Supplementary Information

Heterobimetallic 3d-4f complexes supported by a Schiff-base tripodal ligand

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1. ^{1}H NMR spectroscopic characterisation data for compounds **1**–**5**

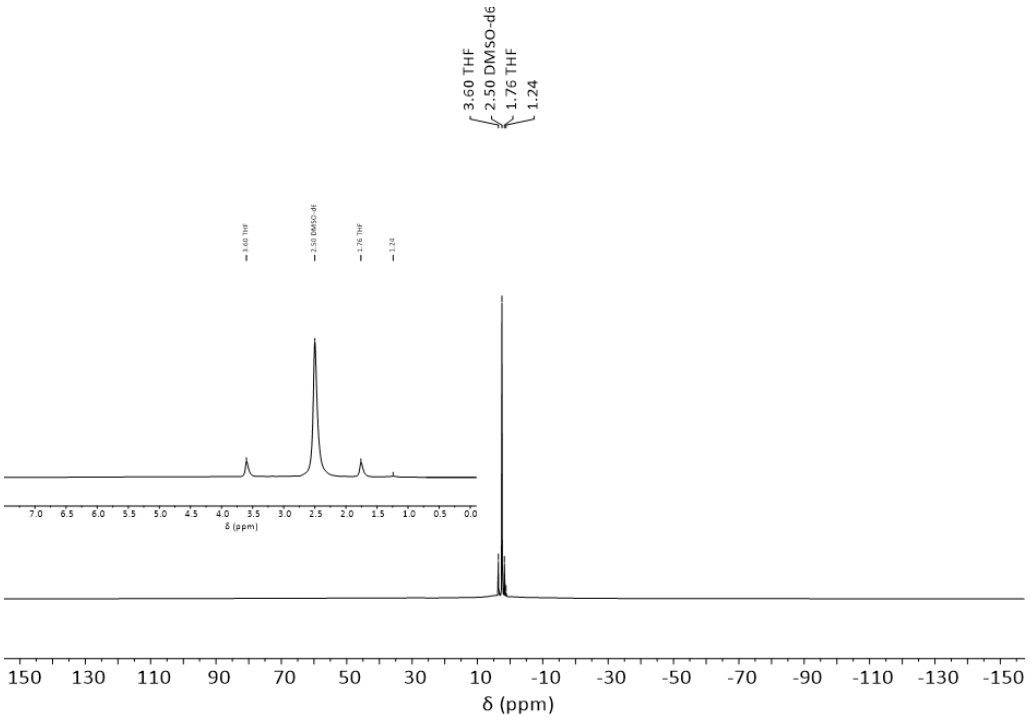

Figure S1: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for compound **1**(NaOTf).

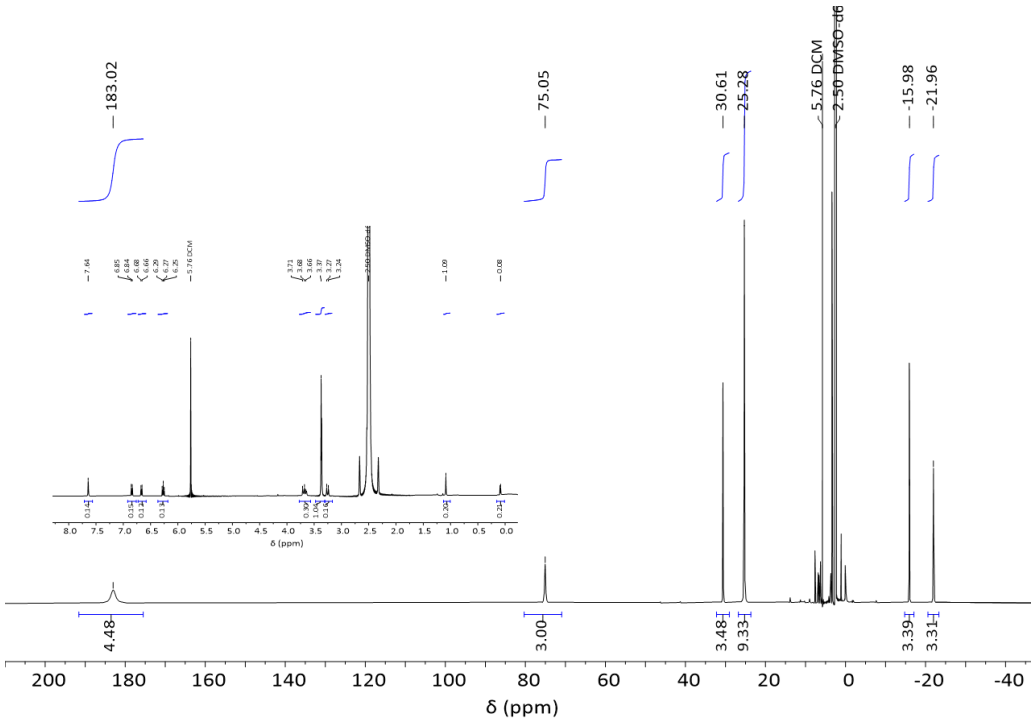

Figure S2: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for compound **2**(NaOTf). Additional peaks in diamagnetic region (e.g. 6.25 – 7.64 ppm) correspond to ligand-based impurities at 5% contamination.

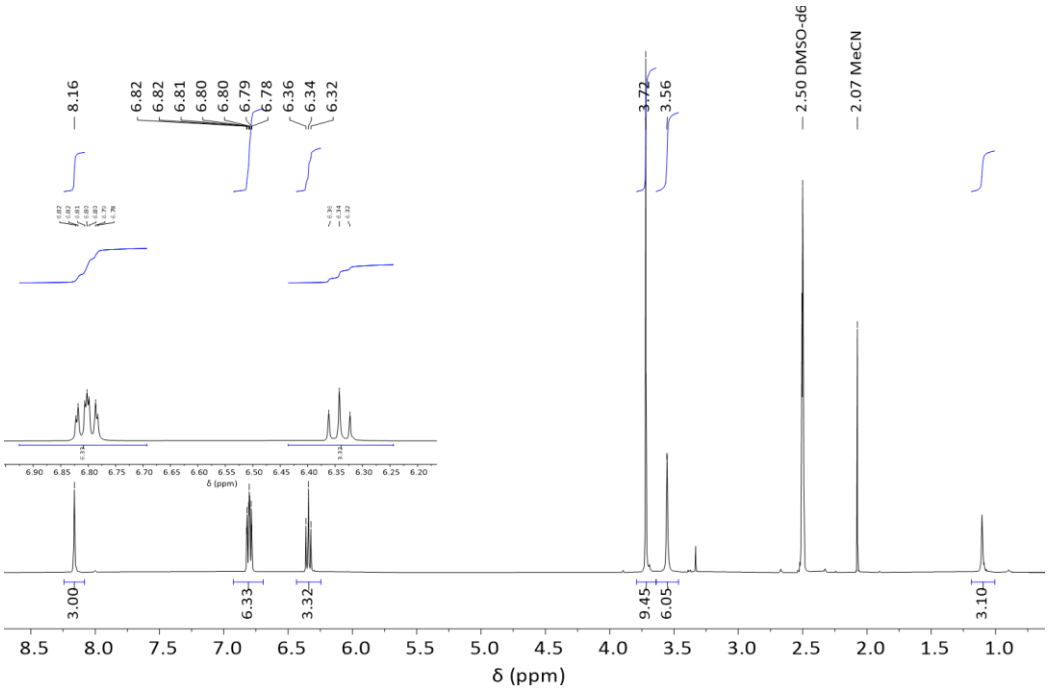

Figure S3: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for compound **3**(NaOTf).

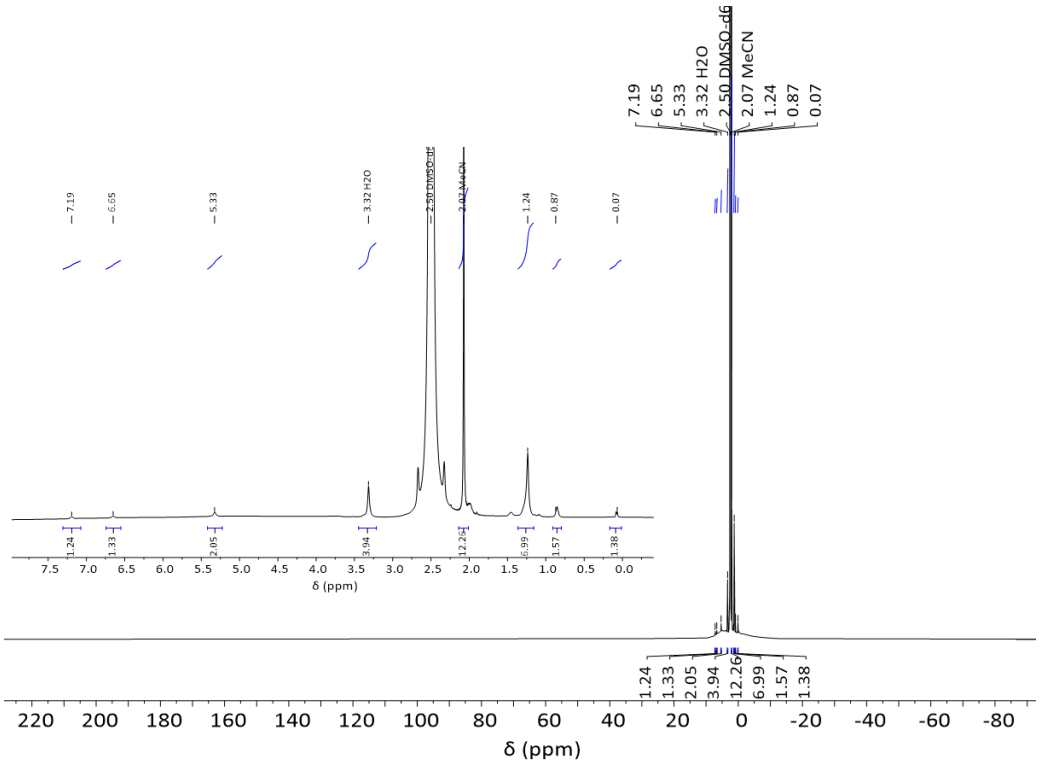

Figure S4: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for compound **4**.

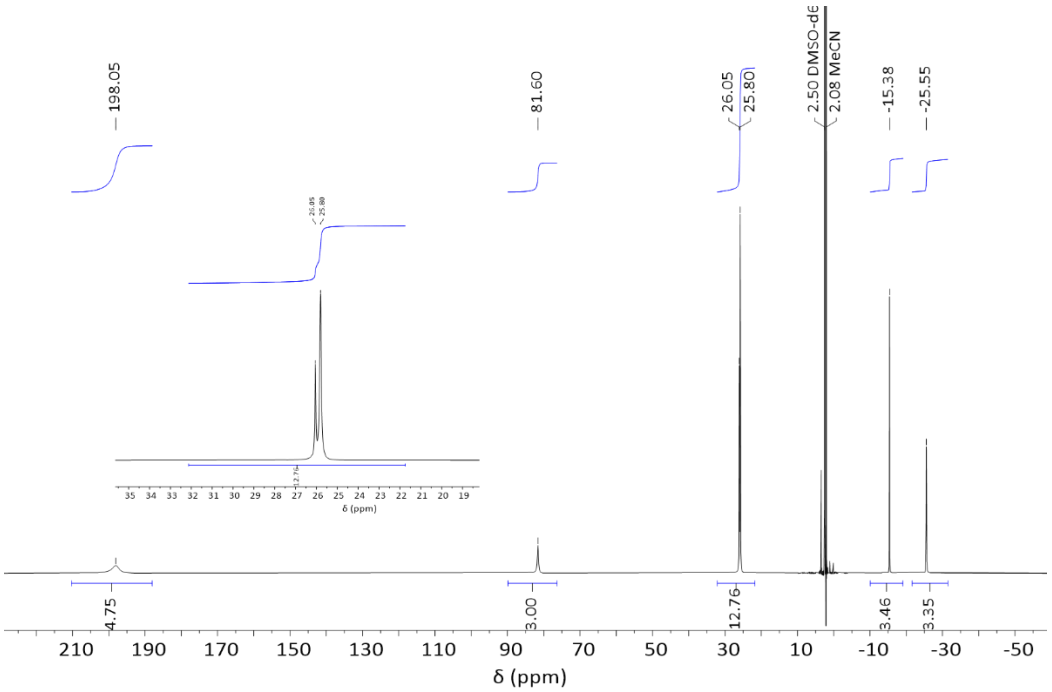

Figure S5: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for compound **5**.

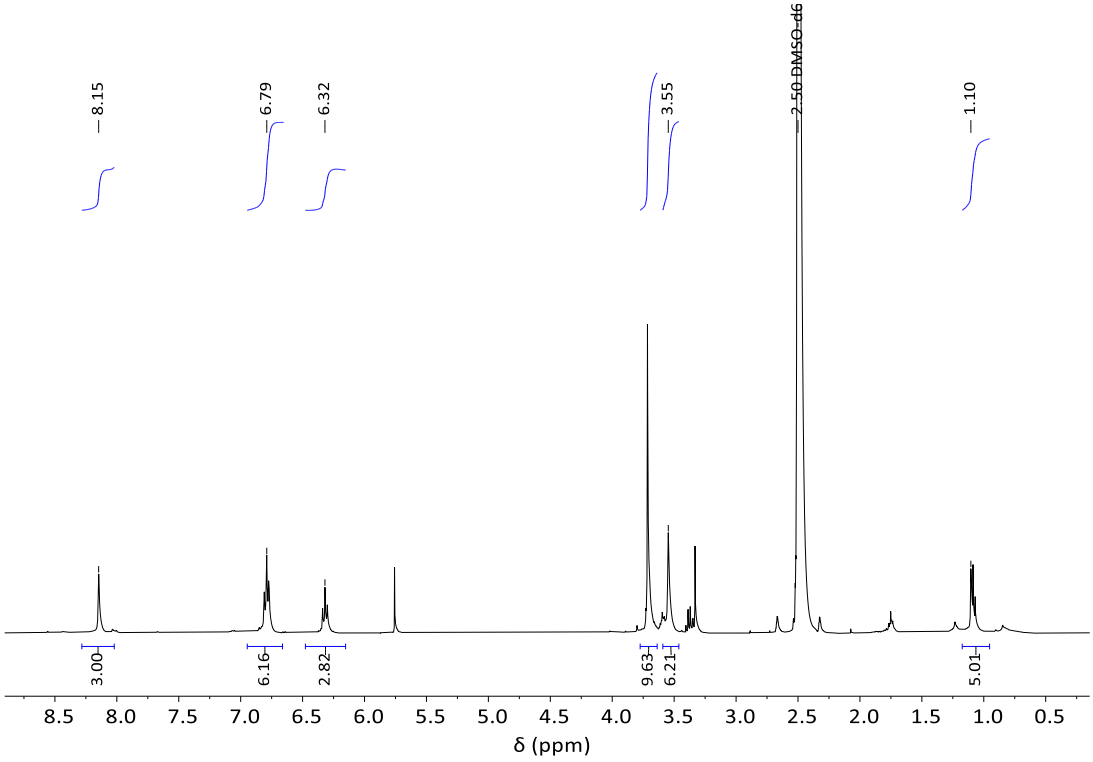

Figure S6: ^{1}H NMR spectrum (400 MHz, d_6-DMSO) for the reaction of compound **3**(NaOTf) with $Co[OTf]_2$ in THF at room temperature for 6 h.

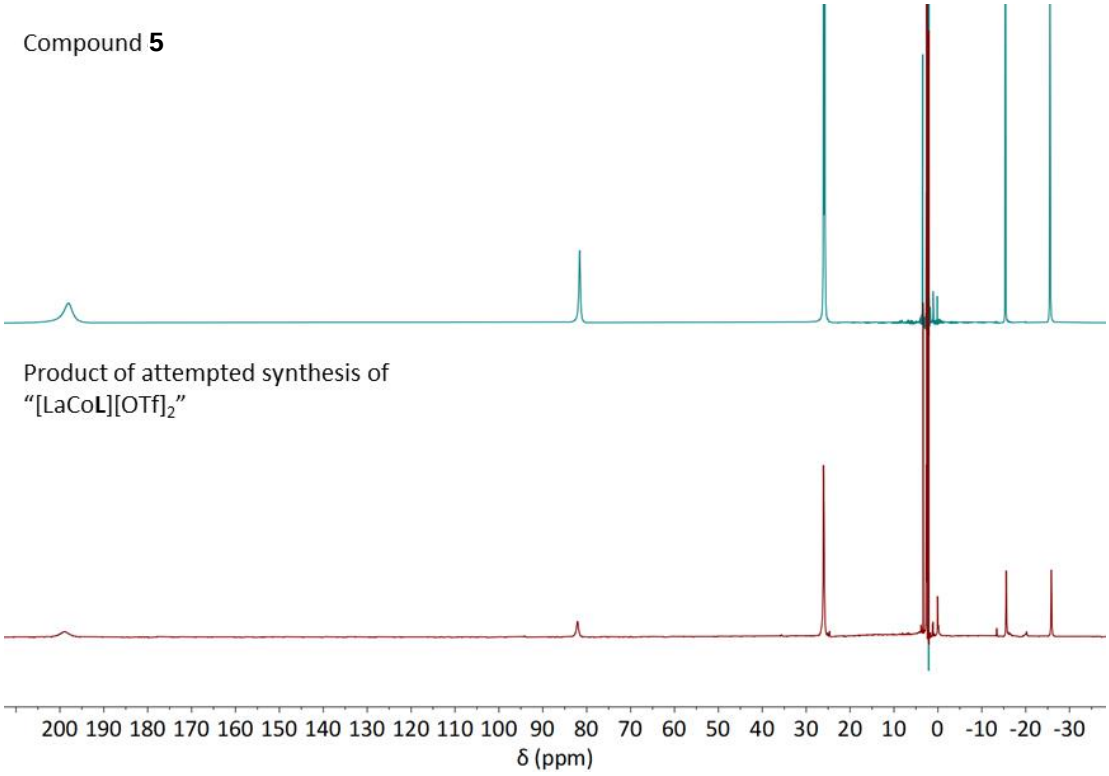

Figure S7: Comparison of ^{1}H NMR spectra (400 MHz, d_6-DMSO) between compound **5** and the attempted synthesis of [LaCo**L**][OTf]$_2$.

