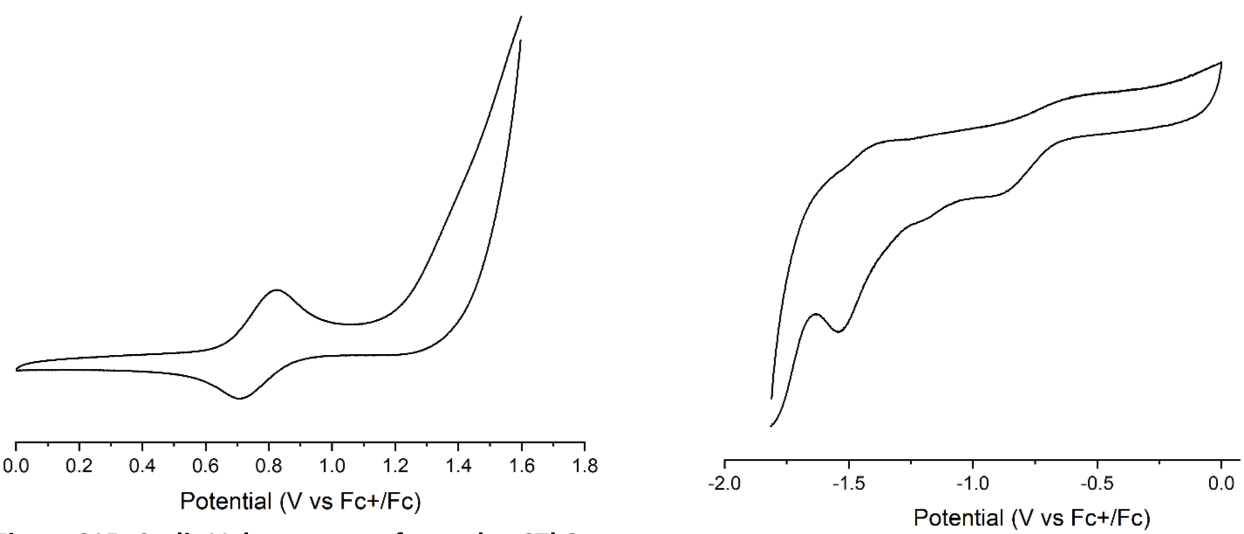


Figure S15. Cyclic Voltammetry of complex CTh3

Transient Absorption Spectroscopy

Overview of fs-TAS results

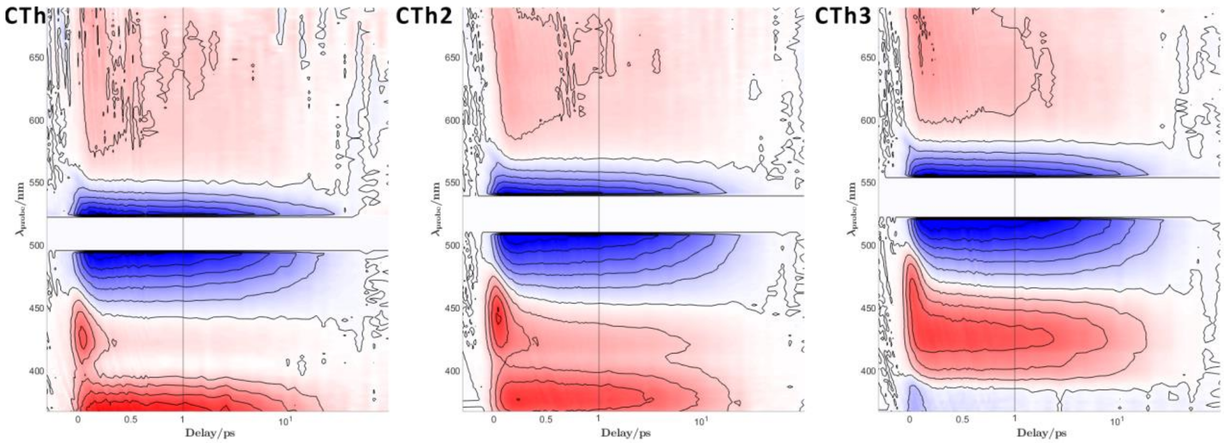


Figure S16. Two-dimensional contour plots of the fs-TAS data of the **CTh** series of molecules. Negative (bleach) signals are in shades of blue, whereas positive ones (induced absorption) are in red. Contour lines are drawn at 10 % increments of maximum absolute signal. Note the delay axis has a break at 1 ps and the scaling becomes logarithmic beyond that delay. The data around bleach maximum were omitted (white gap in 500-550 nm range) due to large noise of the scattered pump light.

Global fit

As described in the main text, all three datasets were subject to a global analysis employing a sequential relaxation scenario, which corresponds to a unidirectional first-order kinetic scheme in conjunction with a convolution with a Gaussian instrument response function (IRF, σ=50-60 fs). The reported time constants correspond to the respective inverse rate coefficients. The minimal number of species/relaxation steps needed to adequately describe the experimental data was decided based on (1) the inspection of the singular values of the data matrix (Fig. S16) and (2) by ensuring that the residuals do not present any systematic features indicative of a missing component. Indeed, as can be seen in Fig. S17, the singular values appear to be almost constant as a function of the singular value index after three (**CTh**) and four (**CTh2** and **CTh3**). This suggests the first hint on the maximum number of components to include in the model.

