Supplementary Information for

Probing The Redox-conversion of Co(II)-disulfide to Co(III)-thiolate Complexes: The Effect of Ligand Field Strength

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Part 3 – Crystallographic Data

Part 4 – Computational Data

Part 1 – Synthesis of Compound $[Co(L^1S)(phen)](SbF_6)_2$

The compound $[Co(L^1S)(phen)](SbF_6)_2$ was prepared in a similar manner as compound [**3**]$(SbF_6)_2$, using 1,10-phenanthroline (phen) instead of bpy. A red powder was obtained in 85% yield. IR (neat, cm^{-1}): 1608s, 1518m, 1485w, 1426s, 1376w, 1344w, 1298w, 1247w, 1225w, 1149w, 1105m, 1091m, 1058m, 1022m, 979w, 955w, 909w, 869w, 847s, 769s, 726s, 649vs, 569m, 526m, 448m, 421s. ESI-MS in acetonitrile calcd. for $[Co(L^1S)(phen)](SbF_6)^+$ *m/z* 732.0, found *m/z* 732.0; calcd. for $[Co(L^1S)(phen)]^{2+}$ *m/z* 248.55, found m/z 248.6; calcd. for $[Co(phen)_3]^{2+}$ *m/z* 299.6, found *m/z* 299.9. Elemental analysis (%) for $[Co(L^1S)(phen)](SbF_6)_2$, calcd. C, 32.23; H, 2.50; N, 7.23; found C, 33.03; H, 2.48; N, 7.18. Single crystals were obtained by vapor diffusion of dry and deoxygenated diethyl ether into the dry and deoxygenated acetonitrile solution of compound $[Co(L^1S)(phen)](SbF_6)_2$.

Part 2 – Experimental Data

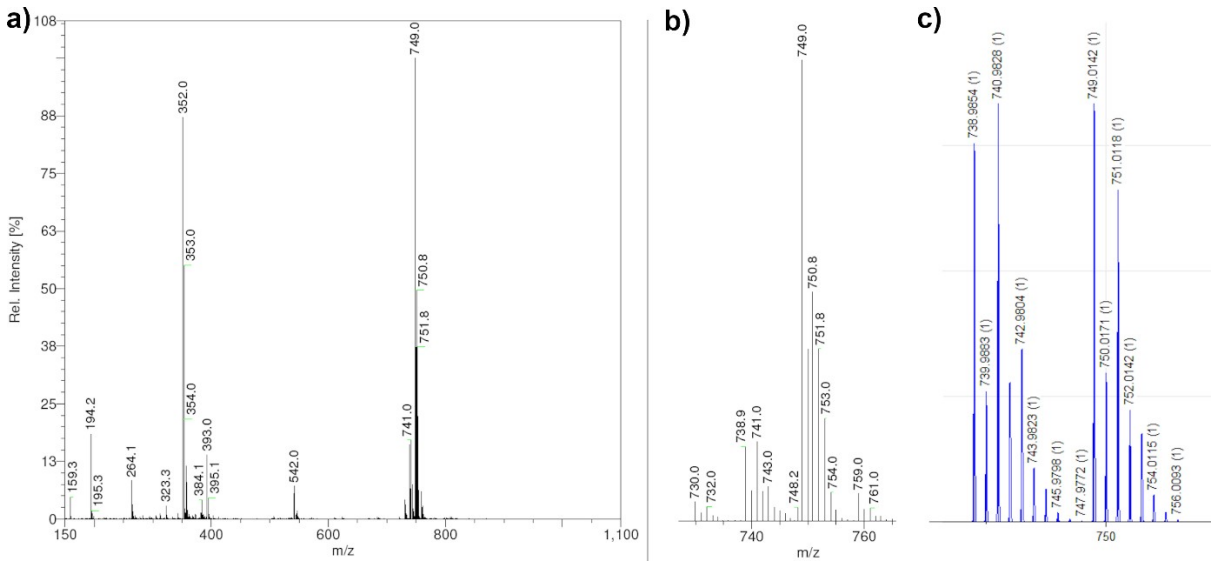

Figure S1. ESI-MS spectrum of a) [$\mathbf{1}_{Cl}$] dissolved in acetonitrile; b) the experimental isotopic distribution of the main signals; c) simulated isotopic distribution of the main signals. ESI-MS found (calcd.) for $[\mathbf{1}_{Cl} - 2Cl^-]^{2+}$ *m/z* 352.0 (352.0), for $[\mathbf{1}_{Cl} - Cl^-]^+$ *m/z* 741.0 (741.0), and for $[\mathbf{1}_{Cl} - 2Cl^- + HCOO^-]^+$ *m/z* 749.0 (749.0).