2. EPR spectra for compounds **2**(NaOTf), **4** and **5**

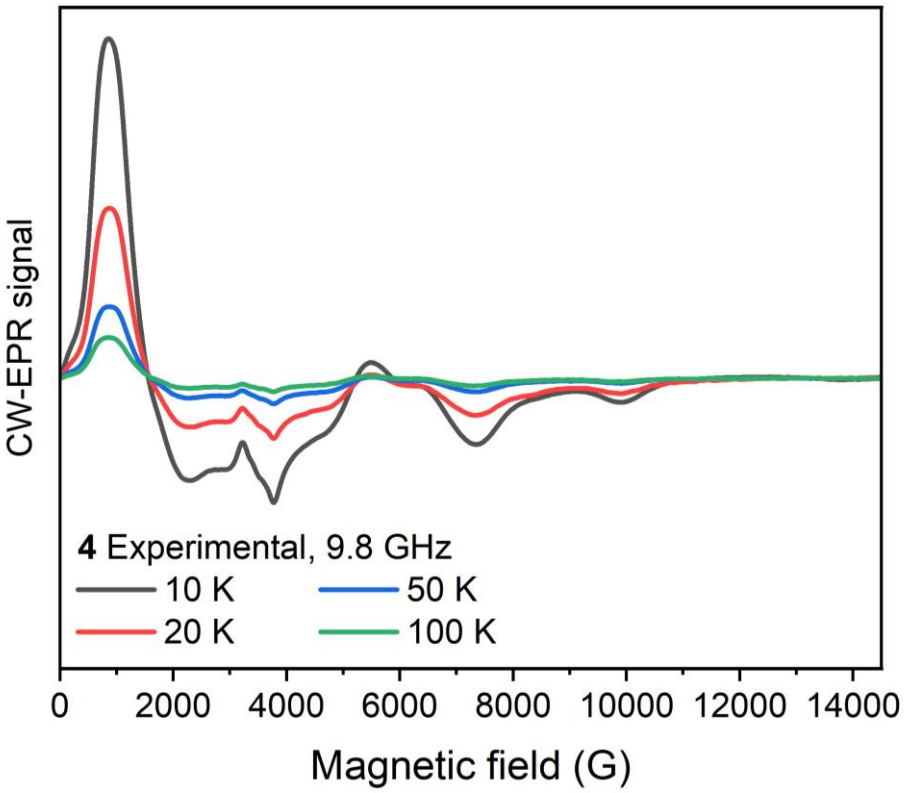

Figure S8: EPR spectra of **4** (5 mM, MeCN) at 10, 20, 50 and 100 K.

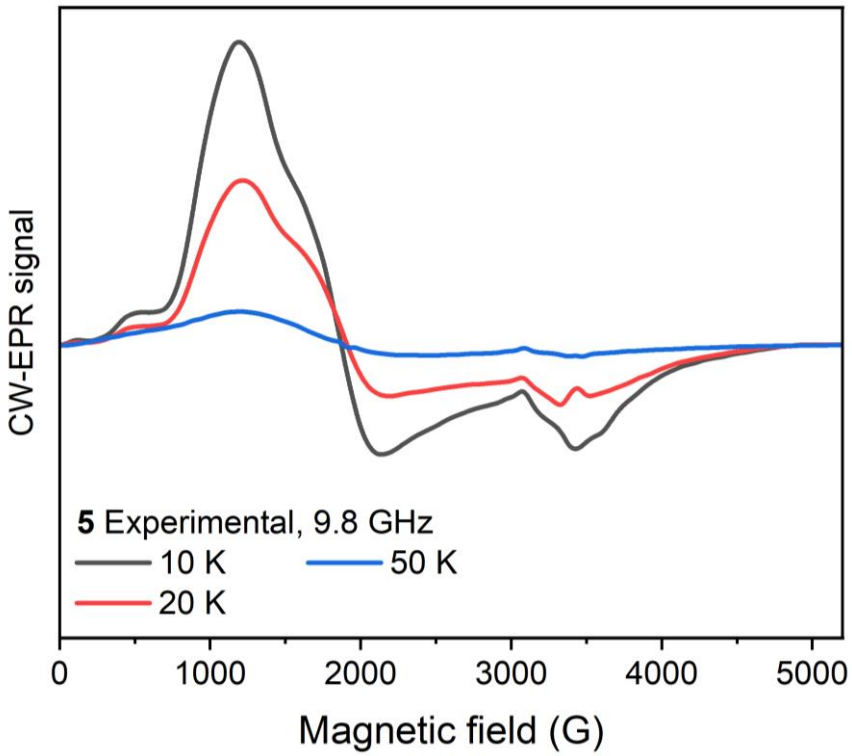

Figure S9: EPR spectra of **5** (5 mM, MeCN) at 10, 20, 50 and 100 K.

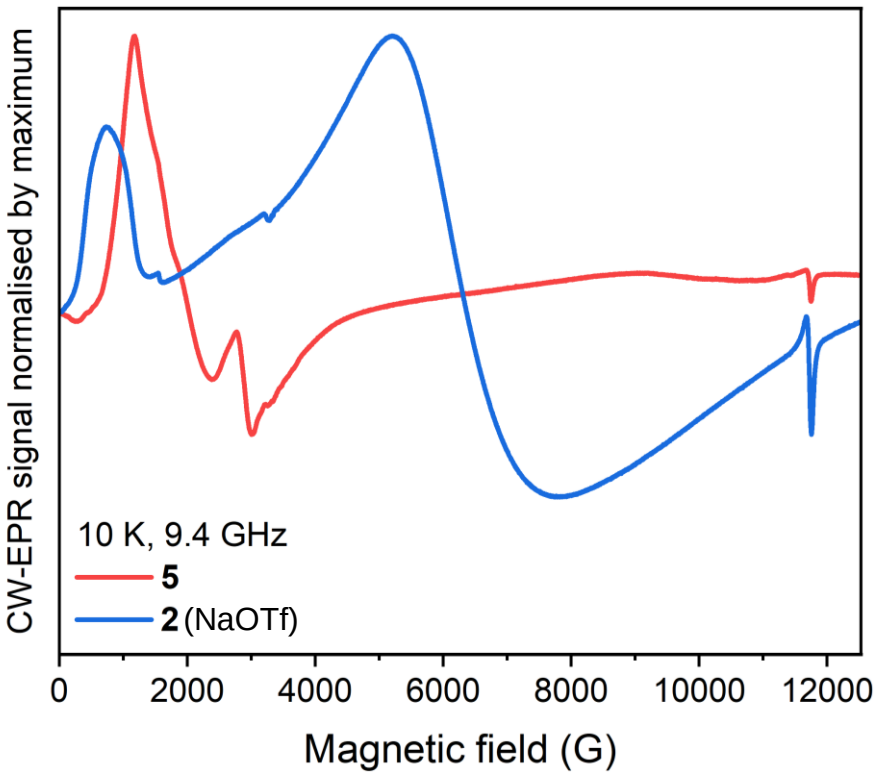

Figure S10: EPR spectra of **2**(NaOTf) and **5** (5 mM, MeCN) at 10 K.

3. UV/Visible absorption spectra for **L**H_3 and compounds **1**–**5**

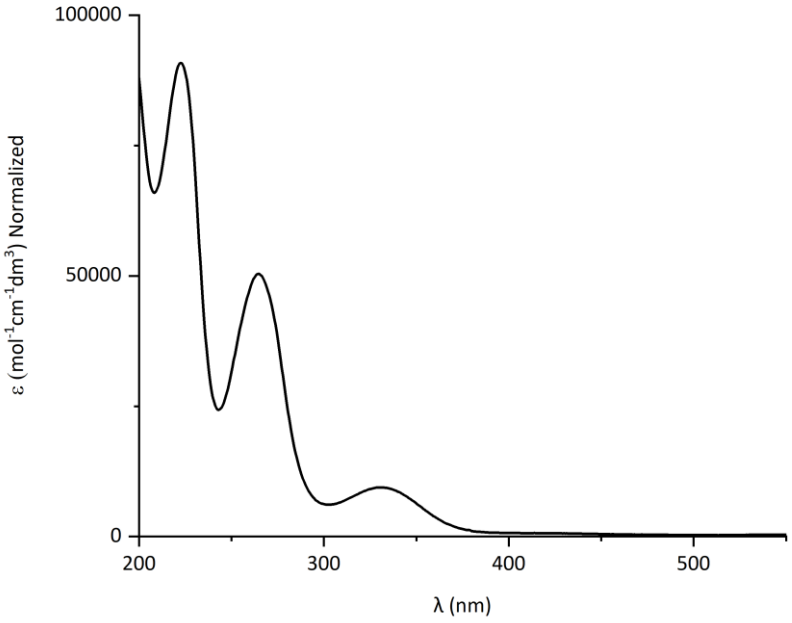

Figure S11: UV/Visible spectrum for compound **L**H_3 in MeCN (20 °C, 1.6 × 10^{-5} M).

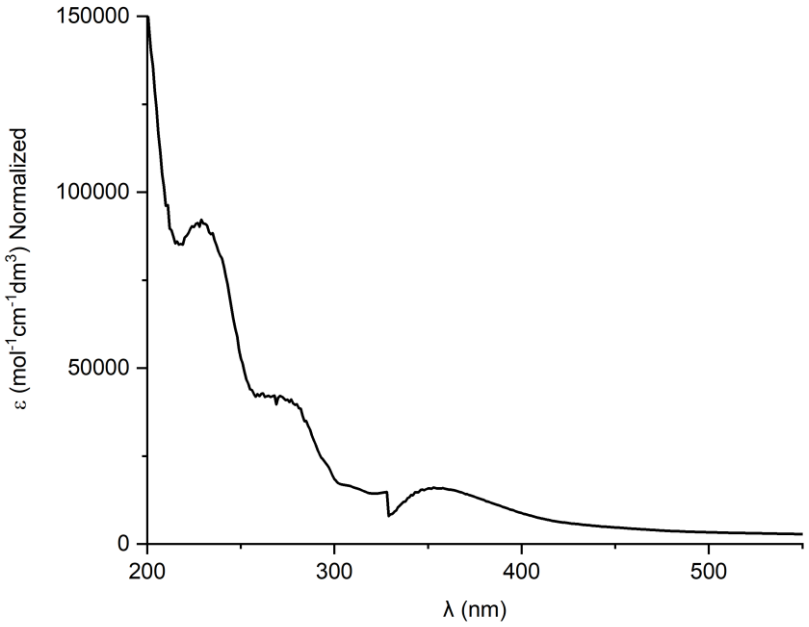

Figure S12: UV/Visible spectrum for compound **1**(NaOTf) in MeCN (20 °C, 1.4 × 10^{-5} M). Feature at 473 nm is an artefact of the spectrometer corresponding to UV lamp switching.

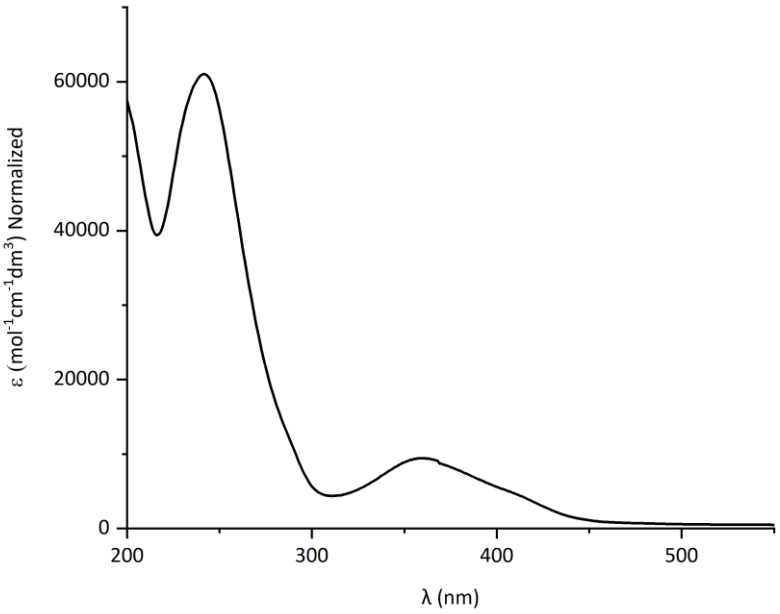

Figure S13: UV/Visible spectrum for compound **2**(NaOTf) in MeCN (20 °C, 4.2×10^{-5} M).

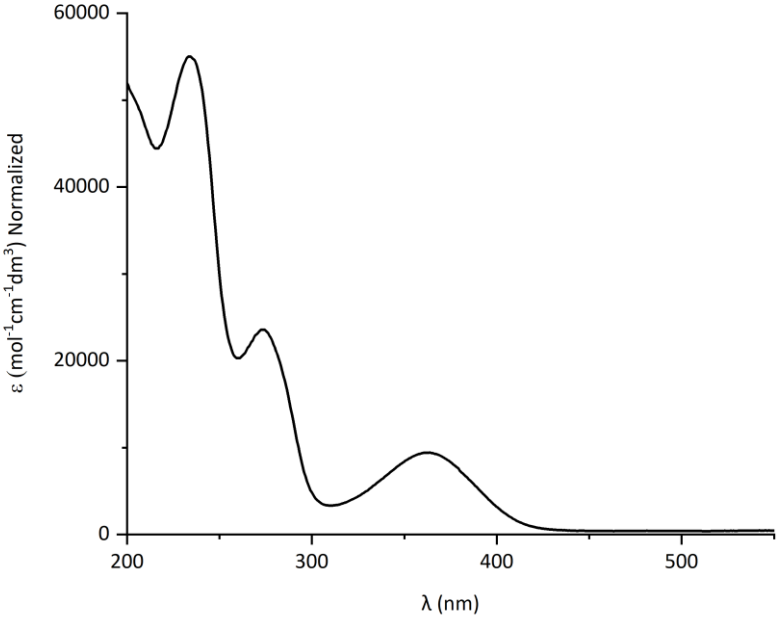

Figure S14: UV/Visible spectrum for compound **3**(NaOTf) in MeCN (20 °C, 3.0×10^{-5} M).

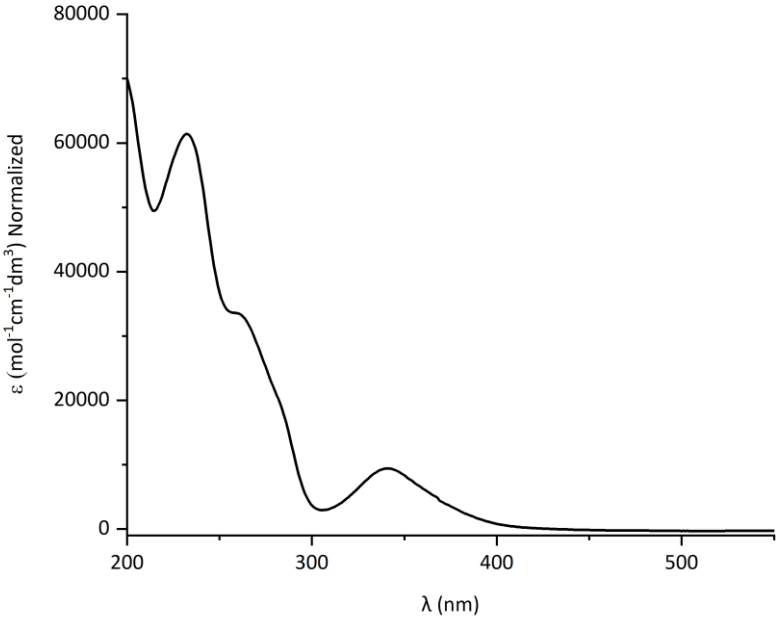

Figure S15: UV/Visible spectrum for compound **4** in MeCN (20 °C, 6.4 × 10^{-5} M).