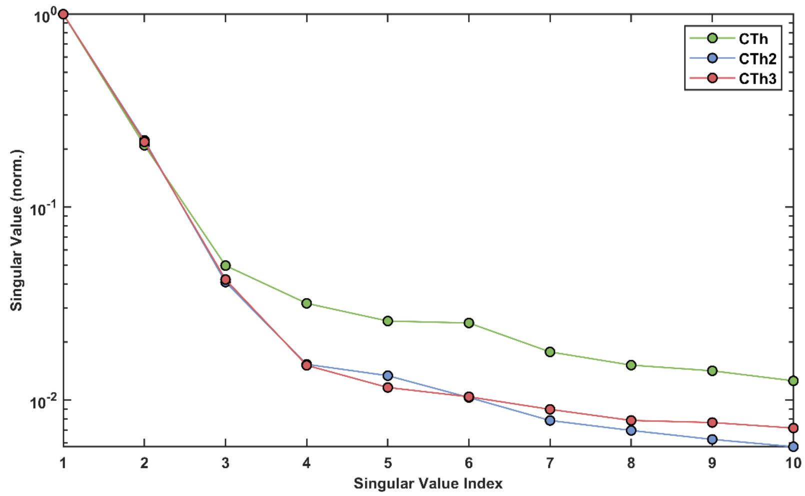


Figure S17. Normalized sorted singular values obtained by the singular value decomposition of the data matrices

We have tried the global sequential analysis with both three and four relaxation steps (+ a so-called coherent artifact contribution having the IRF temporal profile) and it turned out that actually 4 components are necessary for all three datasets **CTh**, **CTh2** and **CTh3**.

Figure S18 shows typical examples that highlight that the global fit with three exponentials does not capture properly the dynamics observed in the data in the 1-10 ps range. The additional time constant introduced by the four-step relaxation model falls in this range (3-5 ps). Note, however, that when fitted with 4 components, the CTh data yield an unphysically short time value of < 10fs for τ_1.

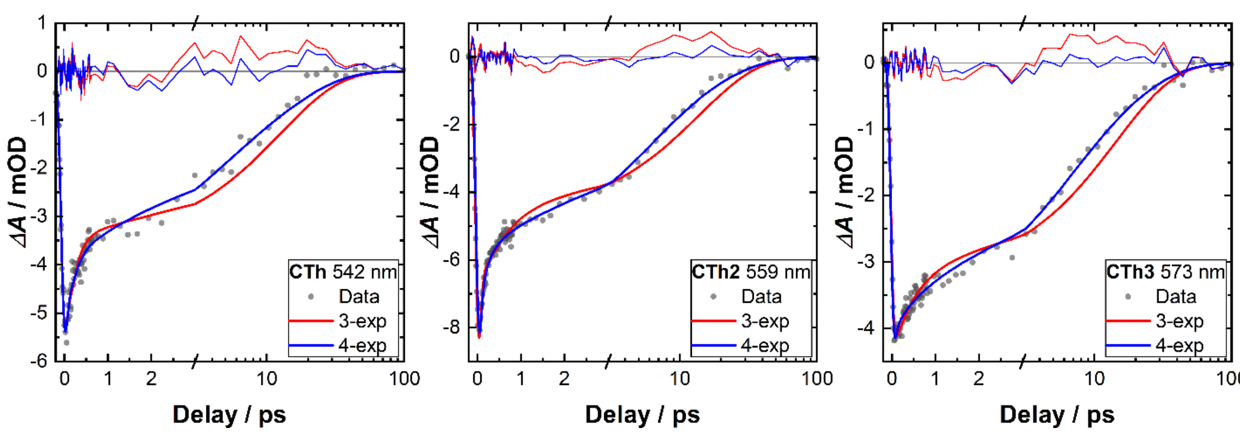


Figure S18. Examples of the results of the global sequential fit with three (red) and four (blue) exponentials at selected wavelengths. Residuals are drawn with thin lines and data are shown as dots.

As mentioned in the main text, given the similarity of the three datasets the evolution associated difference spectra (EADS) also show high resemblance (Fig. S19). Namely, for **CTh2** and **CTh3**, the first one accounts for the ultrafast redshift of the ESA overlapping the main bleach feature and the delayed rise of the latter. This component is attributed to the initial MLCT singlet to triplet conversion. The second sub-picosecond component captures the residual red shift of the ESA features (see e.g. the zero-crossing line for the red and blue curves in the 450-500 nm range) and intensity decrease. This feature can be assigned to vibrational relaxation of a non-thermalized MLCT triplet state. The third and fourth species (blue and green traces in Figure S19) show almost identical spectral shapes and differ mostly in intensities. We tentatively assign the third step (~5 ps relaxation time constant) to residual slower thermalization process which involves vibrational modes that are less strongly coupled to the optical transitions and which therefore leads to little spectral variation. The last, ~15 ps, step corresponds to the return to the ground state in accordance with the relaxation cascade observed for the parent pyridylNHC Fe(II) complexes.[4]