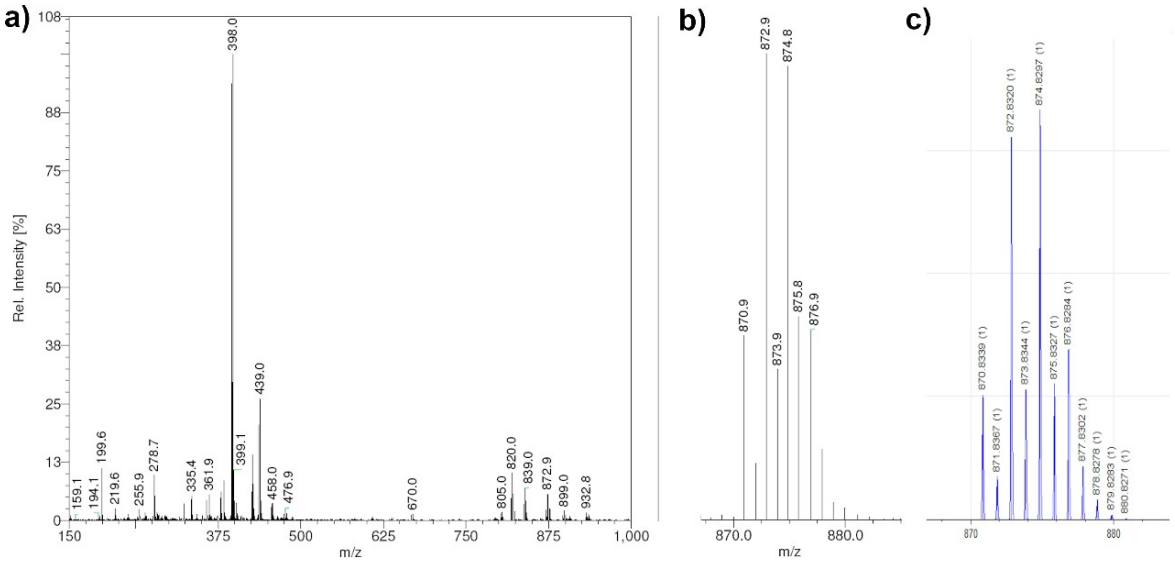

Figure S2. ESI-MS spectrum of a) [$\mathbf{1}_{\mathbf{Br}}$] dissolved in acetonitrile; b) the experimental isotopic distribution; c) simulated isotopic distribution. ESI-MS found (calcd.) for [$\mathbf{1}_{\mathbf{Br}}$ – $2Br^-$]$^{2+}$ *m/z* 398.0 (397.9), for [$\mathbf{1}_{\mathbf{Br}}$ – $2Br^-$ + $HCOO^-$]$^+$ *m/z* 839.0 (838.9), and for [$\mathbf{1}_{\mathbf{Br}}$ – Br^-]$^+$ *m/z* 872.9 (872.8).

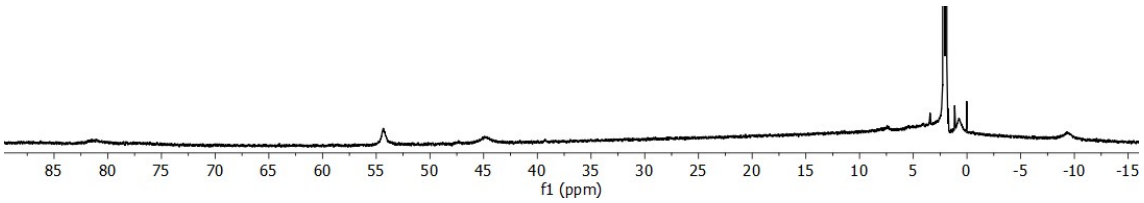

Figure S3. ^{1}H-NMR spectrum of compound [$\mathbf{1}_{\mathbf{Cl}}$] dissolved in CD_3CN.

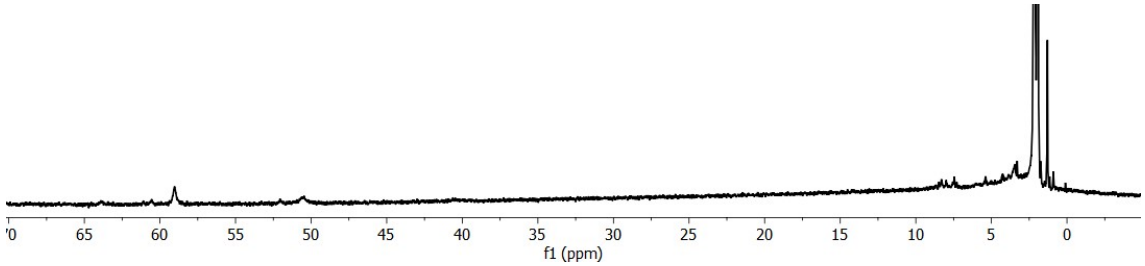

Figure S4. ^{1}H-NMR spectrum of compound [$\mathbf{1}_{\mathbf{Br}}$] dissolved in CD_3CN.