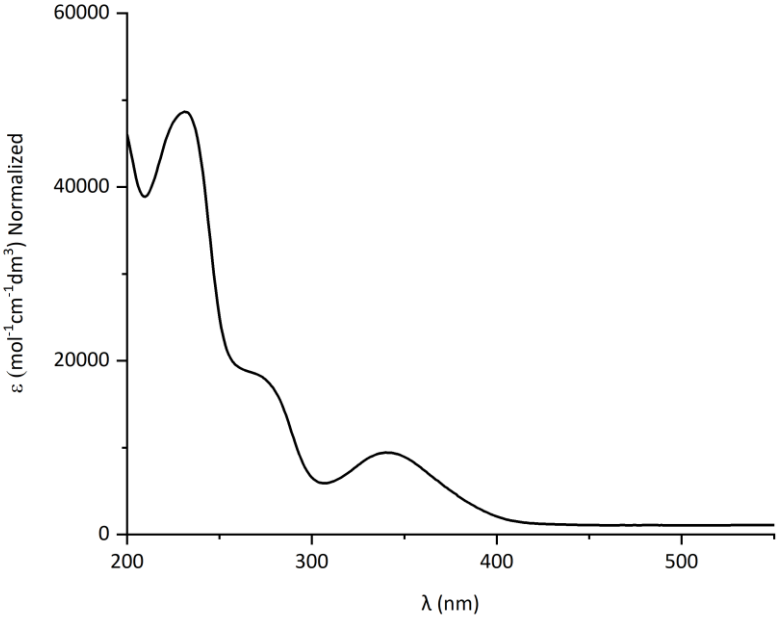

Figure S16: UV/Visible spectrum for compound **5** in MeCN (20 °C, 1.0 × 10^{-5} M).

4. ATR infrared spectra for compounds **1**–**5** and **L**H_3

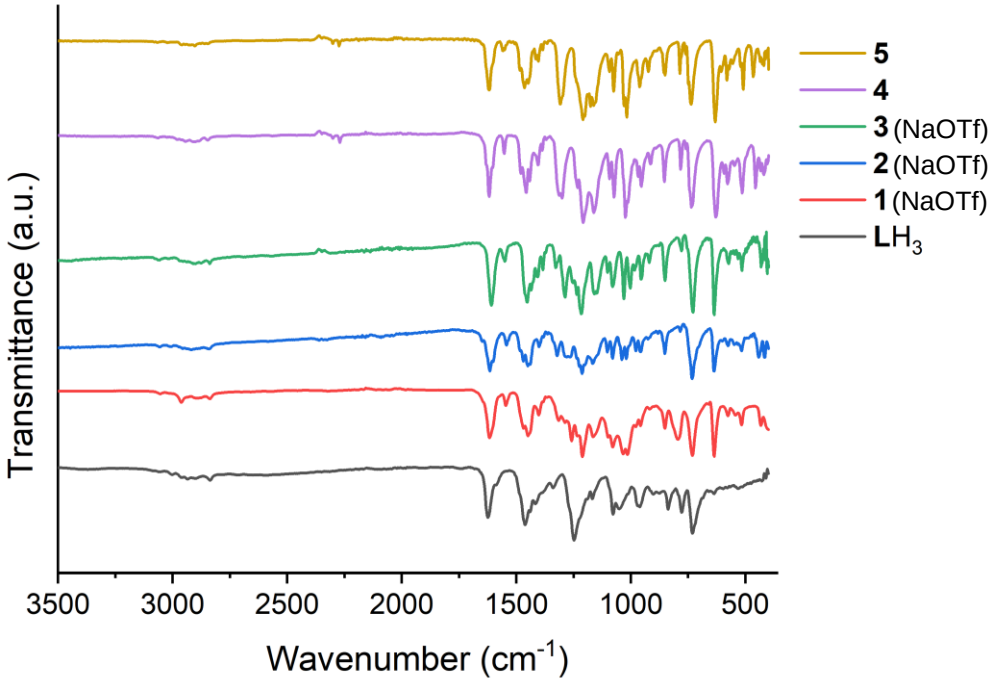

Figure S17: ATR Infrared Spectra for compounds **1**–**5** and **L**H_3.

5. Electrochemistry for **L**H_3 and compounds **2**(NaOTf)**, 4** and **5**

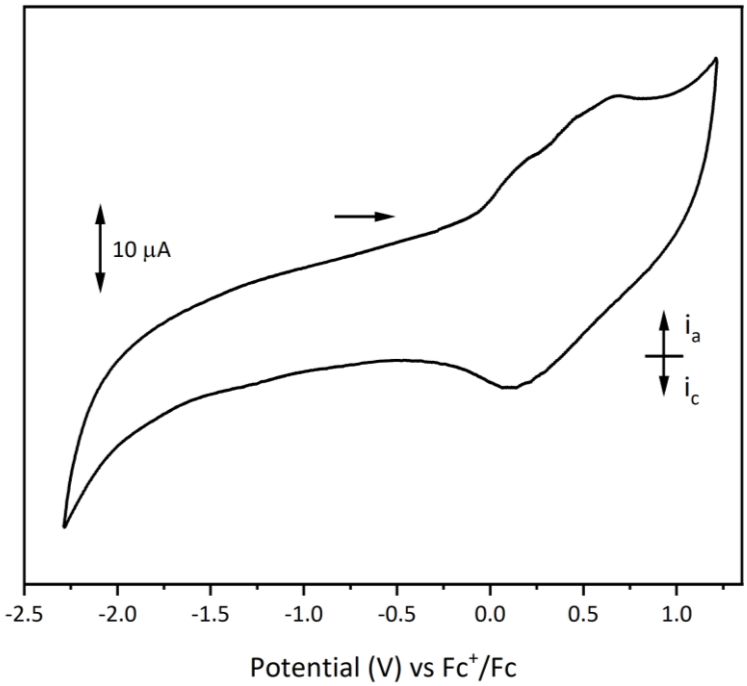

Figure S18: Cyclic voltammogram for compound **L**H_3 at 5 mM in CH_2Cl_2, with 0.25 M [(*n*Bu)$_4$N][PF_6] supporting electrolyte, glassy carbon working and counter electrodes, vs Fc^+/Fc, 0.1 Vs^{-1}, scanning oxidatively. i_a = peak anodic current, i_c = peak cathodic current. A Savitzky-Golay smooth was applied to even out periodic noise in the trace.

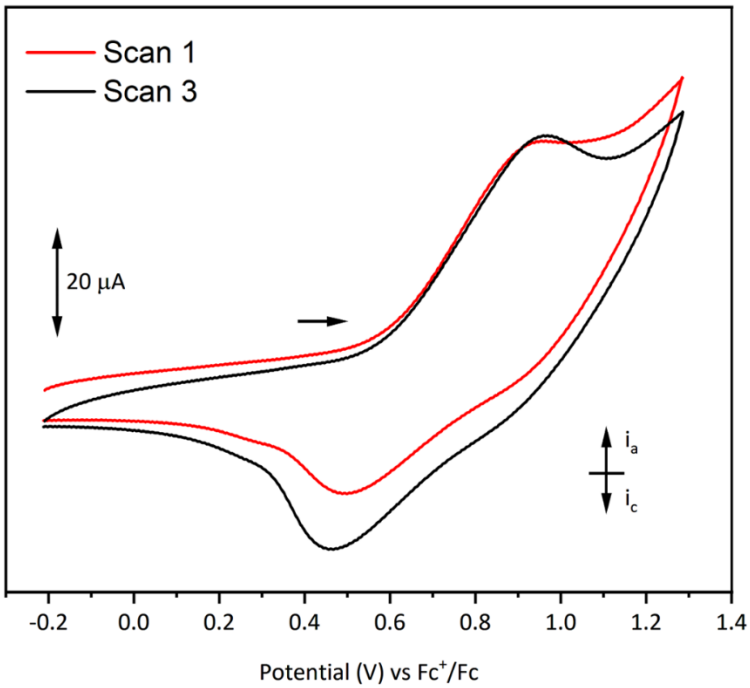

Figure S19: Cyclic voltammogram for compound **2**(NaOTf) at 6.6 mM in CH_2Cl_2, with 0.2 M [(*n*Bu)$_4$N][PF_6] supporting electrolyte, glassy carbon working and counter electrodes, vs Fc^+/Fc, 0.1 Vs^{-1}, scanning oxidatively. i_a = peak anodic current, i_c = peak cathodic current.

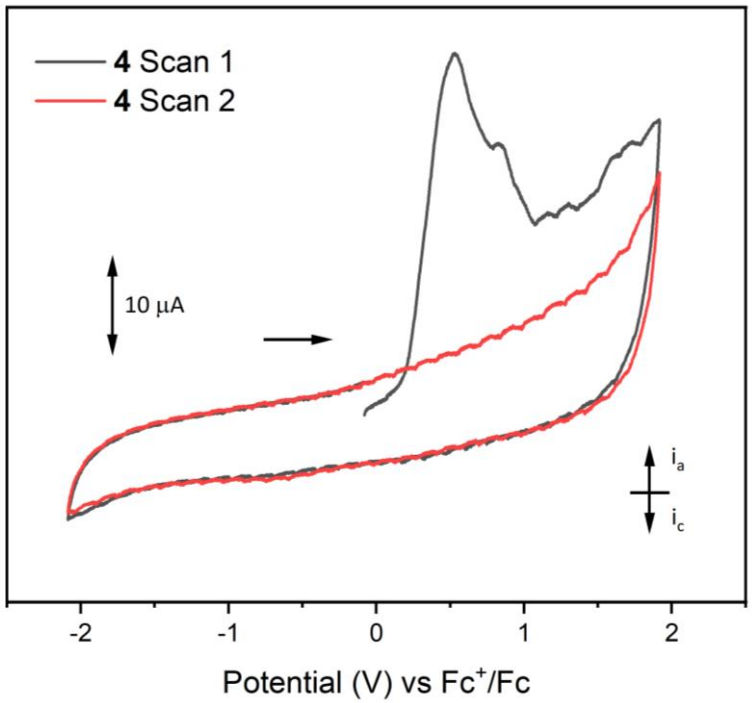

Figure S20: Cyclic voltammogram for compound **4** at 13.3 mM in CH_2Cl_2, with 0.20 M $[(n\text{Bu})_4\text{N}][PF_6]$ supporting electrolyte, glassy carbon working and counter electrodes, vs Fc^+/Fc, 0.2 Vs^{-1}, scanning oxidatively. i_a = peak anodic current, i_c = peak cathodic current. A Savitzky-Golay smooth was applied to even out periodic noise in the trace.

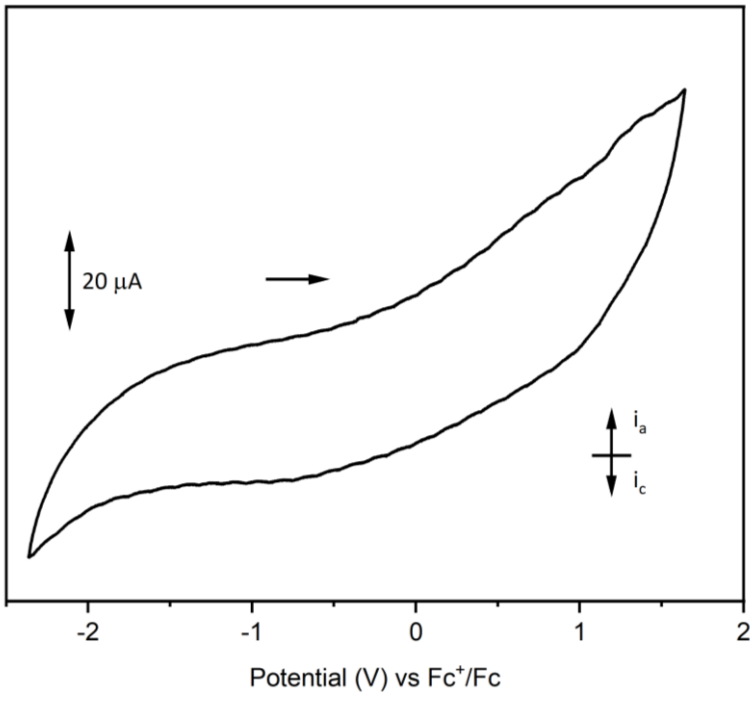

Figure S21: Cyclic voltammogram for compound **5** at 8.5 mM in CH_2Cl_2, with 0.20 M $[(n\text{Bu})_4\text{N}][PF_6]$ supporting electrolyte, glassy carbon working and counter electrodes, vs Fc^+/Fc, 0.2 Vs^{-1}, scanning oxidatively. i_a = peak anodic current, i_c = peak cathodic current. A Savitzky-Golay smooth was applied to even out periodic noise in the trace.

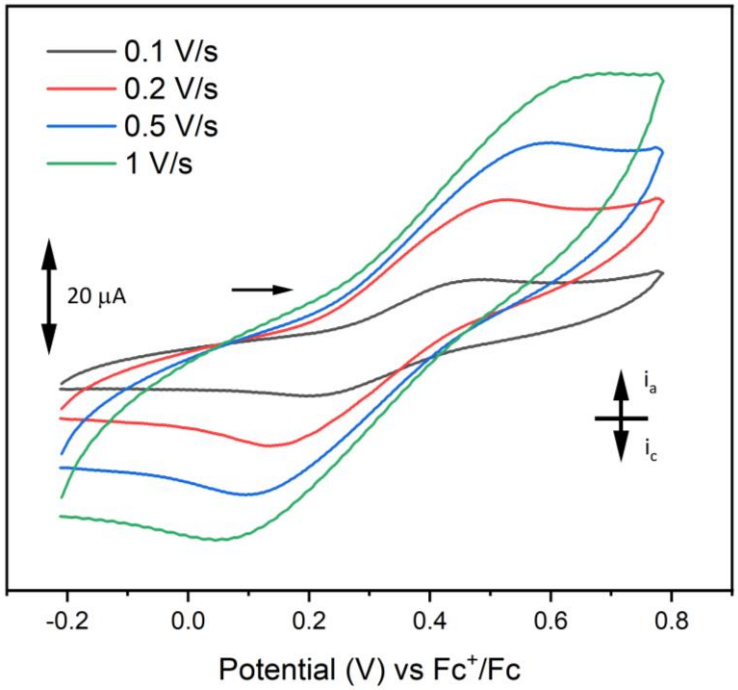

Figure S22: Cyclic voltammogram displaying scan rate dependence of the $Mn^{2+/3+}$ redox couple in **4** at 0.33 V at 7.1 mM in CH_2Cl_2, with 0.20 M $[(n\text{Bu})_4\text{N}][PF_6]$ supporting electrolyte, glassy carbon working and counter electrodes, vs Fc^+/Fc, scanning oxidatively. i_a = peak anodic current, i_c = peak cathodic current. A Savitzky-Golay smooth was applied to even out periodic noise in the trace.

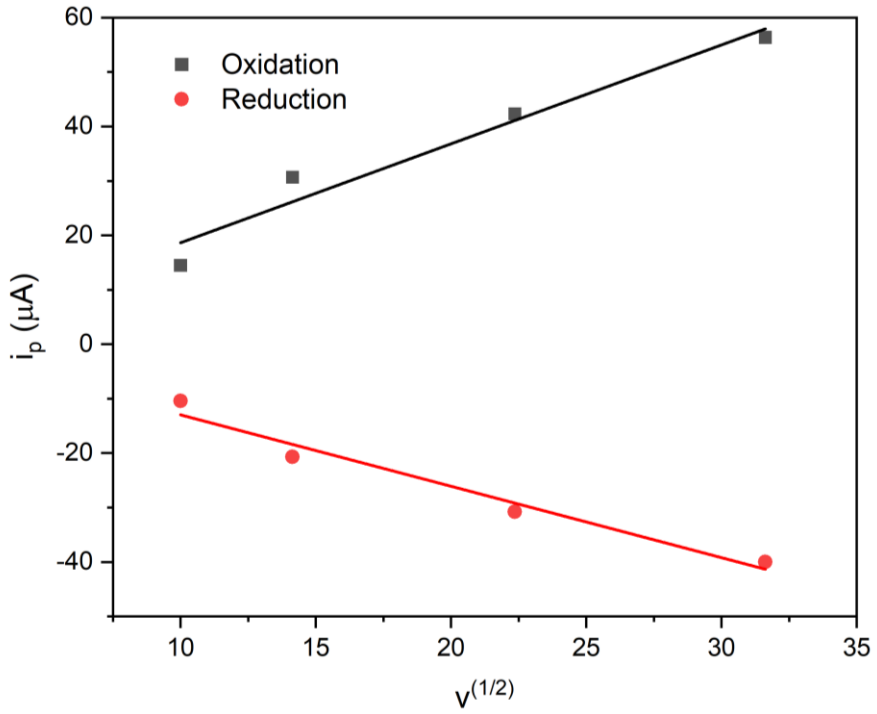

Figure S23: Randles Ševčík plot for the $Mn^{2+/3+}$ redox couple of compound **4** at 0.33 V. v denotes scan rate and i_p is peak current.

6. Evan's magnetometry for compounds **1**(NaOTf), **2**(NaOTf), **4** and **5**

General method: a d_3-MeCN NMR sample of each compound (**1**(NaOTf), **2**(NaOTf), **4** and **5**) with known concentration was prepared. To this NMR sample, a sealed glass reference capillary containing MeCN was added, and a standard ^{1}H NMR spectroscopic experiment was run. The difference in chemical shift (Δδ) between the residual signals of MeCN and d_3-MeCN was used to estimate the effective magnetic moment (μ_{eff}) of each complex.[1, 2]

- The measured molar magnetic susceptibility, χ_{meas} was calculated from the equation

$$\chi_{meas} = \frac{3\Delta\delta}{4\pi f c}$$

  where f denotes frequency of the spectrometer (in this case 400 MHz), Δδ denotes difference in chemical shift between the residual signals of MeCN and d_3-MeCN, and c denotes the concentration of the sample (in mol cm^{-3}).