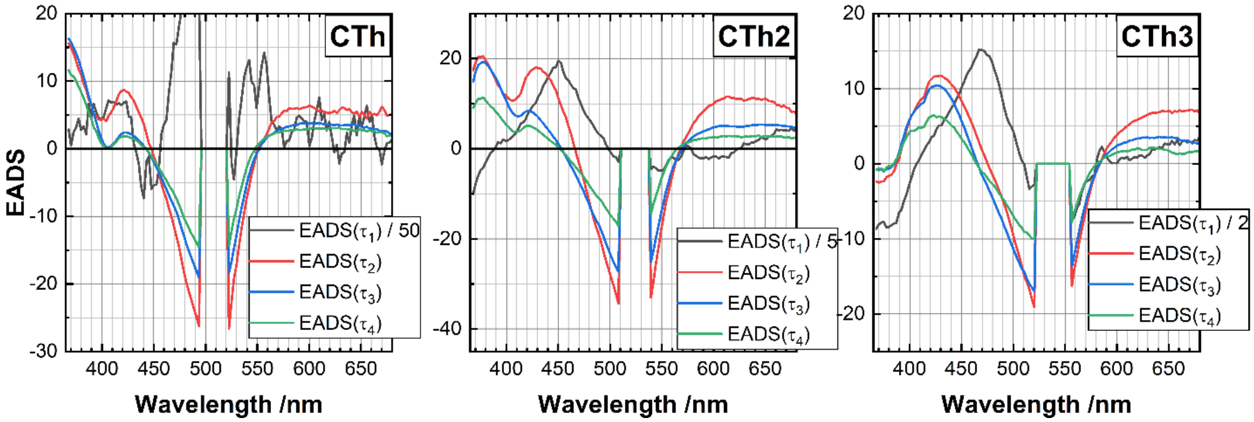
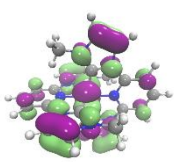


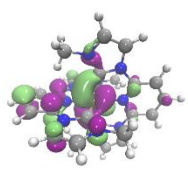
Figure S19. Evolution associated difference spectra obtained by the global sequential analysis with four kinetic components

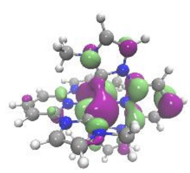
Computational details

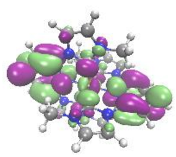
HOMO-LUMO Plots

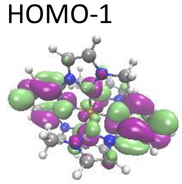
C0


HOMO


HOMO-1


HOMO-2


LUMO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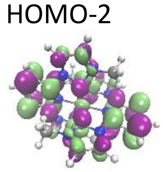
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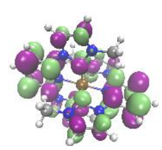
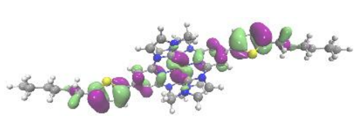

LUMO+3

CTh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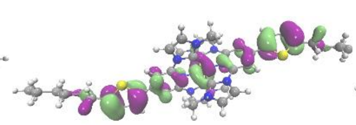
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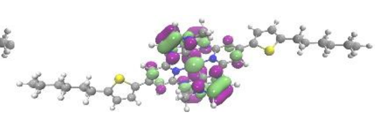
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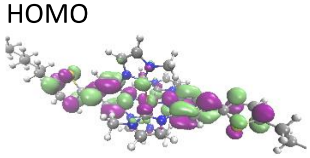
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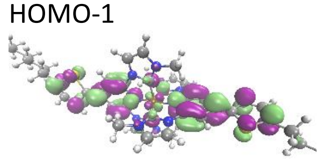
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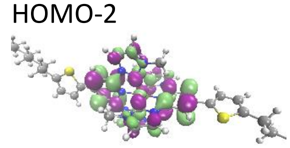
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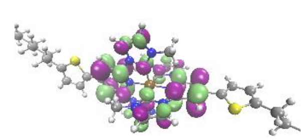
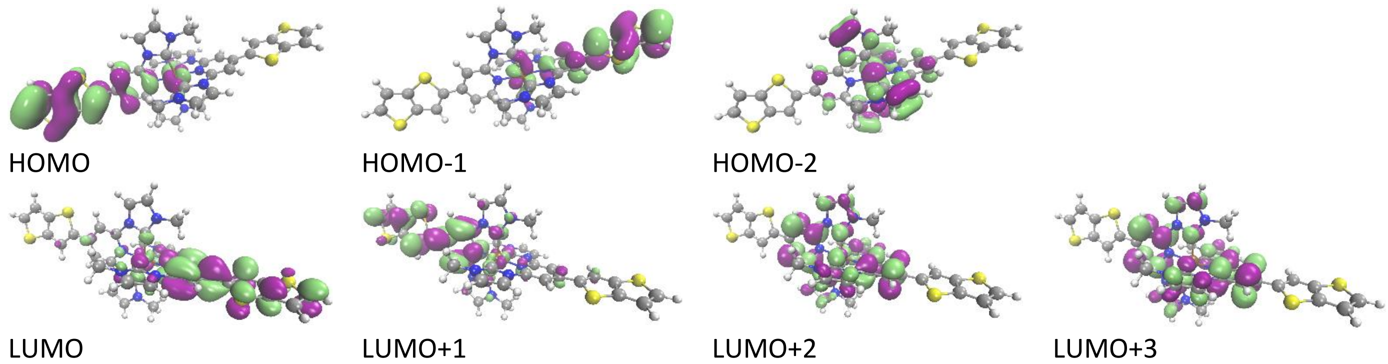
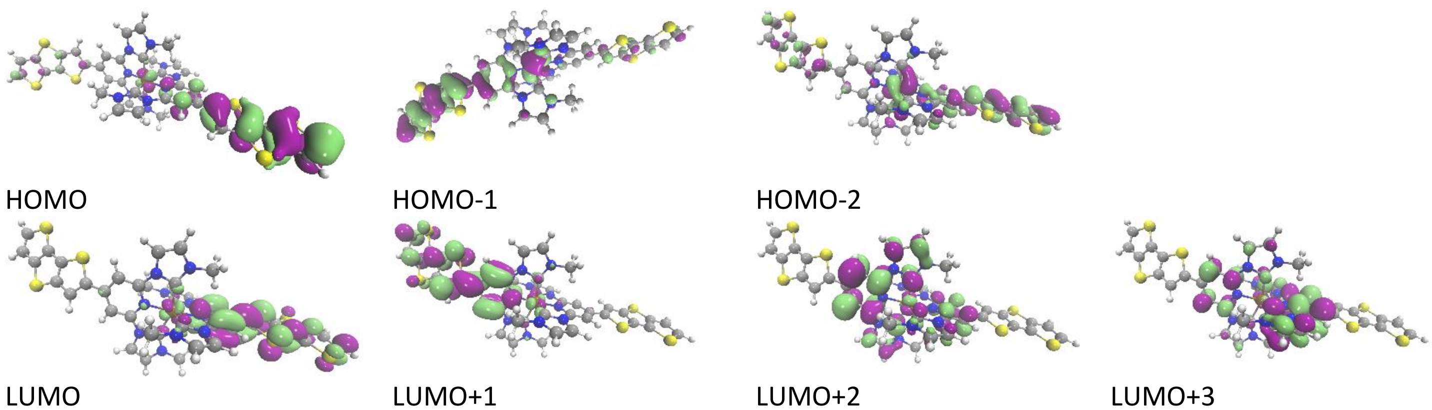