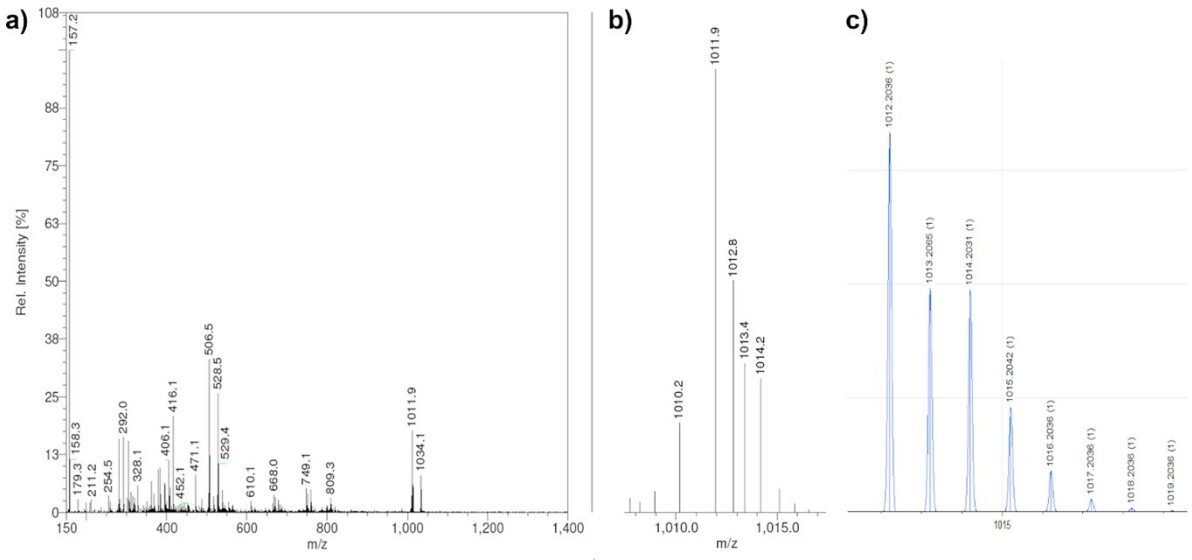

Figure S5. ESI-MS spectrum of a) $[\mathbf{2_{Cl}}](BPh_4)_2$ dissolved in methanol; b) the experimental isotopic distribution; c) simulated isotopic distribution. ESI-MS found (calcd.) for $[\mathbf{2_{Cl}} - Cl^- + OMe^-]^{2+}$ *m/z* 506.5 (506.1), for partially reduced species $[\mathbf{2_{Cl}} - Cl^- + OMe^-]^+$ *m/z* 1011.9 (1012.2).

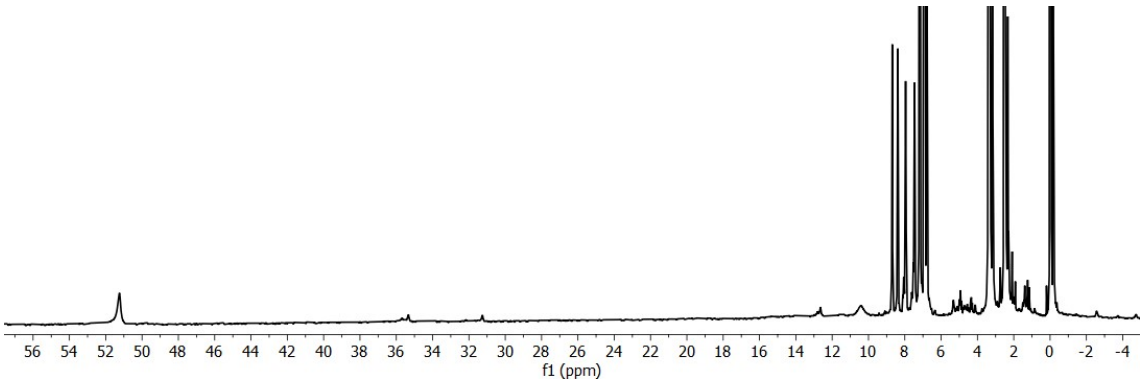

Figure S6. ^{1}H-NMR spectrum of compound $[\mathbf{2_{Cl}}](BPh_4)_2$ dissolved in DMSO-d_6. The diamagnetic region contains peaks that corresponds to the ligand L^1SSL^1 and bipyridine, indicating dissociation of the ligand upon dissolution of the compound.