- χ_P, the paramagnetic contribution to the magnetic susceptibility was calculated using

$$\chi_P = \chi_{meas} - \chi_D$$

  where the diamagnetic component, χ_D, was estimated using the Pascal's constants.[3]

- μ_{eff} was then calculated with the following equation

$$\mu_{eff} = \sqrt{8\chi_P T}$$

  where T denotes temperature (298 K in all cases)

Table S1: Evans magnetometry data

Compound	Δδ (Hz)	c (mol cm^{-3})	X_D (mol cm^{-3})	X_P (mol cm^{-3})	μ_{eff} (μ_B)	g_{eff}
1(NaOTf)	298.55	1.59 × 10^{-5}	–0.00039192	11.6 × 10^{-3}	5.27	1.782
2(NaOTf)	189.97	1.30 × 10^{-5}	–0.00038992	9.13 × 10^{-3}	4.66	2.406
4	406.36	1.61 × 10^{-5}	–0.00047841	15.6 × 10^{-3}	6.09	2.059
5	143.18	1.17 × 10^{-5}	–0.00047641	7.77 × 10^{-3}	4.31	2.226

These values were compared to the expected spin only magnetic moment, given by

$$\mu_{SO} = \sqrt{n(n+2)} \quad \mu_B$$

where *n* is the number of unpaired electrons.

The results for compounds **4** and **5** are broadly in agreement with the EPR and computational analysis which are consistent with *S* = 5/2 for compound **4** and *S* = 3/2 for compound **5**. For compound **4** μ_{eff} = 6.09 implies between five and six unpaired electrons are present (μ_{SO} = 5.92 and 6.93 μB respectively), whilst for **5** μ_{eff} = 4.31 implies between three and four unpaired electrons are present (μ_{SO} = 3.87 and 4.90 μB respectively), supporting the conclusions of EPR and computational analysis. As detailed in the Materials and Methods section, the simulation of the CW-EPR spectrum of **5** was performed by imposing a constraint on the 'true' *g* values, namely (g_1+g_2+g_3)/3 was forced to be equal to g_{eff} = 2.226, obtained from μ_{eff} using the equation

$$\mu_{eff} = g_{eff}\sqrt{S(S+1)} \quad \mu_B$$

The μ_{eff} value for **2**(NaOTf) implies between three and four unpaired electrons and for **1**(NaOTf) between four and five, also consistent with expected electronic structure for each compound.

7. Crystallographic data for compounds **1**–**5**

Author responses to Crystallographic Alerts from checkCIF/PLATON report

[**3**(NaOTf)]·MeCN: PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on La1 1.60 eA–^{3}

There is no chemically sensible species corresponding to the residual density peak about the heavy metal lanthanum atom, and it may be a consequence of thermal restraints in the refinement.

Table S2: Crystal data and structure refinement for [**1**(NaOTf)], [**2**(NaOTf)] and [**3(**NaOTf**)**]·MeCN.

Identification code	[**1**(NaOTf)]	[**2**(NaOTf)]	[**3**(NaOTf)]·MeCN
Empirical formula	$C_{34}H_{36}F_3MnN_5Na_2O_9S$	$C_{30}H_{30}CoF_3N_3Na_2O_9S$	$C_{32}H_{33}F_3LaN_4NaO_9S$
Formula weight	848.66	770.54	868.597
Temperature/K	150	150	150
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/n$
a/Å	11.6556(5)	11.7547(5)	16.0670(1)
b/Å	13.3317(5)	13.2058(5)	13.0765(1)
c/Å	13.5391(6)	13.4600(4)	16.7696(1)
α/°	104.826(4)	104.532(3)	90
β/°	106.697(4)	106.887(3)	101.815(1)
γ/°	105.433(4)	105.274(3)	90
Volume/Å^3	1812.26(14)	1803.25(12)	3448.65(4)
Z	2	2	4
ρ_{calc}g/cm^3	1.555	1.419	1.673
μ/mm^{-1}	4.417	5.115	10.929
F(000)	874.0	790.0	1749.8
Crystal size/mm^3	0.70 × 0.37 × 0.34	0.42 × 0.24 × 0.11	0.32 × 0.26 × 0.14
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.306 to 144.264	7.342 to 144.308	6.94 to 145.16
Index ranges	–14 ≤ h ≤ 11, –16 ≤ k ≤ 15, –16 ≤ l ≤ 16	–14 ≤ h ≤ 14, –16 ≤ k ≤ 16, –16 ≤ l ≤ 15	–19 ≤ h ≤ 19, –16 ≤ k ≤ 16, –20 ≤ l ≤ 20
Reflections collected	12129	12391	59489
Independent reflections	6974 [R_{int} = 0.0336, R_{sigma} = 0.0450]	6933 [R_{int} = 0.0273, R_{sigma} = 0.0405]	6788 [R_{int} = 0.0474, R_{sigma} = 0.0202]
Data/restraints/parameters	6974/6/446	6933/0/446	6788/0/465
Goodness-of-fit on F^2	1.048	1.030	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0504, wR_2 = 0.1428	R_1 = 0.0409, wR_2 = 0.1059	R_1 = 0.0194, wR_2 = 0.0501
Final R indexes [all data]	R_1 = 0.0536, wR_2 = 0.1473	R_1 = 0.0452, wR_2 = 0.1085	R_1 = 0.0200, wR_2 = 0.0505
Largest diff. peak/hole / e Å^{-3}	0.88/–0.55	0.34/–0.34	0.32/–0.93

Table S3: Crystal data and structure refinement for **4** and **5**.

Identification code	**4**	**5**
Empirical formula	$C_{33}H_{33}F_6LaMnN_4O_{12}S_2$	$C_{33}H_{33}CoF_6LaN_4O_{12}S_2$
Formula weight	1049.60	1053.611
Temperature/K	150	150
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a/Å	16.0537(2)	13.4835(1)
b/Å	13.0153(2)	12.9504(1)
c/Å	19.0750(2)	22.0541(2)
α/°	90	90
β/°	99.7480(10)	93.320(1)
γ/°	90	90
Volume/Å^3	3928.06(9)	3844.55(5)
Z	4	4
ρ_{calc}g/cm^3	1.775	1.820
μ/mm^{-1}	12.745	13.729
F(000)	2092.0	2099.6
Crystal size/mm^3	0.46 × 0.35 × 0.29	0.264 × 0.185 × 0.155
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.664 to 143.94	7.5 to 145.08
Index ranges	–19 ≤ h ≤ 19, –15 ≤ k ≤ 11, –23 ≤ l ≤ 21	–16 ≤ h ≤ 16, –16 ≤ k ≤ 16, –26 ≤ l ≤ 24
Reflections collected	14963	71163
Independent reflections	7564 [R_{int} = 0.0342, R_{sigma} = 0.0442]	7553 [R_{int} = 0.0415, R_{sigma} = 0.0180]
Data/restraints/parameters	7564/0/537	7553/0/537
Goodness-of-fit on F^2	1.044	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0360, wR_2 = 0.0911	R_1 = 0.0218, wR_2 = 0.0542
Final R indexes [all data]	R_1 = 0.0393, wR_2 = 0.0939	R_1 = 0.0227, wR_2 = 0.0548
Largest diff. peak/hole / e Å^{-3}	0.89/–1.49	0.53/–1.00

8. Computational Details

Geometry optimizations, frequency calculations, and Natural Bond Order calculations were performed using the Gaussian program package (versions 9 and 16).[4] Optimized geometries in a variety of spin states (**4**: *S*=1/2, *S*=5/2; **5**: *S*=1/2, *S*=3/2), and were calculated in the gas phase from coordinates derived from the X-ray crystal structures. In each case, only the high-spin multiplicities resulted in convergence (and modification of the convergence criteria (e.g. scf=qc, as well as single point calculations on already-optimised high spin configurations) was unsuccessful). Computational methodology was evaluated against the bond metrics taken from single crystal X-ray data for **5**. (summarised in Table S5). The functional and basis sets are outlined in Table S4, along with their replication of X-ray structure bonding parameters with a particular focus on Co–La bond distance. The best replication of bonding parameters was found to be the B3LYP function in combination with def2SVPP(C, H)/def2TZVP(N, O, F, S)/def2TZVPP(La, Mn/Co)[5, 6] along with Grimme's empirical dispersion correction (gd3)[7] used on all atoms. The calculated structures were confirmed to be minima based on the absence of imaginary frequencies from frequency calculations on the optimized geometries. Natural bond order analysis was performed using NBO version 6.0.[8]

Time-dependent (TD) DFT calculations were performed on the optimized structures of **L**H_3, **4** and **5** with def2SVPP(C, H)/def2TZVP(N, O, F, S)/def2TZVPP(La, Mn/Co)[5, 6] in acetonitrile as solvent, using 50 (**L**H_3) or 60 (**4**, **5**) roots. The visible regions of the spectra were well-reproduced for **L**H_3, **4** and **5**. For the optimized structure of **4**, excited states 19 and 21 (351 and 342 nm respectively) reproduce the absorbance at 341 nm well and are comprised of 10 and 8 transitions respectively (Table S7). 346.25 nm. For the optimized structure of **5**, excited states 21 and 24 (352 and 346 nm respectively) reproduce the absorbance at 340 nm well and are each comprised of 12 transitions (Table S8).

Table S4: Methodology development summary.

	Basis Set					
Functional	**H, C**	**N, O, F, S**	**Co, La**	**Modifier**	**Co-La**	**Δcalc-exp**
PBE1	3-21G	3-21G	LANL2DZ		3.4529	0.0902
B3LYP	3-21G	3-21G	LANL2DZ		3.423	0.0603
B3LYP	Def2SVPP	Def2TZVP	Def2TZVPP		3.42424	0.06154
B3LYP	Def2SVPP	Def2TZVP	Def2TZVPP	GD3	3.37548	0.01278
B3LYP	Def2SVPP	Def2TZVPP	LANL2DZ		3.4381	0.0754

Table S5: Comparison of crystallographic and computational bond lengths for complexes **4** and **5**. [a]Where ESD values are quoted for average distances, the highest value is reported. [b]B3LYP-GD3/(Mn/Co/La: def2TZVPP; N/O/F/S: def2TZVP; C/H: def2SVPP basis sets).

Complex		**Distances (Å)**[a]				
			κ^6-N_3O_3 binding site		κ^6-O_6 binding site	
		M···La	M–N_{avg}	M–O_{avg}	La–O_{avg}	
					phenolate	methoxy
4	Experimental	3.398(1)	2.192(3)	2.157(2)	2.446(2)	2.725(3)
(M = Mn)	Computational[b]	3.41	2.220	2.153	2.508	2.743
5	Experimental	3.363(1)	2.103(2)	2.097(2)	2.432(2)	2.715(2)
(M = Co)	Computational[b]	3.38	2.147	2.118	2.464	2.735

	Atom	1	2
1.	La	0.0000	0.1511
2.	Mn	0.1511	0.0000
3.	S	0.0230	0.0004
4.	S	0.0417	0.0015
5.	F	0.0064	0.0002
6.	F	0.0064	0.0002
7.	F	0.0024	0.0001
8.	O	0.1712	0.0019
9.	O	0.2489	0.2014
10.	O	0.2661	0.2201
11.	O	0.1714	0.0019
12.	O	0.1647	0.0028
13.	O	0.2563	0.2152
14.	F	0.0029	0.0002
15.	O	0.3190	0.0015
16.	F	0.0187	0.0004
17.	O	0.0197	0.0003
18.	O	0.0205	0.0001
19.	O	0.0285	0.0006
20.	F	0.0031	0.0003
21.	O	0.2829	0.0013
22.	N	0.0109	0.2433
23.	O	0.2634	0.0068
24.	N	0.0137	0.2573
25.	N	0.0120	0.2503
26.	N	0.2910	0.0063
27.	C	0.0142	0.0193
28.	C	0.0146	0.0104
29.	C	0.0117	0.0096
30.	C	0.0127	0.0092

	Atom	1	2
1.	La	0.0000	0.2408
2.	Mn	0.2408	0.0000 -
3.	S	0.0717	-0.0000
4.	S	0.1643	-0.0001 -
5.	F	0.0084	-0.0000 -
6.	F	0.0085	-0.0000 -
7.	F	0.0008	-0.0000 -
8.	O	0.3242	0.0001 -
9.	O	0.4377	0.3047 -
10.	O	0.4631	0.3154 -
11.	O	0.3220	0.0007 -
12.	O	0.3044	0.0042
13.	O	0.4536	0.3115 -
14.	F	0.0012	0.0000
15.	O	0.5085	0.0011
16.	F	0.0292	0.0001
17.	O	0.0280	0.0000
18.	O	0.0297	-0.0000
19.	O	0.0327	0.0001 -
20.	F	0.0018	-0.0000
21.	O	0.4550	0.0009
22.	N	0.0269	0.3157
23.	O	0.4267	0.0169 -
24.	N	0.0308	0.3290
25.	N	0.0279	0.3208
26.	N	0.4338	0.0092
27.	C	0.0696	0.0171 -
28.	C	0.0578	0.0225 -
29.	C	0.0428	0.0231 -
30.	C	0.0302	-0.0114 -

Figure S24: Select Wiberg bond order values for La, Mn and surrounding atoms for **4**. Right: Select Natural atomic orbital (NAO) bond order values for La, Mn and surrounding atoms for **4**.

	Atom	1	2
1.	La	0.0000	0.0256
2.	Co	0.0256	0.0000
3.	S	0.0059	0.0003
4.	S	0.0054	0.0001
5.	F	0.0012	0.0000
6.	F	0.0006	0.0000
7.	F	0.0009	0.0001
8.	F	0.0010	0.0000
9.	F	0.0010	0.0000
10.	F	0.0004	0.0000
11.	O	0.0661	0.0417
12.	O	0.0394	0.0004
13.	O	0.0656	0.0347
14.	O	0.0408	0.0005
15.	O	0.0635	0.0431
16.	O	0.0406	0.0004
17.	O	0.0783	0.0005
18.	O	0.0096	0.0011
19.	O	0.0074	0.0001
20.	O	0.0754	0.0003
21.	O	0.0060	0.0000
22.	O	0.0065	0.0000
23.	N	0.0031	0.0550
24.	N	0.0028	0.0495
25.	N	0.0027	0.0508
26.	N	0.0715	0.0007
27.	C	0.0000	0.0004
28.	H	0.0000	0.0000
29.	H	0.0000	0.0000
30.	H	0.0000	0.0000

	Atom	1	2
1.	La	0.0000	0.3087
2.	Co	0.3087	0.0000
3.	S	0.0849	0.0021
4.	S	0.0759	-0.0000
5.	F	0.0057	-0.0000
6.	F	0.0004	-0.0000
7.	F	0.0035	-0.0000
8.	F	0.0049	-0.0000
9.	F	0.0051	-0.0000
10.	F	0.0004	-0.0000
11.	O	0.4496	0.2550
12.	O	0.3025	-0.0003
13.	O	0.4451	0.2184
14.	O	0.3059	0.0012
15.	O	0.4390	0.2595
16.	O	0.3091	-0.0004
17.	O	0.4947	0.0028
18.	O	0.0600	0.0085
19.	O	0.0430	0.0004
20.	O	0.4877	0.0005
21.	O	0.0368	0.0000
22.	O	0.0393	0.0000
23.	N	0.0348	0.3112
24.	N	0.0345	0.2787
25.	N	0.0293	0.2868
26.	N	0.4374	0.0023
27.	C	0.0001	0.0047
28.	H	0.0000	0.0001
29.	H	0.0000	0.0001
30.	H	0.0000	0.0001

Figure S25: Select Wiberg bond order values for La, Co and surrounding atoms for **5**. Right: Select Natural atomic orbital (NAO) bond order values for La, Co and surrounding atoms for **5**.