LUMO+3

CTh2

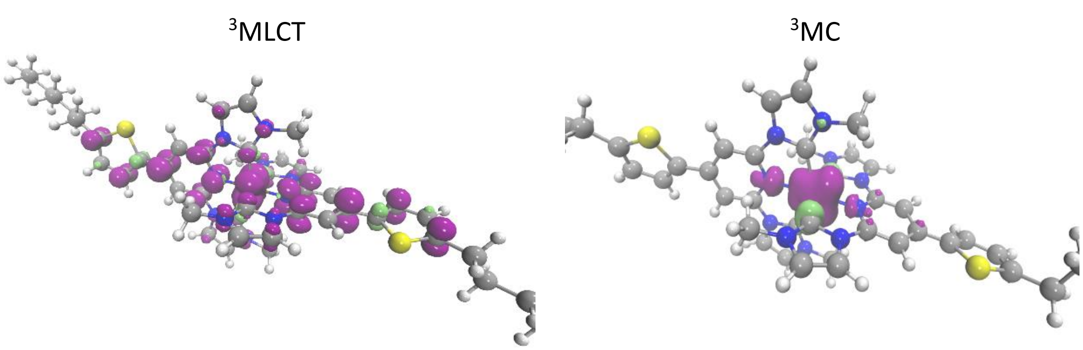


CTh3

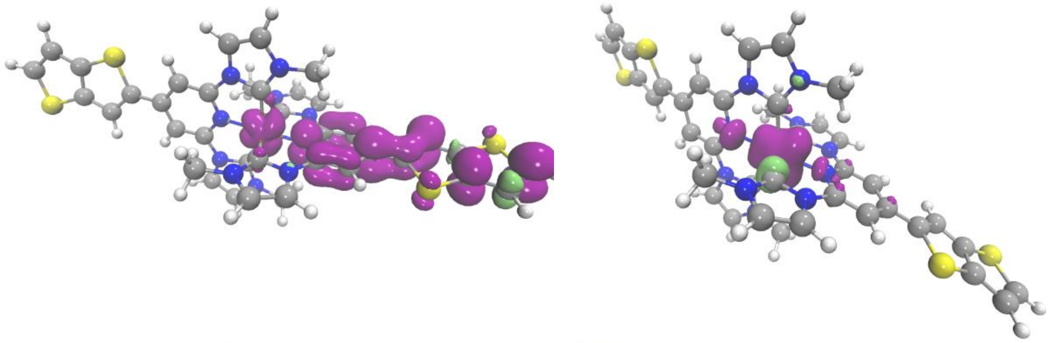


Computation of Geometry and Spin density of the ^{3}MCLT and ^{3}MC state

Complex **CTh**



CTh2



CTh3

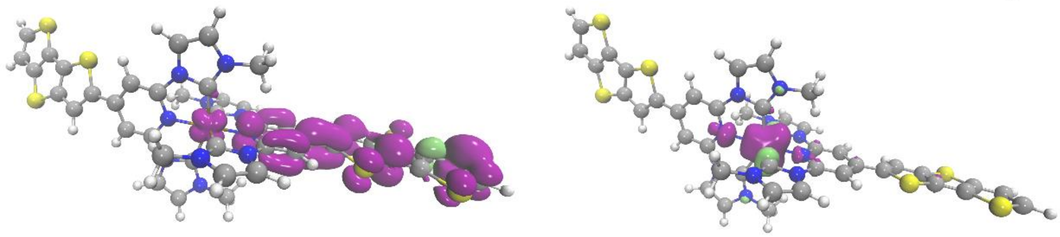


Figure S20. Geometry and Spin density of the ^{3}MLCT and ^{3}MC states of **CTh**, **CTh2** and **CTh3**.