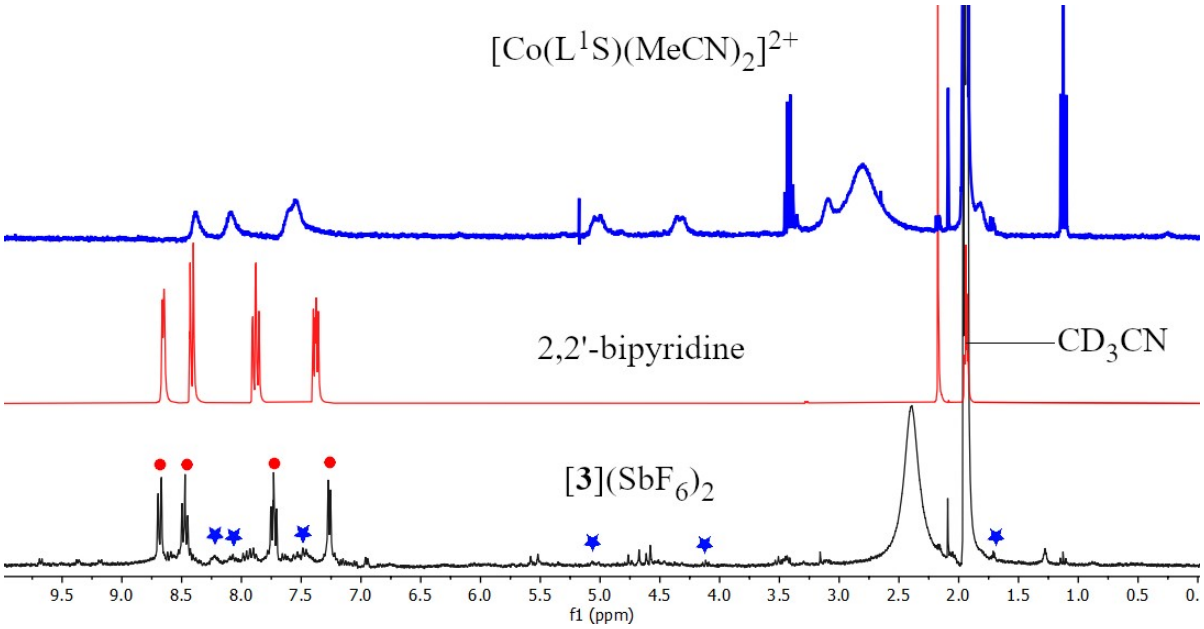

Figure S7. ^{1}H-NMR spectrum of compound [**3**](SbF$_6$)$_2$ (black trace) dissolved in CD$_3$CN. ^{1}H-NMR spectrum of [Co(L^{1}S)(MeCN)$_2$]$^{2+}$ (blue trace) and 2,2'-bipyridine (red trace) dissolved in CD$_3$CN are provided. The red dots and blue stars indicated the presence of 2,2'-bipyridine and [Co(L^{1}S)(MeCN)$_2$]$^{2+}$, respectively.