Coordinates for **4**

La	-0.79150200	-0.05726100	-0.13178600	C	-2.29778600	3.16494800	-4.08355200
Mn	2.59992500	0.19377900	-0.42989100	H	-3.35600400	3.36427300	-3.84437300
S	-4.60990600	0.63525200	-0.01733500	H	-2.22850600	2.76233100	-5.10832800
S	-1.45977300	-3.18727200	0.55612900	H	-1.72872300	4.10858100	-4.02919600
F	-4.76671900	2.14599300	-2.21100000	C	5.78318000	0.34154700	-0.72898000
F	-4.48177000	3.28142000	-0.37580400	C	5.16804600	1.52630500	-1.53734500
F	-6.42492800	2.40714000	-0.82377800	C	2.11319000	-3.36930000	-3.93305800
O	-1.28910000	-1.62160100	-2.26761200	C	3.93534700	0.05341100	2.47807200
O	1.03868200	1.69723200	-0.58944200	C	2.40109700	4.98245100	0.30735500
O	1.07416700	-0.77868300	-1.55622200	C	2.67797600	-0.09399700	3.18622200
O	-0.93670900	-0.09684700	2.58504000	C	2.23332800	-2.34395000	-2.95657000
O	-0.96588900	2.57531600	0.84519200	C	0.87466900	-3.81269900	-4.35782000
O	1.28953600	-0.20100900	1.23291300	C	-1.76307700	2.20420500	-3.12833300
F	-0.58850500	-4.99181300	2.28535600	C	-1.36899500	-3.90322700	2.27780100
O	-3.13950900	0.67934200	-0.20682100	C	-2.19209900	-0.17511600	3.27864700
F	-0.85023800	-3.00971200	3.14290100	C	7.31245100	0.40861000	-0.91616400
O	-4.99086200	0.86260700	1.35490100	C	3.56538200	-1.98426800	-2.51229200
O	-5.25777300	-0.40756900	-0.76357300	C	5.32683000	-1.04085400	-1.26965500
O	-1.90697500	-4.27803400	-0.26231900	C	0.29597900	-0.13298200	4.70873500
F	-2.59057700	-4.24433500	2.71200200	C	2.71400000	-0.10271400	4.60630100
O	-2.38339500	-2.04498200	0.68276100	C	-2.03867200	2.99838700	1.69476300
N	3.83578800	1.90323500	-1.09360600	C	-2.62176000	-2.03078200	-2.62659300
O	-0.10790300	-2.67541500	0.31238800	C	5.50718100	0.48192600	0.78858500
N	3.90527900	-1.14391500	-1.59641600	C	1.55234600	-0.13220200	5.35559100
N	4.13370800	0.17314400	1.21068300	H	7.73873400	1.28905400	-0.40312800
N	-1.35818300	1.45245500	-2.36240000	H	5.85678900	2.39325400	-1.47629300
C	1.17820400	2.88284700	-0.07649400	H	5.93632600	-1.29139700	-2.16015800
C	-0.21179500	-2.24019000	-2.87169000	H	3.31347400	5.57544800	0.18355700
C	0.09617700	3.44426200	0.67335100	H	6.22007800	-0.16918600	1.33057000
C	2.37203200	3.65899200	-0.20502400	H	0.79411900	-4.61011500	-5.10093100
C	3.59988400	3.12407000	-0.76664500	H	1.34995800	6.53734000	1.36926100
C	-0.30158400	-3.24849800	-3.81601100	H	5.73848000	1.52466500	1.07913500
C	0.23213200	-0.12702500	3.32597900	H	-2.79679800	-1.83488600	-3.69918900
C	1.31531400	5.51841600	0.97510400	H	7.57612100	0.47942800	-1.98658300
C	0.15751400	4.73406800	1.17733600	H	4.42133300	3.86153800	-0.86133600
C	1.05396100	-1.75122500	-2.42699100	H	-1.27439400	-3.62219200	-4.13759400
C	1.41673600	-0.14892600	2.52547500	H	5.55948500	-1.79681400	-0.49574200
C	-5.10512000	2.20553200	-0.90147700	H	-2.53599100	3.89060900	1.27855400

H	-1.65857300	3.21052300	2.71042400	H	1.59419900	-0.14311900	6.44765100
H	4.37236000	-2.53781200	-3.03016600	H	-0.61520700	-0.14044600	5.30847900
H	3.02441100	-3.82029900	-4.33929300	H	-2.76634600	-3.09674500	-2.38832100
H	3.68657700	-0.07406800	5.10847200	H	-2.24524400	-1.10541800	3.86629700
H	-0.67850300	5.15520600	1.73731500	H	4.81488700	0.11519200	3.14850400
H	-2.76441600	2.17736900	1.72386200	H	-2.32023700	0.70354700	3.93478000
H	7.80308800	-0.49254100	-0.50652900	H	-2.97761000	-0.18262700	2.51138400
H	5.10959500	1.22217200	-2.59830800	H	-3.30917300	-1.42883500	-2.01471500

Coordinates for **5**

La	-0.78318900	-0.27739600	-0.35525600	H	5.54691500	-1.91401500	0.79965400
Co	2.59083500	-0.18132500	-0.37988900	H	6.05927500	-0.43565500	1.64601300
S	-0.37545900	2.92626400	1.45140900	C	3.51789200	2.46881200	-1.59812300
S	-4.45968200	-1.24516400	-0.77183200	H	4.31655200	3.19922700	-1.82346800
F	-1.56854400	4.77814700	-0.04362000	C	2.21688500	2.85773300	-2.08788300
F	-0.93807700	5.47743600	1.92103600	C	2.08139700	4.14424100	-2.67204600
F	-2.69331200	4.20149200	1.72915600	H	2.96742300	4.78136800	-2.75761300
F	-5.82981700	0.38975000	0.80654600	C	0.85246000	4.60783200	-3.10147400
F	-5.36586500	-1.54355600	1.69536700	H	0.75344600	5.60810000	-3.53045700
F	-6.92759600	-1.38551700	0.18198700	C	-0.29316700	3.79311200	-2.96915500
O	1.11090800	0.82409400	-1.45345100	H	-1.26214600	4.17711600	-3.29042200
O	-1.23297100	1.64325000	-2.24288400	C	-0.18132100	2.52595800	-2.42326000
O	1.13374100	-1.70852800	-0.93438700	C	1.07376600	2.02570000	-1.96812400
O	-0.84550200	-2.96705100	0.21879400	C	-2.56850700	2.14307600	-2.39663000
O	1.17932200	-0.14321900	1.15501200	H	-2.75099400	2.44202700	-3.44411300
O	-1.14228200	-0.46135400	2.33905500	H	-2.73442400	2.99652900	-1.71717800
O	-1.13054700	1.96544300	0.60086100	H	-3.24734900	1.31755200	-2.13489300
O	0.89768400	3.30595200	0.89592600	C	3.73841900	-2.87098600	-1.35182300
O	-0.43881800	2.60861000	2.85627200	H	4.60918800	-3.49446000	-1.63173600
O	-3.24907500	-0.66768800	-0.13551700	C	2.56594300	-3.61697500	-0.93055800
O	-4.90276500	-0.50132000	-1.92713000	C	2.67714000	-5.01194900	-0.70639600
O	-4.40508400	-2.68334000	-0.89411500	H	3.62579100	-5.51126900	-0.93042800
N	3.84910200	1.40980200	-0.93955400	C	1.61689100	-5.73865100	-0.18967600
N	3.87697700	-1.59318900	-1.36283100	H	1.71244800	-6.81342200	-0.01501300
N	3.98119800	-0.59648000	1.25894200	C	0.40539700	-5.08845100	0.13752100
N	-1.63924400	-1.47282000	-2.67021600	H	-0.41292200	-5.66649800	0.57014700
C	7.28266000	-0.16714200	-0.60114400	C	0.27075500	-3.72805000	-0.09085200
H	7.60069300	0.13364500	-1.61558200	C	1.32861400	-2.96567000	-0.67075800
H	7.70756900	-1.16578700	-0.39402700	C	-1.89763800	-3.58355200	0.97167800
H	7.72622100	0.54551800	0.11739800	H	-2.63451000	-2.79705500	1.17534700
C	5.74814500	-0.18370700	-0.48727900	H	-1.49885200	-3.98894500	1.91860600
C	5.25104600	1.28226600	-0.54475900	H	-2.38539200	-4.37654800	0.38071700
H	5.37576000	1.73124100	0.45802600	C	3.72162000	-0.62459800	2.51791700
H	5.89354000	1.85405000	-1.24134100	H	4.56732900	-0.75350900	3.21998600
C	5.18297300	-1.03128200	-1.66924700	C	2.42612800	-0.57079400	3.16286200
H	5.08862000	-0.38339000	-2.55772600	C	2.37252400	-0.76094300	4.56723400
H	5.90465300	-1.83591600	-1.91197200	H	3.31116200	-0.86860800	5.12056800
C	5.37427400	-0.82369100	0.86749000	C	1.16317200	-0.82226600	5.23691900

H	1.13198700	-0.95962400	6.32073600	H	-3.06749300	0.19001800	2.13845700
C	-0.04254600	-0.71843700	4.51278500	C	-1.45584600	4.43466500	1.25589100
H	-0.99544000	-0.77934000	5.04094700	C	-5.72820300	-0.92328300	0.55498800
C	-0.01406700	-0.53360500	3.14036400	C	-2.45763900	-1.96063300	-3.31217100
C	1.21704700	-0.40401800	2.43506400	C	-3.54354600	-2.56578600	-4.06650700
C	-2.36551000	-0.01910300	2.95595800	H	-3.15886500	-3.08687500	-4.95925700
H	-2.17483100	0.90145300	3.52976200	H	-4.25716800	-1.77843900	-4.36107100
H	-2.78228600	-0.81494200	3.59833000	H	-4.07156800	-3.27249000	-3.40399000

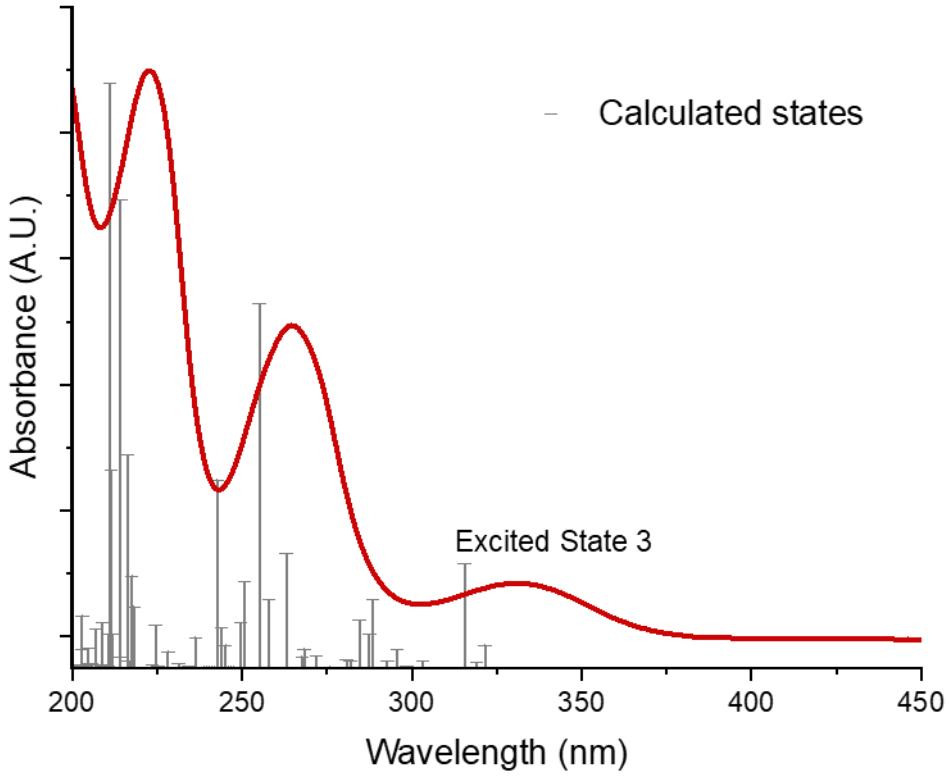

Figure S26: Normalized experimental vs computed (B3LYP-GD3/(N/O: def2TZVP; C/H: def2SVPP basis sets)) absorption spectra of **L**H_3.

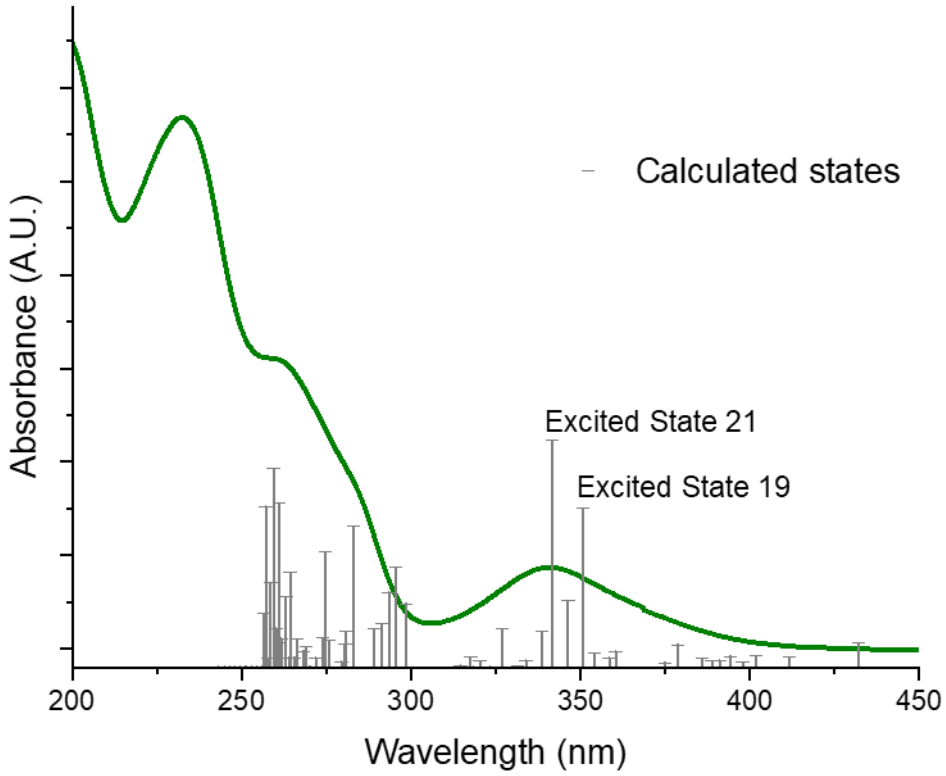

Figure S27: Normalized experimental vs computed (B3LYP-GD3/(Mn/La: def2TZVPP; N/O/F/S: def2TZVP; C/H: def2SVPP basis sets)) absorption spectra of compound **4**.

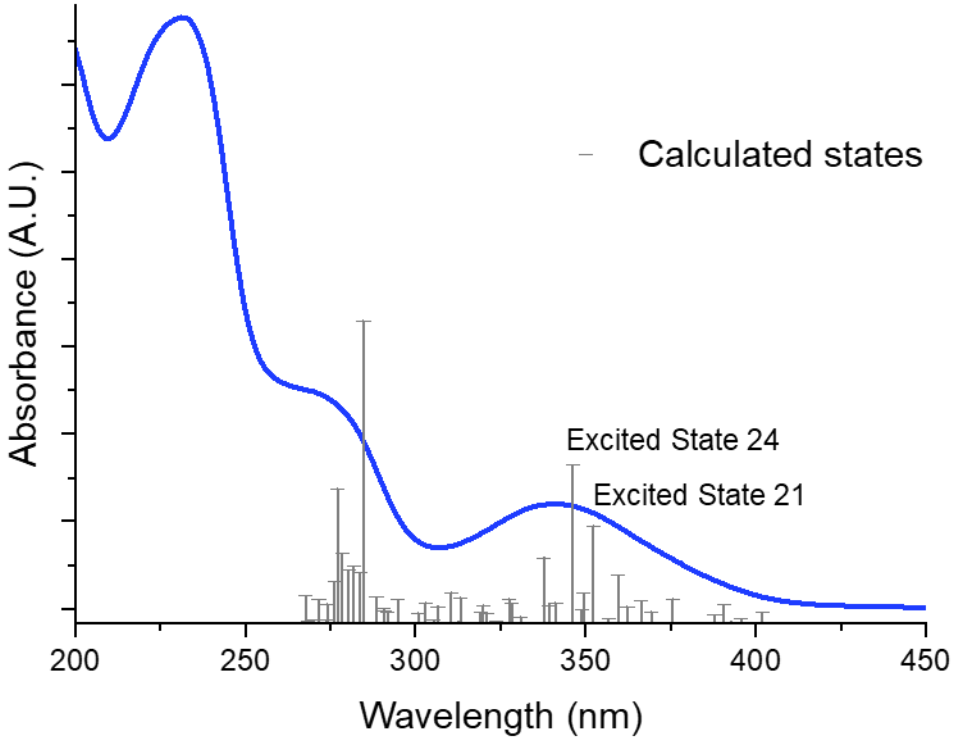

Figure S28: Normalized experimental vs computed (B3LYP-GD3/(Co/La: def2TZVPP; N/O/F/S: def2TZVP; C/H: def2SVPP basis sets)) absorption spectra of compound **5**.

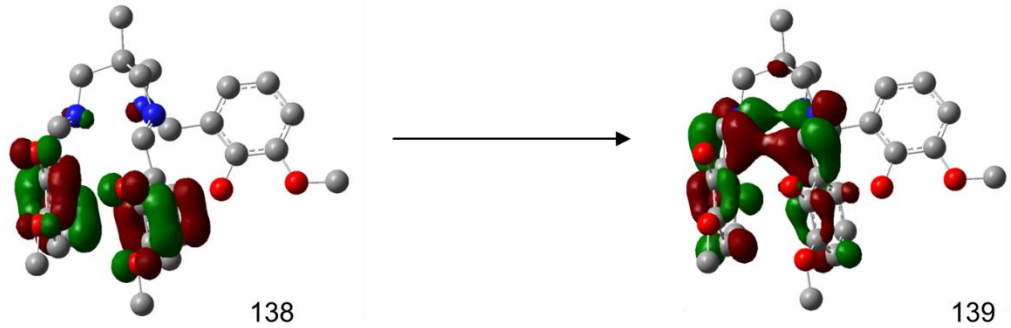

Figure S29: **L**H_3 natural transition orbitals for excited state 3 (orbital 138 (HOMO) and orbital 139 (LUMO) exhibit the largest occupations).