Cartesian coordinates of the optimized structures

Ground state

C0

H	34.74433487615443	29.31776025755730	29.98286176114617
H	38.13051714840139	30.23438856687641	36.56875980411194
C	34.45576208538451	30.07176363702653	30.71389387142452
H	35.62211238883432	29.41617865641120	37.40638086471000
C	37.14060549232064	30.55246919856928	36.24471481930389
C	35.90952882590647	30.15094299996903	36.65557848850518
H	39.73055321502411	31.57498529074572	35.22034389451099
C	39.19538826283620	32.23753965918849	34.53692540818298
H	40.98374909720335	33.09218374293785	33.67346833911478
C	33.22408468214005	30.49023192960887	31.10563091349656
H	32.23475859095891	30.17065774772610	30.78126747339493
C	39.89044614040615	33.09030142123482	33.66827768547441
C	37.79995816801343	32.27152125733563	34.49249136337930

C	39.20086922254798	33.94052109424448	32.79291108756505
N	37.12661972248434	33.08526816101215	33.65476438481037
H	39.74022419040217	34.60490444369594	32.11457829292281
H	30.63241791379465	31.52982529949935	32.10855274384785
C	37.80520372819571	33.90130177065905	32.82347703272950
C	32.56196797481957	32.24772068665145	32.81825791500496
C	31.16658533018128	32.21042197545115	32.77480540285875
N	33.23404252545831	33.08191897854764	33.63664569304039
H	38.14959834353760	35.93640237516838	30.74796334369868
C	30.47021308872404	33.08212789059878	33.62338219872841
C	37.15749233696585	35.61587172355247	31.06273611011013
H	29.37690795758761	33.08212745361185	33.61827951335420
C	32.55419591106968	33.91614796234389	34.44863125205359
C	31.15847504294456	33.95376422952826	34.47846517121783
C	35.92926956059237	36.01218940749209	30.63862834136031
H	30.61810467208011	34.63434864221078	35.13971513495638
C	34.42670521368454	36.08951940313637	36.57430701694143
H	35.64680293018542	36.74432092242842	29.88340674358050
C	33.19910732862693	35.67193164375747	36.16926884049226
H	34.70798004534241	36.84214900288495	37.30955356417647
H	32.20640396368036	35.99067233939971	36.48397722706469
Fe	35.18035128265787	33.08245351670785	33.64566840446061
N	33.45189256822378	31.47487274402368	32.06778274870329
N	33.43668601907962	34.68903946222795	35.20761819570530
C	34.79586017276777	34.48336494345318	35.00481447910067
C	34.80913670677003	31.68058844016695	32.28409505047180
C	35.55364202157625	31.72218296297331	35.04827195807554
C	35.56271088555529	34.44292562736334	32.24554492682585
N	36.91123820848328	31.51527599180681	35.26106887172428

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H	37.38426466029001	31.26058895290116	31.95085800129440
H	37.09645405895866	29.55169377325459	31.51287716082081
H	37.13733765694870	30.81292601052201	30.23777913463475
C	36.81226881044847	35.56302871052979	36.03988806798739
H	37.36900855093540	34.89659927031422	35.37357529351956
H	37.07906878235828	36.60659238371485	35.80560611416524
H	37.09816537416925	35.34655221554812	37.08233959055140
C	33.52839565076628	30.69273306414633	36.11553211373736
H	33.25525202749081	30.92858451403345	37.15713065559371
H	32.97835603797086	31.36036877729815	35.44489788310462
H	33.24079987514135	29.65100932208192	35.89781984315188
C	33.54483114430793	35.45945067866426	31.15144717639846
H	33.28788030250419	35.22059851858656	30.10650272957745
H	32.98967747351662	34.78939393050445	31.81542496514749
H	33.24746466387368	36.49961763661898	31.36374936509174
N	34.97747171764323	35.28922645031157	31.36610716452848
N	34.96257672662095	30.87190999372920	35.91990193378020
N	35.40149763023501	30.80369572752822	31.44020282547078
N	35.37975380293855	35.35856566759558	35.85646494035428

CTh

H	35.920403	29.328696	31.186224
H	38.848638	31.418107	37.772499
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H	36.758070	29.792709	38.575398
C	37.818614	31.367809	37.423744
C	36.789570	30.573813	37.817072
H	39.900387	33.175518	36.486014

C	39.222484	33.633618	35.762555
C	34.112905	29.996542	32.297497
H	33.272279	29.368952	32.009953
C	39.657417	34.702938	34.930269
C	37.911011	33.191971	35.661848
C	38.706267	35.258641	34.027619
N	37.023429	33.724870	34.800538
H	38.990951	36.074800	33.363508
H	31.366519	30.137827	33.347526
C	37.415599	34.744587	34.009254
C	32.936886	31.471091	33.998975
C	31.647029	30.954927	34.012221
N	33.324161	32.491846	34.791369
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C	34.953151	36.239474	31.894674
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C	33.540171	35.646554	37.805261
H	34.446462	36.891302	31.184551
C	32.513769	34.851021	37.408021
H	33.567341	36.428897	38.562467
H	31.481904	34.800803	37.751300
Fe	35.173660	33.108913	34.781517
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N	33.036598	34.033523	36.408057
C	34.379474	34.296328	36.173470