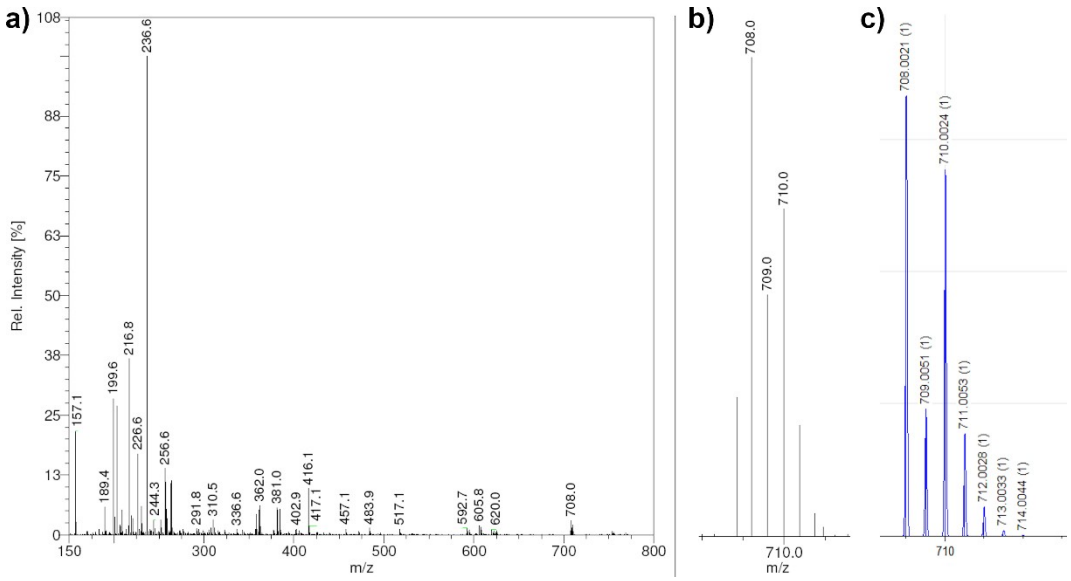

Figure S8. ESI-MS spectrum of a) [**3**](SbF$_6$)$_2$ dissolved in acetonitrile; b) the experimental isotopic distribution; c) simulated isotopic distribution. ESI-MS found (calcd.) for [**3**]$^{2+}$ *m/z* 236.6 (236.55), for [**3**](SbF$_6$)$^{+}$ *m/z* 708.0 (708.0). Species [Co(L^{1}S)(MeCN)$_2$]$^{2+}$ (*m/z* 199.6 (199.55)) and [2,2'-bipyridine + H]$^{+}$ (*m/z* 157.1 (157.0)) are present.

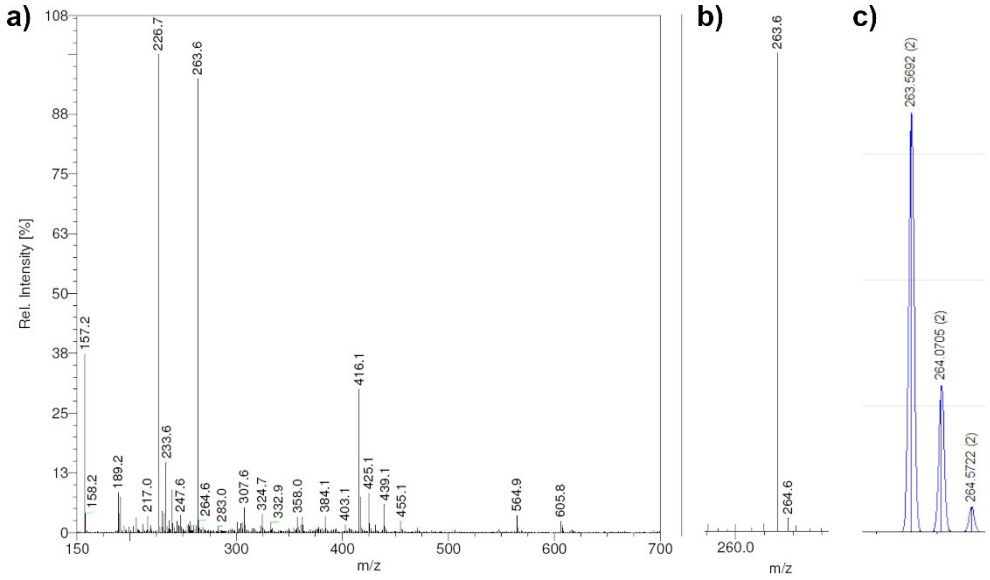

Figure S9. ESI-MS spectrum of a) the isolated brown-reddish powder from the reaction between $[\mathbf{2_{Cl}}](BPh_4)_2$ with $AgSbF_6$, the powder was dissolved in acetonitrile; b) the experimental isotopic distribution; c) simulated isotopic distribution. ESI-MS found (calcd.) for $[(Co(bpy)_3]^{2+}$ *m/z* 263.6 (263.6).