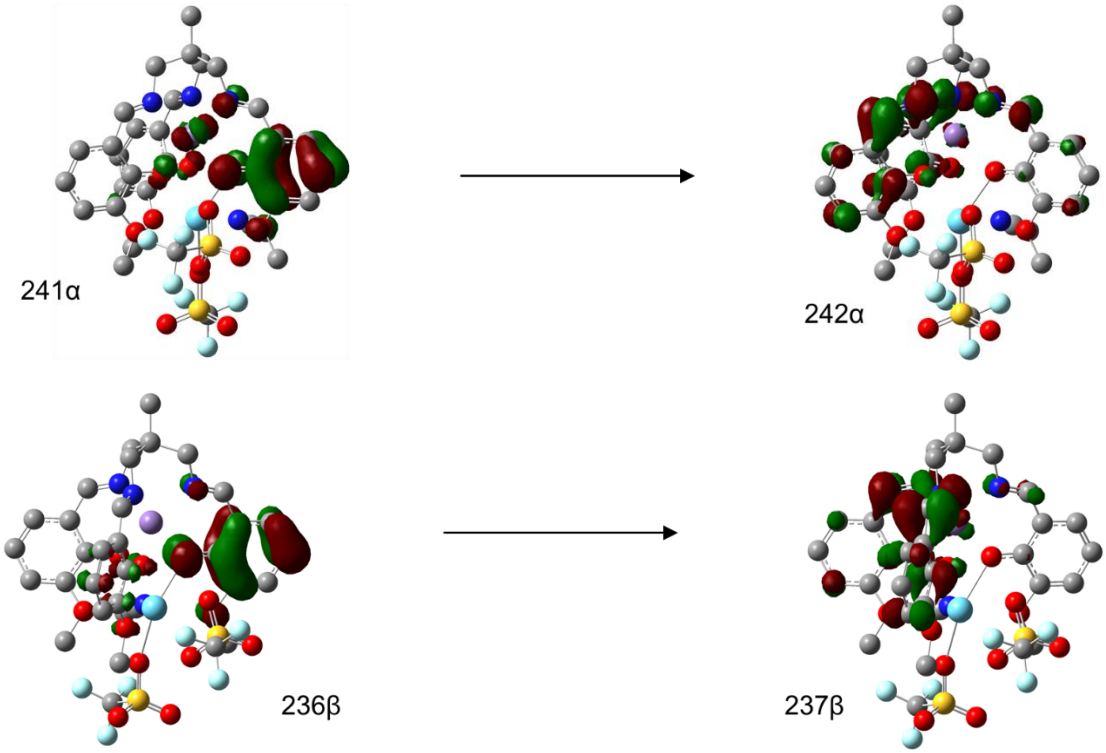

Figure S30: Complex **4** natural transition orbitals for excited state 19 (orbitals 236β, 237β, 241α and 242α exhibit the largest occupations).

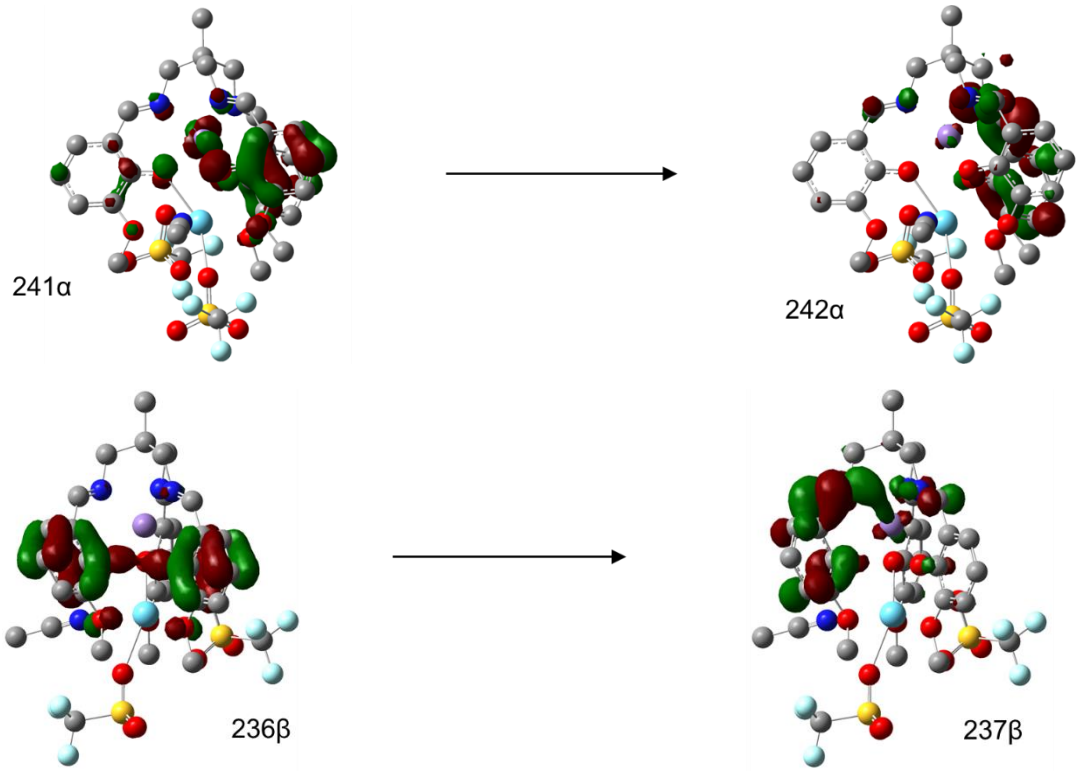

Figure S31: Complex **4** natural transition orbitals for excited state 21 (orbitals 236β, 237β, 241α and 242α exhibit the largest occupations).

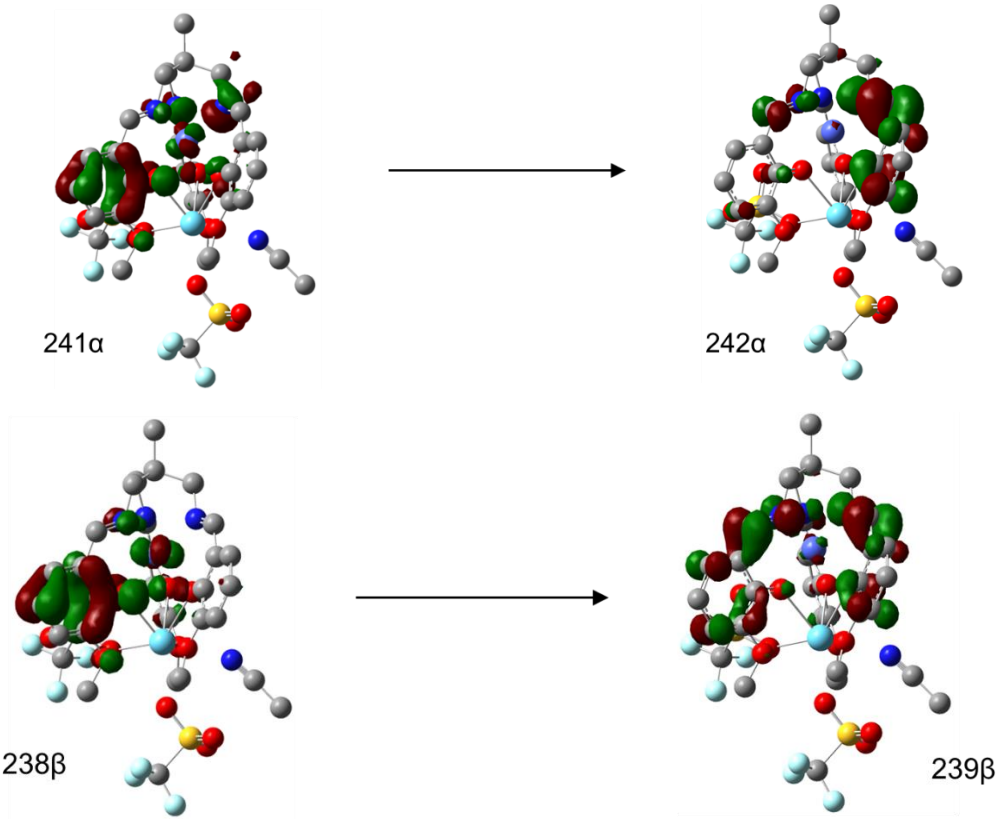

Figure S32: Complex **5** natural transition orbitals for excited state 21 (orbitals 238β, 239β, 241α and 242α exhibit the largest occupations).

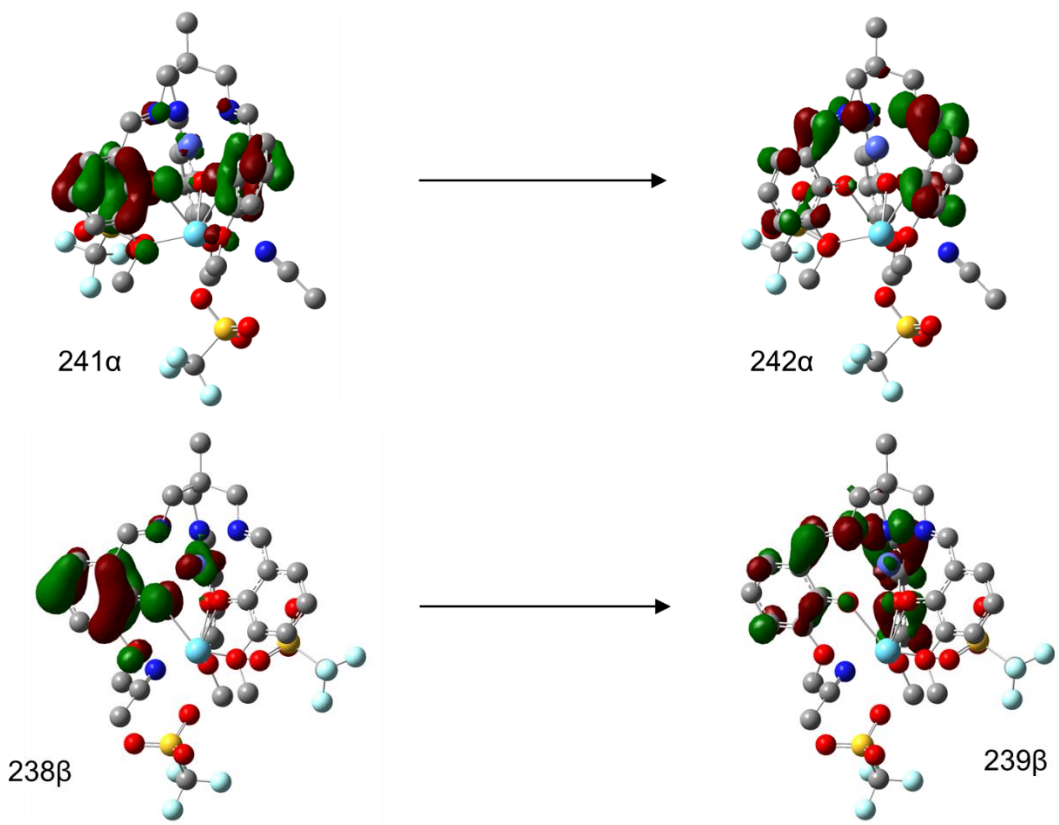

Figure S33: Complex **5** natural transition orbitals for excited state 24 (orbitals 238β, 239β, 241α and 242α exhibit the largest occupations).

Table S6: Selection of excitation wavelengths, oscillator strengths and orbital contributions calculated via time-dependent density functional theory for compound **L**H_3: B3LYP-GD3/(N/O: def2TZVP; C/H: def2SVPP basis sets), NStates = 50. Only excited states with oscillator strengths > 0.01 are shown.

Excited state	Peak information		Orbital contributions			
	λ / nm	Oscillator strength	initial	final	coefficient	percentage
1	321.57	0.0194	134	139	-0.19295	7.45 %
			135	139	-0.31166	19.43 %
			136	139	0.20326	8.26 %
			138	139	0.51945	53.97 %
3	315.59	0.0893	134	139	-0.19295	7.45 %
			135	139	-0.31166	19.43 %
			136	139	0.20326	8.26 %
			138	139	0.51945	53.97 %
6	295.76	0.0152	130	139	-0.10337	2.14 %
			134	139	-0.29519	17.43 %
			134	140	-0.15942	5.08 %
			135	139	0.42899	36.81 %
			135	140	-0.15161	4.60 %
			136	139	0.36629	26.83 %
8	288.41	0.0579	137	141	0.27871	15.54 %
			138	140	-0.15525	4.82 %
			138	141	0.58236	67.83 %
9	187.49	0.0285	137	140	-0.11910	2.84 %
			137	141	0.59162	70.00 %
			138	141	-0.30763	18.93 %
10	284.63	0.0407	132	142	0.10571	2.23 %
			134	140	0.10863	2.36 %
			135	140	0.30785	18.95 %
			136	139	0.15661	4.91 %
			136	140	0.50782	51.58 %
			138	140	-0.17927	6.43 %
15	268.38	0.0161	130	139	-0.14570	4.25 %
			132	139	-0.13716	3.76 %
			133	139	-0.37529	28.17 %
			133	141	-0.15070	4.54 %
			134	139	0.10366	2.15 %
			134	141	0.50730	51.47 %
17	263.10	0.0979	130	139	0.41880	35.08 %
			131	141	0.21275	9.05 %
			132	139	0.12936	3.35 %
			132	141	-0.13825	3.82 %
			133	139	-0.19252	7.41 %
			133	141	0.17774	6.32 %
			134	139	-0.14408	4.15 %
			134	140	-0.10730	2.30 %
			134	141	0.14209	4.04 %
			135	141	0.30511	18.62 %
18	257.90	0.0587	130	139	-0.14420	4.16 %
			131	139	0.50401	50.81 %
			132	139	0.32836	21.56 %
			133	139	-0.25434	12.94 %
			134	141	-0.15668	4.91 %
19	255.14	0.3112	131	141	0.20918	8.75 %
			132	139	0.38867	30.21 %
			132	141	-0.14958	4.47 %
			133	139	0.22239	9.89 %
			133	140	-0.12129	2.94 %
			133	141	0.13334	3.56 %
			134	141	0.28282	16.00 %
			135	141	-0.25725	13.24 %
20	250.71	0.0742	130	139	0.39080	30.54 %
			131	139	0.14415	4.16 %
			131	141	-0.20766	8.62 %

			132	139	0.11632	2.71 %
			132	140	0.13378	3.58 %
			132	141	0.20598	8.49 %
			133	139	0.10181	2.07 %
			133	140	-0.14920	4.45 %
			133	141	-0.36672	26.90 %
21	249.62	0.0392	130	139	0.13160	3.46 %
			131	140	0.37651	28.35 %
			132	140	-0.34909	24.37 %
			133	140	0.39380	31.02 %
			133	141	-0.16493	5.44 %
22	245.30	0.0194	130	141	-0.12762	3.26 %
			131	140	0.12166	2.96 %
			131	141	-0.15505	4.81 %
			132	140	-0.33351	22.25 %
			132	141	0.34213	23.41 %
			133	140	-0.22816	10.41 %
			133	141	0.34544	23.87 %
			134	141	0.10632	2.26 %
23	243.90	0.0337	131	141	-0.10469	2.19 %
			132	140	0.30967	19.18 %
			132	141	0.23382	10.93 %
			133	140	0.46818	43.84 %
			133	141	0.26667	14.22 %
			134	141	0.10340	2.14 %
24	242.71	0.1607	130	140	-0.34198	23.39 %
			131	140	0.43480	37.81 %
			132	140	0.22509	10.13 %
			133	139	-0.11104	2.47 %
			133	141	0.11061	2.45 %
			134	140	-0.22054	9.73 %
			134	141	-0.10614	2.25 %
			136	142	-0.11774	2.77 %
25	236.32	0.0260	130	140	0.54809	60.08 %
			131	140	0.27992	15.67 %
			132	140	0.24655	12.16 %
			136	142	-0.15804	5.00 %
29	228.29	0.0137	137	143	0.48185	46.44 %
			137	144	0.32402	21.00 %
			138	**143**	-0.25717	13.23 %
			138	144	-0.28096	15.79 %
31	224.60	0.0362	134	142	0.36195	26.20 %
			135	142	0.45675	41.72 %
			135	143	0.13268	3.52 %
			136	142	-0.26789	14.35 %
			137	142	0.18027	6.50 %
34	218.21	0.0521	129	139	0.13491	3.64 %
			135	143	0.22128	9.79 %
			135	144	-0.20499	8.40 %
			136	143	0.35731	25.53 %
			136	144	0.36125	26.10 %
			137	144	-0.24018	11.54 %
			138	143	-0.13029	3.40 %
			138	144	-0.11574	2.68 %
35	217.70	0.0785	129	139	-0.20281	8.23 %
			135	143	0.22559	10.18 %
			135	144	0.36029	25.96 %
			136	142	0.14101	3.98 %
			136	143	0.37003	27.38 %
			137	144	0.25241	12.74 %
			138	143	0.11848	2.81 %
37	216.39	0.1823	129	139	0.28630	16.39 %
			134	142	0.11318	2.56 %
			134	143	0.11934	2.85 %
			135	143	0.12258	3.01 %
			135	144	0.36113	26.08 %