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C	35.110525	34.552840	33.417678
N	37.301512	32.184203	36.419928
N	36.335373	35.185069	33.231900
C	37.500757	31.256967	32.400891
H	37.787420	32.136232	32.988621
H	38.098194	30.392961	32.736327
H	37.715833	31.449078	31.337036
C	35.949931	35.956377	37.195840
H	36.643064	35.566447	36.444613
H	35.841536	37.043482	37.051385
H	36.366626	35.766370	38.199390
C	34.382668	30.265287	37.197232
H	33.963824	30.454777	38.199969
H	33.691636	30.656802	36.444894
H	34.490009	29.178161	37.051969
C	32.858992	34.962845	32.390667
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H	32.260579	35.826513	32.725238
N	34.280956	35.223346	32.579458
N	35.674357	30.922295	37.050476
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C	41.010061	35.218455	35.018431
C	41.558358	36.363389	34.440639
C	42.910861	36.583968	34.789046
C	43.428167	35.618144	35.642035

S	42.228178	34.419930	35.995746
H	40.989608	37.051258	33.809189
H	43.498165	37.437271	34.438460
C	44.798290	35.512438	36.247261
C	29.339331	30.991226	34.994103
C	28.795081	29.845095	34.414789
C	27.441815	29.622103	34.758732
C	26.919887	30.587270	35.609646
S	28.116441	31.787799	35.966930
H	29.367178	29.158238	33.785258
H	26.857251	28.767548	34.406634
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C	45.944635	35.250638	35.246745
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H	45.750066	34.311667	34.695703
C	47.295376	35.187956	35.966751
H	47.407177	36.101765	36.582701
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H	47.280317	34.352842	36.695699
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C	49.836112	35.015820	35.830100
H	49.888704	35.911459	36.479889
C	51.085399	34.944546	34.952532
H	49.825210	34.158559	36.532659
H	51.149977	35.808970	34.267358
H	51.091601	34.037998	34.320034

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H	25.334935	29.748402	36.749548
C	24.404059	30.953656	35.207543
H	25.546725	31.483449	36.979869
H	24.393455	30.149856	34.447112
H	24.600208	31.892958	34.657632
C	23.051868	31.016207	35.924817
H	22.938157	30.101583	36.539173
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H	21.924564	32.081331	34.397547
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H	20.458279	30.293798	36.433180
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H	20.522046	32.046625	36.487541
H	19.199777	30.398303	34.219230
H	19.258447	32.169256	34.273325
H	18.346817	31.274745	35.518624

CTh2

H	35.862946	29.283279	31.019970
H	38.968205	31.400683	37.499555
C	35.368905	29.934721	31.739379
H	36.926052	29.725033	38.322656
C	37.929649	31.343142	37.178384
C	36.925479	30.521595	37.579933
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C	39.235773	33.696430	35.552113
C	34.083377	29.945331	32.177652

H	33.240410	29.308242	31.919195
C	39.619695	34.796442	34.735365
C	37.942456	33.203179	35.449389
C	38.647176	35.316863	33.834504
N	37.029617	33.712714	34.600455
H	38.897020	36.148407	33.175605
H	31.367252	30.073473	33.304524
C	37.379543	34.752271	33.814774
C	32.946722	31.416491	33.908831
C	31.662686	30.891098	33.962280
N	33.349819	32.441334	34.688203
H	36.988553	36.823585	31.804144
C	30.731739	31.440263	34.889904
C	36.160921	36.187514	32.110219
C	32.480707	32.969033	35.571514
C	31.175678	32.517151	35.706632
C	34.859857	36.175771	31.720761
H	30.512117	32.966916	36.448125
C	33.633465	35.594452	37.698965
H	34.328437	36.808807	31.011894
C	32.601006	34.794275	37.328768
H	33.676751	36.375522	38.456793
H	31.579912	34.737120	37.701803
Fe	35.191885	33.068494	34.622498
N	34.009624	30.984650	33.103416
N	33.100484	33.981899	36.312921
C	34.435005	34.252018	36.041614
C	35.233743	31.625918	33.258879
C	36.031263	31.883521	35.987917

C	35.073701	34.508355	33.257922
N	37.373373	32.168210	36.202778
N	36.281578	35.163321	33.048228
C	37.465542	31.227345	32.187403
H	37.758144	32.113641	32.761788
H	38.075470	30.369872	32.517026
H	37.655092	31.410830	31.117236
C	36.022838	35.919621	37.033365
H	36.707300	35.534684	36.271962
H	35.904698	37.005883	36.890117
H	36.456575	35.732857	38.030128
C	34.509866	30.178133	37.009093
H	34.091334	30.369297	38.011671
H	33.807801	30.545642	36.254986
H	34.642420	29.092686	36.874542
C	32.797877	34.867208	32.265654
H	32.571185	34.657870	31.207377
H	32.531705	33.991937	32.868805
H	32.192052	35.726646	32.597620
N	34.218315	35.153445	32.426158
N	35.785852	30.862270	36.846345
N	36.049006	30.958557	32.404586
N	34.733341	35.253505	36.907263
C	40.938169	35.387510	34.841003
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C	42.714137	36.883108	34.673204
C	43.317774	35.884885	35.464428
S	42.214712	34.582901	35.769694
H	40.750308	37.273218	33.727055