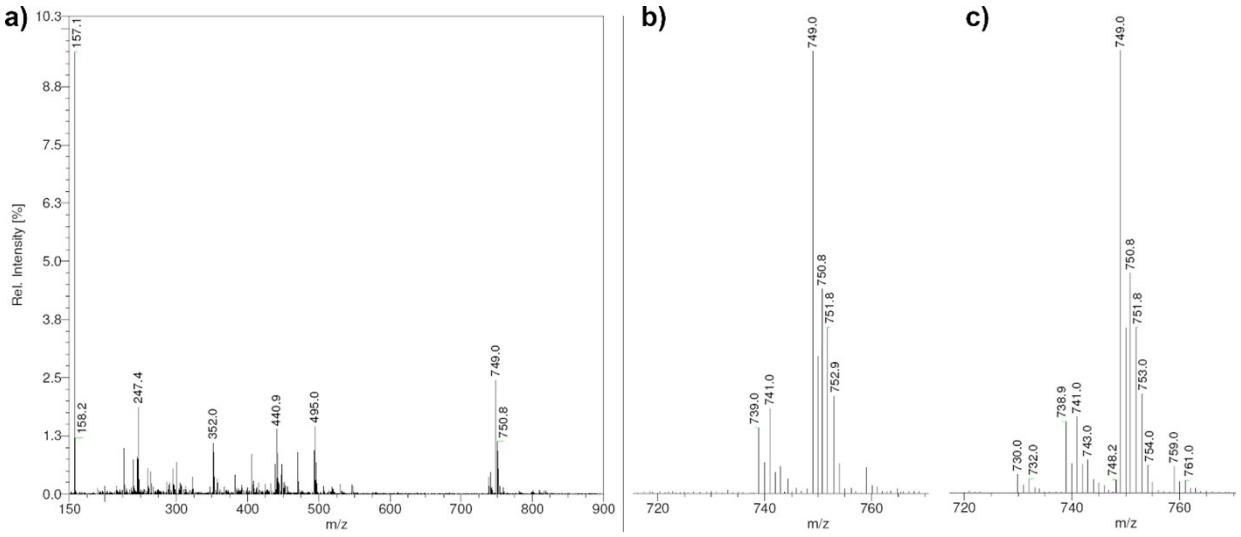

Figure S10. ESI-MS spectrum of a) the isolated purple powder from the reaction between $[\mathbf{3}](SbF_6)_2$ with NEt_4Cl, the powder was dissolved in acetonitrile; b) the experimental isotopic distribution; c) the experimental isotopic distribution for compound $[\mathbf{1_{Cl}}]$. ESI-MS found (calcd.) for $[\mathbf{1_{Cl}} - 2Cl^-]^{2+}$ *m/z* 352.0 (352.0), for $[\mathbf{1_{Cl}} - Cl^-]^+$ *m/z* 741.0 (741.0), and for $[\mathbf{1_{Cl}} - 2Cl^- + HCOO^-]^+$ *m/z* 749.0 (749.0).

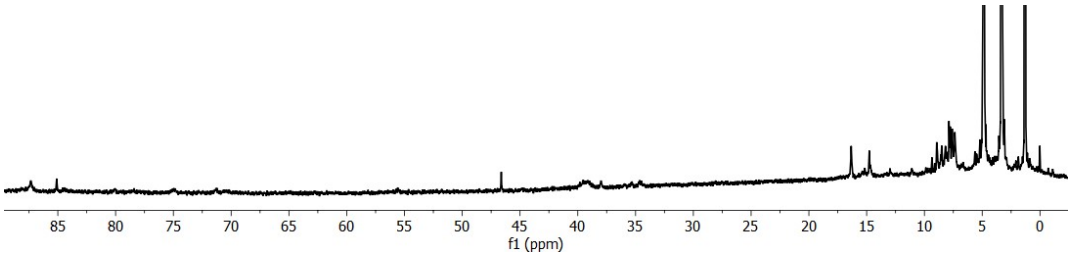

Figure S11. ^{1}H-NMR spectrum of the isolated purple powder from the reaction between [**3**](SbF$_6$)$_2$ with NEt$_4$Cl, the powder was dissolved in CD$_3$CN.

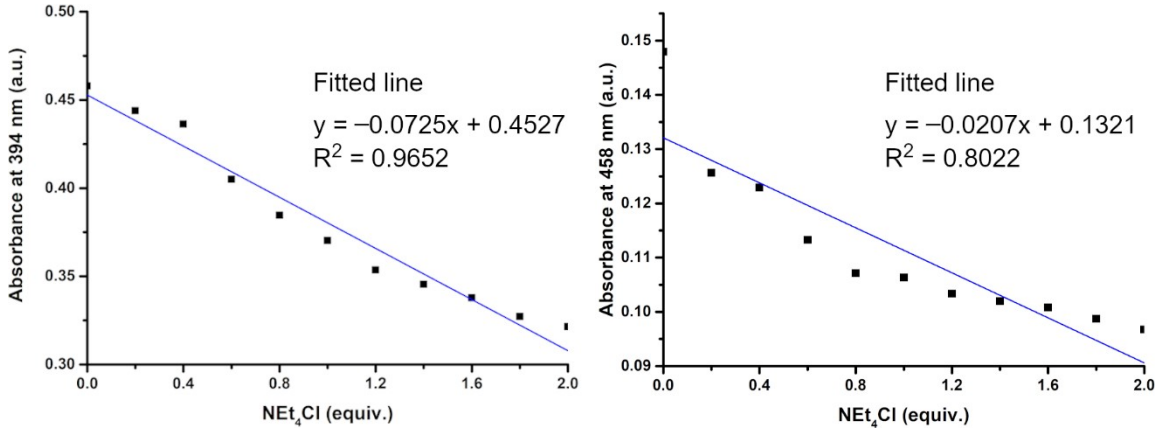

Figure S12. Changes of absorbance at 394 nm and 458 nm as a function of the amount of added NEt$_4$Cl to 5 mM solution of [**3**](SbF$_6$)$_2$. Linear fitting details are provided.