			136	142	0.14609	4.27 %
			136	144	-0.21816	9.52 %
			137	144	-0.29353	17.23 %
			138	143	-0.19798	7.84 %
38	214.37	0.4000	134	143	-0.19330	7.47 %
			135	142	0.29918	17.90 %
			135	144	-0.13911	3.87 %
			136	142	0.48250	46.56 %
40	211.89	0.0285	129	139	-0.15590	4.86 %
			131	142	-0.20168	8.13 %
			132	142	-0.29978	17.97 %
			133	142	0.14838	4.40 %
			134	142	-0.13337	3.56 %
			135	142	0.11297	2.55 %
			135	143	-0.10005	2.00 %
			135	144	0.10067	2.03 %
			135	145	0.12857	3.31 %
			136	143	-0.16590	5.50 %
			136	144	0.16361	5.35 %
			136	145	0.37126	27.57 %
			138	144	-0.12556	3.15 %
41	211.53	0.1685	129	139	0.47529	45.18 %
			136	144	0.14235	4.05 %
			136	145	0.13943	3.89 %
			137	143	0.12712	3.23 %
			137	144	0.16891	5.71 %
			138	143	0.19866	7.89 %
			138	144	0.26367	13.90 %
42	211.15	0.4998	129	139	-0.27221	14.82 %
			136	142	-0.14195	4.03 %
			136	144	0.10773	2.32 %
			137	143	0.34123	23.29 %
			137	144	-0.25534	13.04 %
			138	144	0.34836	24.27 %
43	210.82	0.0283	132	142	0.13625	3.71 %
			135	143	-0.11105	2.47 %
			135	144	0.32028	20.52 %
			136	143	-0.23120	10.69 %
			136	144	0.48209	46.48 %
			136	145	-0.18826	7.09 %
44	208.84	0.0390	133	143	0.14814	4.39 %
			134	143	0.15721	4.94 %
			134	144	0.60766	73.85 %
			137	147	-0.10337	2.14 %
			138	150	-0.10550	2.23 %
45	207.05	0.0328	132	143	0.16065	5.16 %
			133	143	0.47382	44.90 %
			133	144	-0.15335	4.70 %
			134	144	-0.19581	7.67 %
			137	146	0.20029	8.02 %
			137	147	-0.18476	6.83 %
			137	148	-0.11612	2.70 %
			138	146	-0.21639	9.36 %
46	204.72	0.0171	133	143	0.25323	12.83 %
			137	146	-0.28603	16.36 %
			137	147	-0.12026	2.89 %
			137	149	0.11978	2.87 %
			138	145	-0.12667	3.21 %
			138	146	0.50918	51.85 %
			138	147	0.10090	2.04 %
49	203.00	0.0445	131	143	-0.29229	17.09 %
			131	144	-0.13053	3.41 %
			132	143	0.43002	36.98 %
			132	144	0.27048	14.63 %
			133	144	0.21668	9.39 %
			138	147	-0.13506	3.65 %

			138	150	-0.11531	2.66 %
50	202.78	0.0151	131	143	0.17798	6.34 %
			131	144	0.10442	2.18 %
			132	143	-0.18546	6.88 %
			133	142	0.12059	2.91 %
			133	143	0.20813	8.66 %
			133	144	0.48749	47.53 %
			134	144	-0.10449	2.18 %
			137	146	0.16281	5.30 %
			137	147	0.10754	2.31 %
			138	147	-0.10554	2.23 %

Table S7: Selection of excitation wavelengths, oscillator strengths and orbital contributions calculated via time-dependent density functional theory for compound **4**: B3LYP-GD3/(Mn/La: def2TZVPP; N/O/F/S: def2TZVP; C/H: def2SVPP basis sets), NStates = 60. Only excited states with oscillator strengths > 0.01 are shown.

Excited state	Peak information		Orbital contributions			
	λ / nm	Oscillator strength	initial	final	coefficient	percentage
6	432.07	0.0102	237A	242A	0.16067	5.16 %
			237A	243A	0.21165	8.96 %
			237A	244A	0.14935	4.46 %
			239A	242A	0.26003	13.52 %
			239A	243A	0.39664	31.46 %
			239A	244A	0.37066	27.48 %
			240A	242A	-0.11372	2.59 %
			241A	242A	0.45615	41.61 %
			241A	243A	0.38860	30.20 %
			234B	237B	0.12964	3.36 %
			236B	237B	0.15262	4.66 %
			236B	238B	0.13703	3.76 %
			236B	239B	0.19917	7.93 %
19	350.72	0.0666	237A	242A	-0.11723	2.75 %
			237A	243A	-0.14609	4.27 %
			238A	242A	-0.23457	11.00 %
			238A	243A	-0.49781	49.56 %
			239A	244A	0.24179	11.69 %
			240A	244A	0.29567	17.48 %
			241A	244A	-0.11397	2.60 %
			234B	237B	-0.31452	19.78 %
			235B	237B	0.53704	57.68 %
			236B	239B	-0.21842	9.54 %
21	341.52	0.0950	237A	242A	0.80463	129.49 %
			237A	243A	0.22307	9.95 %
			238A	242A	0.12858	3.31 %
			241A	242A	-0.10754	2.31 %
			234B	237B	-0.30413	18.50 %
			234B	239B	-0.14036	3.94 %
			235B	238B	-0.18841	7.10 %
			236B	239B	-0.21444	9.20 %
22	338.60	0.0152	237A	243A	0.53684	57.64 %
			237A	244A	0.36226	26.25 %
			238A	243A	-0.26147	13.67 %
			238A	244A	-0.21507	9.25 %
			240A	243A	-0.11503	2.65 %
			234B	238B	0.36566	26.74 %
			234B	239B	0.32282	20.84 %
			235B	237B	-0.12967	3.36 %
			235B	239B	0.10305	2.12 %
			236B	239B	-0.30052	18.06 %
25	326.98	0.0161	237A	243A	-0.13674	3.74 %
			237A	244A	0.31567	19.93 %
			238A	242A	-0.10112	2.05 %

			238A	244A	0.74696	111.59 %
			239A	244A	-0.14279	4.08 %
			240A	244A	0.11268	2.54 %
			234B	238B	-0.14981	4.49 %
			234B	239B	0.36082	26.04 %
			235B	238B	-0.16627	5.53 %
			236B	239B	-0.10332	2.14 %
31	298.47	0.0266	232A	242A	0.22323	9.97 %
			233A	242A	0.16898	5.71 %
			236A	242A	0.76782	117.91 %
			236A	243A	0.28061	15.75 %
			238A	242A	-0.10068	2.03 %
			231B	237B	-0.12291	3.02 %
			233B	237B	0.35413	25.08 %
32	295.61	0.0419	232A	242A	-0.19677	7.74 %
			233A	242A	0.32704	21.39 %
			235A	242A	0.75802	114.92 %
			236A	242A	-0.18250	6.66 %
			236A	243A	0.17318	6.00 %
			236A	244A	0.12949	3.35 %
			231B	237B	-0.13946	3.89 %
			231B	238B	-0.12785	3.27 %
			232B	237B	-0.18506	6.85 %
			233B	237B	0.17905	6.41 %
			233B	239B	-0.10817	2.34 %
33	293.41	0.0315	233A	242A	-0.13714	3.76 %
			233A	243A	0.32830	21.56 %
			235A	242A	-0.21087	8.89 %
			235A	243A	0.60029	72.07 %
			236A	242A	-0.18106	6.56 %
			236A	243A	0.53802	57.89 %
			232B	237B	-0.15204	4.62 %
			232B	238B	0.14868	4.42 %
34	291.17	0.0183	232A	242A	-0.11172	2.50 %
			232A	243A	0.18429	6.79 %
			233A	242A	-0.19377	7.51 %
			233A	243A	-0.15172	4.60 %
			234A	242A	-0.18009	6.49 %
			234A	243A	-0.11402	2.60 %
			235A	242A	-0.11793	2.78 %
			235A	243A	-0.43096	37.15 %
			235A	244A	-0.15368	4.72 %
			236A	242A	-0.13923	3.88 %
			236A	243A	0.30790	18.96 %
			231B	237B	0.32535	21.17 %
			232B	237B	0.11289	2.55 %
			232B	238B	0.14627	4.28 %
			233B	237B	0.52922	56.01 %
35	289.09	0.0161	232A	243A	-0.28877	16.68 %
			234A	242A	-0.16143	5.21 %
			234A	243A	-0.21323	9.09 %
			234A	244A	-0.10163	2.07 %
			235A	243A	0.39374	31.01 %
			235A	244A	-0.21750	9.46 %
			236A	243A	-0.36785	27.06 %
			236A	244A	0.18165	6.60 %
			229B	237B	0.15465	4.78 %
			231B	239B	-0.12535	3.14 %
			232B	237B	0.26249	13.78 %
			233B	237B	0.44147	38.98 %
			233B	238B	-0.12350	3.05 %
			233B	239B	-0.19403	7.53 %
36	283.03	0.0591	232A	244A	0.11032	2.43 %
			233A	244A	0.15038	4.52 %
			234A	242A	0.38656	29.89 %
			235A	244A	0.19925	7.94 %
			236A	244A	0.53767	57.82 %

			230B	237B	0.19095	7.29 %
			230B	238B	0.12008	2.88 %
			230B	239B	0.17204	5.92 %
			231B	237B	0.39833	31.73 %
			231B	238B	0.17706	6.27 %
			232B	237B	0.26629	14.18 %
			232B	238B	-0.11513	2.65 %
			233B	239B	-0.13154	3.46 %
37	280.77	0.0152	234A	242A	0.35073	24.60 %
			235A	244A	-0.14557	4.24 %
			236A	243A	0.15368	4.72 %
			229B	237B	0.12163	2.96 %
			230B	237B	-0.21362	9.13 %
			230B	238B	-0.11220	2.52 %
			230B	239B	-0.13330	3.55 %
			231B	237B	-0.28720	16.50 %
			231B	238B	-0.16956	5.75 %
			232B	237B	0.55683	62.01 %
			232B	238B	0.15609	4.87 %
			233B	237B	-0.15167	4.60 %
			233B	238B	0.44342	39.32 %
40	275.84	0.0112	232A	244A	0.22798	10.39 %
			233A	242A	-0.22024	9.70 %
			233A	243A	-0.12485	3.12 %
			234A	244A	0.22118	9.78 %
			235A	244A	-0.21369	9.13 %
			236A	244A	0.49291	48.59 %
			228B	237B	0.10676	2.28 %
			229B	237B	-0.12299	3.03 %
			231B	237B	-0.35624	25.38 %
			231B	238B	0.19585	7.67 %
			232B	237B	-0.15373	4.73 %
			232B	238B	0.16842	5.67 %
			233B	239B	0.41176	33.91 %
41	274.67	0.0485	231A	243A	0.12639	3.19 %
			232A	243A	0.16307	5.32 %
			234A	242A	-0.13871	3.85 %
			234A	243A	0.68462	93.74 %
			235A	243A	0.12234	2.99 %
			235A	244A	-0.11463	2.63 %
			236A	243A	-0.18310	6.71 %
			236A	244A	0.13985	3.91 %
			230B	237B	-0.19847	7.88 %
			230B	238B	-0.12053	2.91 %
			230B	239B	-0.15007	4.50 %
			231B	237B	0.21679	9.40 %
			231B	238B	-0.34214	23.41 %
			233B	239B	-0.17974	6.46 %
42	273.81	0.0124	231A	242A	-0.19776	7.82 %
			232A	242A	-0.12819	3.29 %
			233A	242A	0.17453	6.09 %
			233A	243A	0.11842	2.80 %
			233A	244A	-0.13488	3.64 %
			234A	242A	-0.21921	9.61 %
			234A	243A	0.19489	7.60 %
			235A	244A	-0.17639	6.22 %
			230B	237B	0.30442	18.53 %
			230B	238B	0.20840	8.69 %
			230B	239B	0.26134	13.66 %
			231B	237B	-0.18656	6.96 %
			231B	238B	0.15977	5.11 %
			231B	239B	0.28202	15.91 %
			232B	237B	0.27426	15.04 %
			232B	238B	0.46756	43.72 %
			233B	237B	-0.10922	2.39 %
			233B	239B	-0.13710	3.76 %
47	266.24	0.0120	231A	242A	0.13964	3.90 %

			232A	242A	-0.10849	2.35 %
			232A	244A	-0.10267	2.11 %
			233A	242A	-0.11363	2.58 %
			234A	244A	-0.22350	9.99 %
			240A	245A	-0.14132	3.99 %
			241A	245A	0.14291	4.08 %
			241A	246A	0.72574	105.34 %
			241A	247A	0.27334	14.94 %
			229B	237B	0.11026	2.43 %
			236B	240B	-0.33158	21.99 %
49	264.32	0.0399	231A	243A	-0.34989	24.48 %
			232A	242A	0.52342	54.79 %
			232A	243A	-0.15225	4.64 %
			233A	243A	-0.17643	6.23 %
			234A	242A	-0.17785	6.33 %
			235A	242A	0.12149	2.95 %
			236A	242A	-0.10245	2.10 %
			240A	245A	-0.16218	5.26 %
			241A	247A	0.26006	13.53 %
			222B	238B	0.10056	2.02 %
			231B	238B	-0.22161	9.82 %
			231B	239B	0.13777	3.80 %
			232B	238B	0.13861	3.84 %
			232B	239B	0.16724	5.59 %
			233B	239B	-0.16256	5.29 %
			236B	240B	0.18333	6.72 %
51	263.08	0.0296	231A	243A	-0.22718	10.32 %
			232A	243A	0.21698	9.42 %
			233A	242A	-0.11789	2.78 %
			233A	243A	-0.17534	6.15 %
			233A	244A	-0.11361	2.58 %
			234A	244A	-0.18411	6.78 %
			235A	243A	0.15265	4.66 %
			241A	246A	-0.20867	8.71 %
			241A	247A	0.23746	11.28 %
			228B	237B	-0.28411	16.14 %
			228B	238B	0.51209	52.45 %
			229B	237B	-0.13548	3.67 %
			231B	238B	0.21583	9.32 %
			236B	240B	0.16979	5.77 %
52	261.65	0.0122	231A	243A	0.69794	97.42 %
			232A	243A	0.15841	5.02 %
			233A	243A	-0.29531	17.44 %
			234A	243A	-0.17675	6.25 %
			235A	243A	0.14404	4.15 %
			240A	245A	-0.17131	5.87 %
			241A	247A	0.34500	23.81 %
			228B	238B	-0.12127	2.94 %
			231B	239B	0.17964	6.45 %
			232B	238B	-0.10275	2.11 %
53	261.23	0.0104	231A	243A	-0.20682	8.55 %
			233A	242A	-0.25911	13.43 %
			233A	243A	0.41049	33.70 %
			235A	242A	0.11547	2.67 %
			235A	243A	-0.17760	6.31 %
			240A	245A	-0.18685	6.98 %
			240A	246A	-0.24722	12.22 %
			240A	247A	0.12682	3.22 %
			241A	246A	-0.31477	19.82 %
			241A	247A	0.36819	27.11 %
			241A	248A	-0.10844	2.35 %
			241A	249A	-0.12686	3.22 %
			228B	237B	0.12964	3.36 %
			228B	238B	-0.18891	7.14 %
			231B	239B	0.11338	2.57 %
			232B	238B	-0.12862	3.31 %
			236B	240B	-0.21852	9.55 %

			236B	245B	-0.12605	3.18 %
54	260.87	0.0687	231A	242A	0.14470	4.19 %
			232A	242A	-0.19044	7.25 %
			233A	242A	-0.18593	6.91 %
			233A	243A	0.13971	3.90 %
			233A	244A	-0.16483	5.43 %
			234A	244A	-0.40317	32.51 %
			236A	242A	0.11602	2.69 %
			236A	244A	0.10601	2.25 %
			240A	246A	0.11962	2.86 %
			228B	237B	0.16398	5.38 %
			228B	238B	-0.27942	15.62 %
			231B	239B	0.18173	6.61 %
			232B	239B	0.12969	3.36 %
			233B	239B	0.18539	6.87 %
			236B	240B	0.44749	40.05 %
			236B	244B	0.19106	7.30 %
			236B	245B	0.20526	8.43 %
			236B	246B	0.10767	2.32 %
55	260.19	0.0165	231A	243A	0.14351	4.12 %
			231A	244A	0.13296	3.54 %
			232A	242A	0.52340	54.79 %
			232A	243A	0.29445	17.34 %
			233A	242A	-0.12111	2.93 %
			233A	243A	0.43015	37.01 %
			234A	242A	-0.12522	3.14 %
			234A	243A	-0.12898	3.33 %
			235A	242A	0.11391	2.60 %
			235A	243A	-0.12806	3.28 %
			236A	242A	-0.11342	2.57 %
			236A	243A	-0.15947	5.09 %
			241A	246A	0.13233	3.50 %
			241A	247A	-0.23439	10.99 %
			232B	239B	-0.16055	5.16 %
			236B	240B	0.10467	2.19 %
56	259.33	0.0834	231A	242A	0.22333	9.98 %
			232A	242A	0.16314	5.32 %
			232A	243A	0.24879	12.38 %
			233A	242A	0.34434	23.71 %
			234A	244A	-0.33307	22.19 %
			235A	242A	-0.14363	4.13 %
			236A	242A	-0.10596	2.25 %
			239A	245A	0.22785	10.38 %
			239A	246A	0.17996	6.48 %
			239A	247A	-0.12073	2.92 %
			240A	245A	-0.14894	4.44 %
			240A	246A	-0.19019	7.23 %
			241A	248A	-0.15181	4.61 %
			228B	238B	-0.13394	3.59 %
			229B	237B	0.11819	2.79 %
			231B	239B	-0.21524	9.27 %
			232B	239B	-0.14161	4.01 %
			233B	239B	0.23667	11.20 %
			236B	241B	-0.10811	2.34 %
57	258.43	0.0356	231A	243A	0.14767	4.36 %
			232A	243A	-0.20716	8.58 %
			233A	243A	0.16057	5.16 %
			233A	244A	0.19116	7.31 %
			235A	244A	-0.20821	8.67 %
			239A	245A	0.24276	11.79 %
			239A	246A	0.25650	13.16 %
			239A	247A	-0.16002	5.12 %
			240A	245A	-0.23735	11.27 %
			240A	246A	-0.20313	8.25 %
			241A	248A	-0.16039	5.14 %
			228B	238B	0.20483	8.39 %
			232B	238B	0.11986	2.87 %