S	43.823000	38.196885	34.385980
C	29.389448	30.908657	35.014877
C	28.878687	29.727493	34.478948
C	27.534980	29.511601	34.850017
C	26.997052	30.525648	35.667269
S	28.171154	31.761719	35.978121
H	29.464746	29.032681	33.872936
S	26.351239	28.265992	34.555527
C	45.051633	37.386411	35.315966
C	44.660430	36.170740	35.831043
H	46.022894	37.871433	35.441037
H	45.307001	35.531921	36.436027
C	25.181346	29.125486	35.516649
C	25.645841	30.307789	36.047661
H	24.184824	28.695296	35.644754
H	25.041577	30.971487	36.669290

CTh3

H	36.742194	30.034408	31.548795
H	38.598279	32.200540	38.487097
C	36.072691	30.575457	32.215816
H	36.562571	30.466679	39.200345
C	37.609649	32.055769	38.053344
C	36.604934	31.212434	38.407503

H	39.767962	33.637847	36.881847
C	39.074691	34.123998	36.191725
C	34.741015	30.425440	32.436450
H	34.022916	29.746277	31.981194
C	39.535961	35.069085	35.230911
C	37.731532	33.775904	36.192726
C	38.564784	35.685584	34.391776
N	36.835951	34.312866	35.342616
H	38.871352	36.403108	33.630756
H	31.939133	30.151468	33.123085
C	37.244142	35.269003	34.482454
C	33.193026	31.629667	34.045533
C	31.997374	30.951504	33.861772
N	33.336880	32.646148	34.919413

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C	36.066818	36.730998	32.775350
C	32.271186	33.023685	35.652838
C	31.030099	32.411932	35.551122
C	34.789194	36.694750	32.316241
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S	42.16179556469589	34.68634783454635	35.88902766161190
H	40.72429901204182	37.26777747449535	33.64952141269577
S	43.75096909396597	38.27708362595077	34.35055050102495
C	29.38559873622807	30.95370197293990	35.02873122236268
C	28.84360209673736	29.79108168309601	34.47917366169700
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C	26.98537706888909	30.62479683287406	35.67908508207816
S	28.19027036155861	31.82561289642383	36.00484640367340
H	29.41109027374290	29.08796500906465	33.86510027742744
S	26.27853099433286	28.39675672982392	34.53908587880432
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C	44.56645966538238	36.34036101204241	35.93504995518922
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H	45.20659185256697	35.74813175370659	36.59250573969926
C	25.13334598725388	29.27650547008935	35.51053939461393
C	25.62931175553588	30.43960897979817	36.05646076800413
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H	39.768996	33.651224	36.888877
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H	36.73053072938792	31.37753788837268	38.45678522816099
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H	33.18013109661228	34.66595316612253	30.01508397069182
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C	43.89068353273088	34.78932405788444	32.48812456393566
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C	34.61158057687447	36.16474555481983	32.29975990615099
H	30.39265039436008	32.59229944413795	36.47771507187522
C	33.31860511023498	34.96871794920705	38.37492197548070
H	33.96793360230064	36.76028903512363	31.65405495550967
C	32.40299161974486	34.08326534596497	37.89897259391626
H	33.25814146057780	35.68063122846124	39.19686667783517
H	31.39110964900003	33.86168514405693	38.23548920398236
Fe	35.43485033052775	32.99377689645130	35.07466648233220
N	34.22153840258864	30.83794345702792	33.36327161646455
N	33.02062751730627	33.43397914224077	36.83167539037243
C	34.30940191127291	33.89497907061829	36.62808179666736
C	35.41078815717733	31.51059773443338	33.58847172688506
C	36.55264969579843	31.94306410553287	36.35914661914998
C	35.10283905926580	34.49213883471187	33.76744437628403
N	37.86348503782651	32.39953202834518	36.50938460887849
N	36.22821493814145	35.26769318490438	33.48384624281959
C	37.67208262609859	31.31924146103843	32.56831489609640
H	37.89333963867985	32.10517715166839	33.29908991625690
H	38.31412464238588	30.44791884644620	32.77951829981421
H	37.89311774820053	31.69227132205702	31.55417298267538
C	35.66677602116118	35.63577193810523	37.78316375302845
H	36.40071786949056	35.36382551637940	37.01547089823826