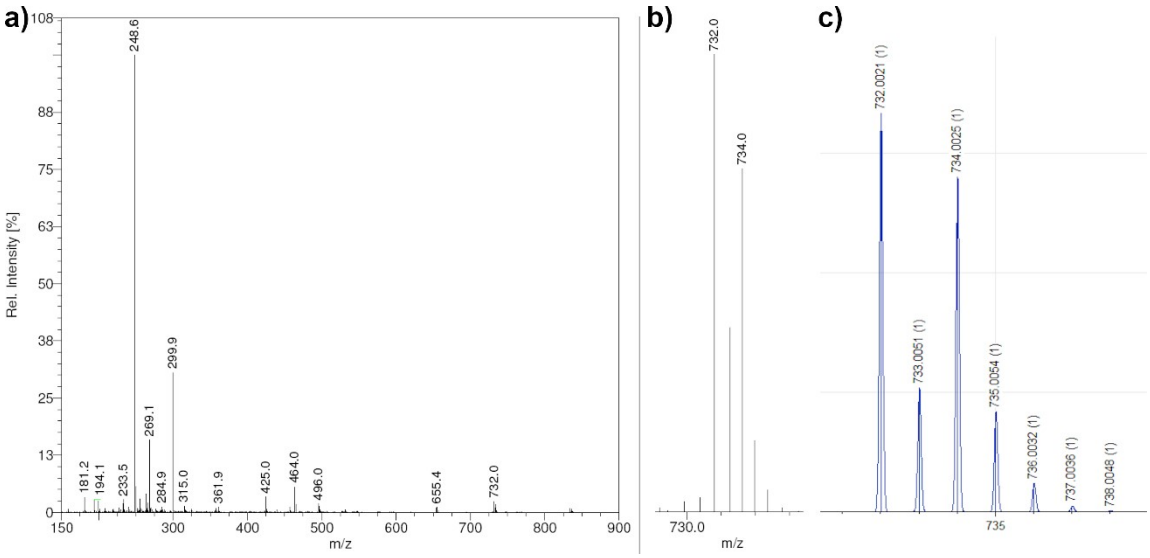

Figure S13. ESI-MS spectrum of a) $[Co(L^1S)(phen)](SbF_6)_2$, the powder was dissolved in acetonitrile; b) the experimental isotopic distribution; c) simulated isotopic distribution. ESI-MS found (calcd.) for $[Co(L^1S)(phen)]^{2+}$ *m/z* 248.6 (248.55) and for $[Co(L^1S)(phen)](SbF_6)^+$ *m/z* 732.0 (732.0). The species $[Co(phen)_3]^{2+}$ is also found (calcd.) at *m/z* 299.9 (299.6).

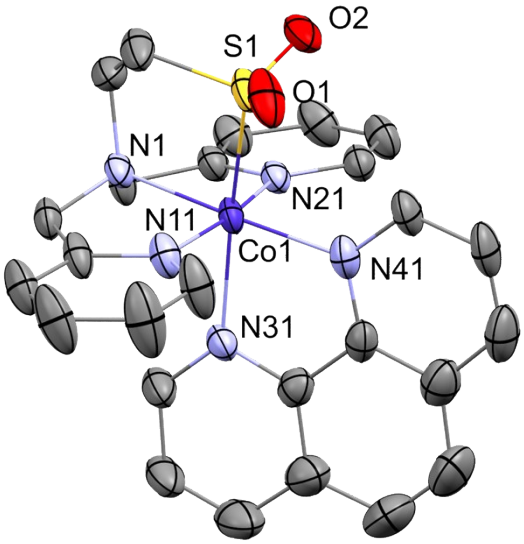

Figure S14. Displacements ellipsoid plot (50% probability level) of the oxidized compound $[Co(L^1SO_2)(phen)](SbF_6)_2$ at 110(2) K. Hydrogen atoms, non-coordinated anions, and lattice solvent molecules are omitted for clarity.