			232B	239B	0.29689	17.63 %
			233B	239B	0.10362	2.15 %
			236B	242B	-0.14121	3.99 %
			236B	243B	0.14592	4.26 %
			236B	244B	0.13656	3.73 %
			236B	245B	0.15996	5.12 %
			236B	246B	0.13715	3.76 %
59	257.08	0.0674	231A	243A	-0.31634	20.01 %
			232A	242A	-0.19956	7.96 %
			232A	243A	0.14304	4.09 %
			233A	243A	-0.19842	7.87 %
			234A	244A	0.16619	5.52 %
			235A	243A	0.12068	2.91 %
			239A	245A	0.20343	8.28 %
			239A	246A	0.37463	28.07 %
			239A	247A	-0.10832	2.35 %
			240A	245A	-0.19746	7.80 %
			240A	246A	-0.11367	2.58 %
			240A	248A	-0.10508	2.21 %
			241A	246A	0.13510	3.65 %
			241A	247A	-0.24115	11.63 %
			228B	237B	0.15196	4.62 %
			228B	238B	-0.12268	3.01 %
			231B	239B	0.15364	4.72 %
			232B	238B	-0.15661	4.91 %
			232B	239B	-0.32991	21.77 %
			233B	239B	-0.15595	4.86 %
60	256.49	0.0225	232A	243A	0.12769	3.26 %
			233A	242A	0.16585	5.50 %
			239A	245A	0.23875	11.40 %
			239A	246A	-0.28963	16.78 %
			240A	245A	-0.43558	37.95 %
			240A	246A	0.30349	18.42 %
			241A	246A	-0.10275	2.11 %
			241A	247A	-0.20162	8.13 %
			241A	248A	0.49922	49.84 %
			241A	249A	-0.14659	4.30 %
			236B	241B	0.11995	2.88 %

Table S8: Selection of excitation wavelengths, oscillator strengths and orbital contributions calculated via time-dependent density functional theory for compound **5**: B3LYP-GD3/(Co/La: def2TZVPP; N/O/F/S: def2TZVP; C/H: def2SVPP basis sets), NStates = 60. Only excited states with oscillator strengths > 0.01 are shown.

Excited state	Peak information		Orbital contributions			
	λ / nm	Oscillator strength	initial	final	coefficient	percentage
15	375.54	0.0111	238A	242A	-0.14305	4.09 %
			239A	242A	0.20265	8.21 %
			240A	242A	0.18401	6.77 %
			240A	243A	0.11780	2.78 %
			241A	242A	-0.45921	42.17 %
			241A	243A	-0.27259	14.86 %
			235B	242B	0.14428	4.16 %
			236B	239B	-0.11552	2.67 %
			237B	239B	0.62881	79.08 %
			237B	240B	-0.14782	4.37 %
			238B	240B	-0.10025	2.01 %
			238B	241B	-0.10377	2.15 %
17	366.24	0.0102	236A	244A	0.10684	2.28 %
			237A	242A	0.16002	5.12 %
			238A	242A	-0.24683	12.19 %
			239A	242A	0.50182	50.36 %
			241A	243A	0.27137	14.73 %
			235B	240B	-0.11153	2.49 %

			236B	239B	-0.19457	7.57 %
			237B	240B	0.58636	68.76 %
			238B	240B	-0.18341	6.73 %
19	359.49	0.0219	234A	242A	-0.10689	2.29 %
			237A	242A	0.11804	2.79 %
			237A	243A	0.10661	2.27 %
			238A	243A	-0.18844	7.10 %
			239A	242A	0.13833	3.83 %
			239A	243A	0.37467	28.08 %
			239A	244A	-0.16474	5.43 %
			240A	242A	0.40606	32.98 %
			240A	243A	0.21885	9.58 %
			241A	242A	0.18408	6.78 %
			241A	244A	0.10976	2.41 %
			236B	239B	0.10976	2.41 %
			236B	242B	-0.10641	2.26 %
			237B	241B	-0.19285	7.44 %
21	352.21	0.0450	237A	243A	0.23523	11.07 %
			237A	244A	0.14527	4.22 %
			238A	244A	0.11076	2.45 %
			239A	242A	-0.21625	9.35 %
			239A	243A	0.52288	54.68 %
			239A	244A	0.17431	6.08 %
			240A	242A	-0.30242	18.29 %
			240A	243A	0.20380	8.31 %
			240A	244A	0.10095	2.04 %
			236B	241B	-0.10528	2.22 %
			237B	241B	0.19461	7.57 %
			238B	241B	-0.51937	53.95 %
22	349.40	0.0136	236A	243A	-0.11426	2.61 %
			237A	242A	-0.17097	5.85 %
			237A	243A	0.10887	2.37 %
			237A	244A	0.10465	2.19 %
			238A	242A	-0.34056	23.20 %
			238A	243A	0.35109	24.65 %
			238A	244A	-0.14657	4.30 %
			239A	242A	-0.12083	2.92 %
			239A	243A	-0.15752	4.96 %
			240A	242A	-0.25081	12.58 %
			240A	243A	0.44664	39.90 %
			241A	243A	-0.12853	3.30 %
			241A	244A	0.19406	7.53 %
			236B	240B	0.26755	14.32 %
			236B	241B	0.11171	2.50 %
			237B	240B	0.12209	2.98 %
			237B	241B	-0.20529	8.43 %
			238B	241B	0.27984	15.66 %
24	346.25	0.0734	238A	242A	-0.13902	3.87 %
			239A	244A	0.11279	2.54 %
			240A	242A	0.13157	3.46 %
			241A	244A	0.56471	63.78 %
			235B	239B	-0.11116	2.47 %
			235B	240B	-0.11839	2.80 %
			236B	239B	0.18048	6.51 %
			236B	240B	-0.41653	34.70 %
			236B	241B	-0.10376	2.15 %
			237B	241B	0.44878	40.28 %
			238B	241B	0.24519	12.02 %
			238B	242B	0.22274	9.92 %
27	337.78	0.0302	238A	242A	-0.15309	4.69 %
			238A	244A	-0.10098	2.04 %
			239A	244A	-0.20792	8.65 %
			240A	243A	-0.12268	3.01 %
			231B	239B	-0.10114	2.05 %
			235B	239B	-0.37726	28.47 %
			235B	240B	-0.20357	8.29 %
			236B	239B	-0.10727	2.30 %

			236B	241B	0.12353	3.05 %
			237B	239B	0.13503	3.65 %
			237B	241B	-0.23281	10.84 %
			237B	242B	-0.15075	4.55 %
			238B	241B	-0.18497	6.84 %
			238B	242B	0.65058	84.65 %
30	327.52	0.0109	237A	243A	0.10400	2.16 %
			238A	244A	0.12352	3.05 %
			239A	244A	-0.23231	10.79 %
			239A	247A	0.11805	2.79 %
			240A	244A	0.26120	13.65 %
			241A	249A	0.12686	3.22 %
			231B	240B	0.12991	3.38 %
			233B	239B	-0.11754	2.76 %
			234B	239B	-0.15676	4.91 %
			235B	240B	0.52763	55.68 %
			235B	248B	-0.10674	2.28 %
			236B	241B	-0.10982	2.41 %
			237B	242B	0.37134	27.58 %
			237B	243B	-0.11924	2.84 %
			238B	242B	0.32791	21.50 %
36	313.18	0.0116	235A	242A	-0.17681	6.25 %
			237A	243A	0.11030	2.43 %
			239A	246A	0.11111	2.47 %
			239A	247A	0.16306	5.32 %
			239A	249A	0.13295	3.54 %
			240A	248A	-0.17246	5.95 %
			241A	246A	0.10977	2.41 %
			241A	247A	0.16705	5.58 %
			241A	249A	0.13222	3.50 %
			232B	239B	-0.20795	8.65 %
			232B	240B	0.13200	3.48 %
			233B	239B	0.10319	2.13 %
			233B	240B	-0.23791	11.32 %
			234B	239B	0.38791	30.09 %
			234B	240B	-0.30508	18.61 %
			234B	242B	0.10557	2.23 %
			234B	243B	0.15556	4.84 %
			235B	240B	-0.16791	5.64 %
			235B	243B	0.12773	3.26 %
			236B	247B	0.12462	3.11 %
			236B	248B	-0.15865	5.03 %
			236B	249B	-0.10080	2.03 %
			238B	238B	0.13273	3.52 %
			238B	246B	-0.13057	3.41 %
			238B	247B	-0.10166	2.07 %
			238B	248B	-0.21746	9.46 %
38	310.51	0.0140	240A	244A	0.12109	2.93 %
			240A	247A	-0.10279	2.11 %
			240A	248A	-0.18694	6.99 %
			231B	240B	-0.13693	3.75 %
			232B	240B	-0.10177	2.07 %
			233B	240B	0.27160	14.75 %
			234B	240B	0.50703	51.42 %
			234B	243B	-0.12175	2.96 %
			235B	239B	0.15374	4.73 %
			235B	242B	0.20251	8.20 %
			236B	241B	-0.23931	11.45 %
			236B	242B	-0.22187	9.85 %
			236B	247B	0.16416	5.39 %
			237B	242B	-0.29519	17.43 %
			237B	249B	-0.13274	3.52 %
			238B	247B	-0.13327	3.55 %
43	294.82	0.0108	236A	243A	-0.11571	2.68 %
			231B	239B	0.21329	9.10 %
			231B	242B	-0.25113	12.61 %
			232B	239B	-0.13129	3.45 %

			233B	240B	0.12375	3.06 %
			233B	242B	0.12906	3.33 %
			234B	239B	0.26951	14.53 %
			234B	240B	0.14956	4.47 %
			234B	242B	0.30984	19.20 %
			235B	239B	-0.29101	16.94 %
			235B	242B	-0.33592	22.57 %
			236B	242B	-0.38028	28.92 %
			237B	242B	0.39410	31.06 %
			238B	243B	-0.15650	4.90 %
47	288.62	0.0120	234A	244A	-0.17852	6.37 %
			235A	244A	-0.10016	2.01 %
			236A	244A	-0.20295	8.24 %
			237A	242A	0.24439	11.95 %
			237A	243A	-0.31512	19.86 %
			237A	244A	0.60173	72.42 %
			238A	244A	-0.19418	7.54 %
			231B	240B	-0.15697	4.93 %
			233B	240B	-0.10880	2.37 %
			233B	241B	0.11035	2.44 %
			234B	241B	0.20640	8.52 %
			235B	241B	-0.14884	4.43 %
			237B	243B	0.13532	3.66 %
			238B	243B	0.32155	20.68 %
48	284.66	0.1407	234A	243A	0.15540	4.83 %
			235A	242A	-0.28169	15.87 %
			235A	243A	-0.11526	2.66 %
			236A	242A	0.50155	50.31 %
			236A	243A	-0.17270	5.97 %
			237A	242A	0.10883	2.37 %
			231B	240B	0.18524	6.86 %
			232B	239B	0.45320	41.08 %
			232B	240B	0.25360	12.86 %
			232B	242B	-0.16200	5.25 %
			233B	239B	0.20760	8.62 %
			233B	240B	-0.25274	12.78 %
			234B	240B	0.16524	5.46 %
			238B	243B	0.12744	3.25 %
			238B	244B	0.11388	2.59 %
49	283.79	0.0233	234A	244A	-0.11053	2.44 %
			235A	242A	-0.24370	11.88 %
			236A	242A	-0.15502	4.81 %
			236A	243A	0.20986	8.81 %
			237A	244A	0.27982	15.66 %
			230B	240B	-0.10726	2.30 %
			231B	239B	0.41214	33.97 %
			231B	241B	0.10221	2.09 %
			232B	239B	0.24561	12.06 %
			232B	240B	0.23407	10.96 %
			232B	242B	-0.11922	2.84 %
			233B	240B	0.44350	39.34 %
			235B	242B	0.14116	3.99 %
			238B	243B	-0.25620	13.13 %
			238B	244B	-0.15664	4.91 %
			238B	245B	-0.15483	4.79 %
50	281.86	0.0264	235A	242A	0.24850	12.35 %
			236A	242A	0.21568	9.30 %
			236A	243A	-0.17563	6.17 %
			237A	244A	-0.11243	2.53 %
			231B	239B	0.74226	110.19 %
			232B	239B	-0.19808	7.85 %
			233B	240B	-0.16841	5.67 %
			234B	242B	-0.12050	2.90 %
			235B	239B	-0.12652	3.20 %
			235B	242B	0.28511	16.26 %
			236B	242B	0.11363	2.58 %
51	280.39	0.0243	235A	242A	0.31957	20.42 %

			236A	242A	-0.13027	3.39 %
			230B	240B	-0.17344	6.02 %
			231B	239B	-0.10833	2.35 %
			232B	239B	-0.17078	5.83 %
			232B	240B	0.81542	132.98 %
			234B	240B	0.13448	3.62 %
			238B	245B	0.10885	2.37 %
52	278.47	0.0322	234A	242A	-0.45539	41.48 %
			234A	243A	-0.10813	2.34 %
			234A	244A	-0.12655	3.20 %
			235A	242A	-0.10843	2.35 %
			235A	243A	0.28938	16.75 %
			236A	242A	0.57823	66.87 %
			236A	243A	0.11197	2.51 %
			236A	244A	0.27207	14.80 %
			237A	244A	0.13843	3.83 %
			231B	239B	-0.12739	3.25 %
			231B	241B	0.12300	3.03 %
			232B	239B	-0.19805	7.84 %
			232B	240B	0.11069	2.45 %
			233B	240B	0.21774	9.48 %
53	277.13	0.0624	234A	242A	-0.26905	14.48 %
			234A	243A	-0.11879	2.82 %
			235A	242A	-0.31749	20.16 %
			235A	243A	-0.13790	3.80 %
			236A	242A	-0.27087	14.67 %
			236A	243A	-0.38794	30.10 %
			237A	242A	-0.16129	5.20 %
			237A	243A	-0.16285	5.30 %
			230B	240B	-0.16292	5.31 %
			231B	240B	0.51147	52.32 %
			232B	239B	-0.14611	4.27 %
			233B	241B	0.19046	7.26 %
			235B	240B	-0.11357	2.58 %
			236B	243B	0.12162	2.96 %
			238B	244B	0.12580	3.17 %
			238B	245B	0.10215	2.09 %
54	276.11	0.0189	234A	242A	0.20794	8.65 %
			234A	243A	0.42607	36.31 %
			235A	242A	0.19922	7.94 %
			235A	243A	0.56030	62.79 %
			236A	243A	0.16764	5.62 %
			237A	243A	0.21351	9.12 %
			237A	244A	0.11977	2.87 %
			231B	240B	0.41021	33.65 %
			233B	241B	0.19548	7.64 %
57	271.47	0.0108	234A	242A	-0.18683	6.98 %
			234A	243A	0.40814	33.32 %
			234A	244A	0.15422	4.76 %
			235A	242A	-0.14957	4.47 %
			235A	243A	0.12145	2.95 %
			235A	244A	0.34564	23.89 %
			236A	242A	-0.20976	8.80 %
			236A	243A	-0.23795	11.32 %
			236A	244A	0.41029	33.67 %
			237A	242A	-0.13067	3.41 %
			237A	244A	0.18835	7.10 %
			231B	240B	-0.16447	5.41 %
			231B	241B	-0.15057	4.53 %
			233B	240B	-0.14392	4.14 %
			233B	241B	-0.23062	10.64 %
			238B	244B	-0.20087	8.07 %
			238B	245B	-0.16125	5.20 %
60	267.65	0.0125	234A	244A	-0.10105	2.04 %
			235A	244A	-0.11345	2.57 %
			232B	240B	-0.15880	5.04 %
			232B	241B	0.11702	2.74 %

233B	243B	0.11128	2.48 %
234B	243B	0.12291	3.02 %
235B	243B	-0.19466	7.58 %
236B	243B	0.66467	88.36 %
236B	244B	0.10086	2.03 %
237B	243B	0.46519	43.28 %
238B	243B	-0.17279	5.97 %

References

1. D. F. Evans, *J. Chem. Soc.*, 1959, 2003-2005.
2. A. A. Pavlov, G. L. Denisov, M. A. Kiskin, Y. V. Nelyubina and V. V. Novikov, *Inorg. Chem.*, 2017, **56**, 14759-14762.
3. G. A. Bain and J. F. Berry, *J. Chem. Educ.*, 2008, **85**, 532-536.
4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenburg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyey, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. L. Fox, *Gaussian 09, Revision B.01*, Wallingford CT, 2010.
5. F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065.
6. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
7. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
8. E. D. Glendening, C. R. Landis and F. Weinhold, *J. Comput. Chem.*, 2013, **34**, 1429-1437.