H	35.43273819785014	36.70864462405612	37.68806870260755
H	36.09931698926004	35.44551794288314	38.77987815390016
C	35.29668775907125	30.07645492498708	37.41133915484517
H	34.91121035656472	30.20902575194426	38.43589264211515
H	34.53348978522001	30.40156093627084	36.69467001267040
H	35.52926053660530	29.01226803790822	37.24396822891585
C	32.73182290840225	34.65691274271139	33.00517160426573
H	32.45664697798480	34.27108727630770	32.00962196797602
H	32.59631647245116	33.86875419477339	33.75103838087489
H	32.07696616679235	35.50639195964736	33.25733372475761
N	34.12877549288233	35.07712539111171	33.03055986638555
N	36.48694127324621	30.89205832788989	37.20647924987187
N	36.26507689868605	30.95936943871070	32.69452839067742
N	34.46428389525355	34.83715652992849	37.58686562403879
C	41.12897605907582	35.58010722483108	34.43736019643730
C	41.50883255746842	36.56846750885111	33.52753697820218
C	42.90078917413418	36.77050146953439	33.50962163215320
C	43.61473605644834	35.94724945645117	34.40277444254752
S	42.53762435855884	34.91528860958459	35.28828085693263
H	40.81258326407492	37.12135277683478	32.89360342006449
S	43.98678902012887	37.79298822231421	32.60876212629415
C	29.36353867902462	30.90075468064495	34.57427053047895
C	28.78090343695403	30.35765432135008	33.43146748293521
C	27.37587946325258	30.27463952961562	33.53750941908581
C	26.86478548151457	30.73721117268338	34.76457728670028
S	28.14511957601366	31.27419567203542	35.80586315552903
H	29.33989545789091	30.06372304164487	32.53953280883854
S	26.08343706218887	29.75370692464622	32.48904128930154
C	45.35405894695063	37.09988045024228	33.43534343345601

C	45.02217918628421	36.13663965711245	34.36423025685780
H	46.35714783666959	37.45339401691242	33.18122290088697
H	45.75073296236022	35.59651218800108	34.97242504305162
C	24.90666626818864	30.15297998148755	33.70883350681197
C	25.44894321078876	30.66304250394571	34.86717243381518
H	23.84840446376676	29.97908763169849	33.50074742395186
H	24.85476528412611	30.96681150914166	35.73153630282867

CTh3

H	36.321495	29.899038	31.148601
H	38.714886	32.154140	38.192288
C	35.686934	30.437492	31.850643
H	36.708205	30.420644	38.991074
C	37.718511	31.992534	37.782803
C	36.729598	31.149837	38.182151
H	39.884615	33.400795	36.514548
C	39.196227	33.945034	35.865715
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H	33.630743	29.597008	31.738055
C	39.680806	34.900480	34.924278
C	37.835740	33.677326	35.899390
C	38.724523	35.550752	34.087345
N	36.961556	34.291678	35.107163
H	39.048112	36.274899	33.338859
H	31.598392	29.936969	33.039525
C	37.384743	35.196707	34.223470
C	32.888626	31.464461	33.839296
C	31.696007	30.762105	33.745328

N	33.055374	32.480366	34.695177
H	37.078020	37.439472	32.417144
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C	36.236802	36.773250	32.597408
C	32.069196	32.849289	35.520305
C	30.840438	32.208211	35.531701
C	34.958000	36.823749	32.138270
H	30.051425	32.525774	36.216003
C	32.664180	35.586456	37.757884
H	34.476260	37.529382	31.462780
C	31.789097	34.657313	37.287938
H	32.534191	36.364000	38.508959
H	30.747177	34.475609	37.546488
Fe	34.896974	33.393301	34.860532
N	34.086687	31.229843	33.129209
N	32.488158	33.926646	36.329801
C	33.798458	34.386210	36.191650
C	35.213289	31.988040	33.451135
C	35.903100	32.323034	36.411968
C	35.070551	35.033309	33.540900
N	37.201216	32.700457	36.700759
N	36.295130	35.674593	33.452516
C	37.568316	31.907498	32.632918

H	37.696106	32.680592	33.396192
H	38.235204	31.060608	32.862076
H	37.835753	32.319913	31.645643
C	35.065757	36.203266	37.316867
H	35.844060	35.868019	36.621585
H	34.853404	37.271305	37.146348
H	35.421088	36.062973	38.351299
C	34.389024	30.631439	37.448755
H	33.920429	30.822773	38.428631
H	33.711036	30.962884	36.655098
H	34.568176	29.549732	37.337706
C	32.861521	35.478480	32.483069
H	32.685718	35.275761	31.413501
H	32.573984	34.596869	33.070529
H	32.240014	36.334625	32.793611
N	34.271637	35.758520	32.723198
N	35.642381	31.364942	37.334295
N	36.176254	31.471384	32.651701
N	33.870942	35.403995	37.078932
C	41.103209	35.138669	34.798629
C	41.795588	35.990449	33.934139
C	43.194200	35.893789	34.085080

C	43.591429	34.960750	35.068615
S	42.224923	34.211034	35.813229
H	41.306611	36.653997	33.217096
S	44.575526	36.664162	33.312886
C	29.365399	30.427038	34.596878
C	28.916376	29.469489	33.679855
C	27.619467	29.013352	33.968370
C	27.055956	29.600425	35.126094
S	28.143395	30.737007	35.846924
H	29.506851	29.123806	32.827436
S	26.531062	27.862116	33.206294
C	45.669685	35.720928	34.312967
C	44.994983	34.862354	35.197912
S	46.115102	33.945204	36.160541
C	25.333476	28.168139	34.452884
C	25.758486	29.116918	35.404586
C	24.029317	27.661952	34.702194
C	47.086958	35.638564	34.413172
C	47.460200	34.720099	35.369081
H	48.475355	34.443695	35.665279
H	47.794777	36.219166	33.817837
S	24.537957	29.378137	36.619055
C	23.490655	28.228707	35.836001

H	22.507235	28.030903	36.270125
H	23.500991	26.933767	34.083845

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