Part 3 – Crystallographic Data

	[$\mathbf{1}_{Br}$]	[$\mathbf{2}_{Cl}$](BPh$_4$)$_2$	[Co(L^{1}SO$_2$)(phen)](SbF$_6$)$_2$
Chemical formula	$C_{28}H_{32}Br_4Co_2N_6S_2$, CH_4O	$C_{48}H_{48}Cl_2Co_2N_{10}S_2$, 2($C_{24}H_{20}B$), 2($C_3H_6O$), 0.42(O)	$C_{26}H_{24}CoN_5O_2S$, 2(F_6Sb), 0.566($C_4H_{10}O$), 1.434(C_2H_3N)
M_r	986.26	1779.17	1101.82
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$C2/c$	$P2_1/c$
Cell lengths (*a, b, c*) (Å)	15.7651(7), 11.9665(5), 19.6343(8)	19.0139(7), 20.1121(7), 27.0156(13)	21.5627 (5), 13.6523 (4), 14.0315 (4)
Cell angles (α, β, γ) (°)	90, 103.345(4), 90	90, 108.171(4), 90	90, 103.059 (3), 90
Cell volume (Å^3)	3604.1 (3)	9815.8 (7)	4023.8 (2)
Z	4	4	4
μ (mm^{-1})	5.50	0.49	1.89
Crystal size (mm)	0.11 × 0.08 × 0.02	0.26 × 0.19 × 0.10	0.29 × 0.09 × 0.05
Temperature (K)	110(2)	110(2)	110(2)
Diffractometer	SuperNova, Dual, Cu at zero, Atlas detector	SuperNova, Dual, Cu at zero, Atlas detector	SuperNova, Dual, Cu at zero, Atlas detector
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α
T_{min}, T_{max}	0.734, 0.982	0.520, 1.000	0.439, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28658, 6355, 4720	38544, 11261, 8613	50549, 7091, 5615
R_{int}	0.065	0.038	0.049
(sin θ/λ)$_{max}$ (Å^{-1})	0.595	0.650	0.595
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.110, 1.04	0.043, 0.105, 1.02	0.039, 0.102, 1.04
No. of reflections	6355	11261	7091
No. of parameters	411	652	661
No. of restraints	39	309	404
H-atom treatment	H-atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.94, -0.58	0.56, -0.31	0.79, -0.77

Table S1.Crystallographic Data for the crystal structures in the present work.

Table S2. Selected bond distances and bond angles in $[Co(L^1SO_2)(phen)](SbF_6)_2$.

Atoms	distance (Å)	Atoms	Bond angles (°)
Co1–N1	1.976(4)	S1−Co1−N1	86.78(11)
Co1–N11	1.921(4)	S1−Co1−N11	88.59(13)
Co1–N21	1.929(4)	S1−Co1−N21	95.64(11)
Co1–N31	2.084(4)	S1−Co1−N31	172.01(12)
Co1–N41	1.969(4)	S1−Co1−N41	92.32(12)
Co1–S1	2.1866(13)	N31−Co1−N41	82.36(16)
S1–O1	1.460(4)	N31−Co1−N1	98.77(15)
S1–O2	1.456(4)	N21−Co1−N1	84.00(16)

Part 4 – Computational Data

Table S3. Bond energies and coordinates of the optimized structures of [**1***] and [**4**]$^{2+}$.

[**1***] E = −4845.07 kcal/mol			
1.C	2.844744	6.382931	15.971685
2.Co	3.386012	8.479512	13.894811
3.H	3.806330	6.749578	16.320430
4.C	0.630152	7.294129	13.186178
5.Cl	4.160892	7.699974	11.877657
6.Cl	5.401121	8.524228	15.084964
7.H	0.963185	6.719459	12.312007
8.H	-0.468560	7.265252	13.189977
9.N	2.337893	7.008872	14.892136
10.N	1.167871	8.645361	13.056652
11.N	2.832228	10.450830	14.190168
12.C	1.517070	10.739125	14.240323
13.C	1.055172	12.029467	14.479685
14.H	-0.015117	12.222206	14.513083
15.C	0.972497	9.154997	11.695599
16.H	1.474817	8.495985	10.985626
17.H	1.412781	10.151820	11.609553
18.H	0.426011	4.093677	16.586330
19.C	2.198266	5.333140	16.605779
20.H	2.658506	4.863296	17.472281
21.C	1.974770	13.056275	14.664189
22.H	1.634753	14.074028	14.849059
23.C	3.332649	12.760444	14.594965
24.H	4.091563	13.529311	14.723199
25.C	3.717862	11.447921	14.360959
26.H	4.766855	11.166158	14.316009
27.C	0.598254	9.569623	14.042648
28.H	0.512465	9.038219	14.998775
29.H	-0.412798	9.911644	13.786780
30.C	1.144570	6.603320	14.416475
31.C	0.432026	5.563610	15.008922
32.H	-0.534062	5.273564	14.600911
33.C	0.966737	4.912028	16.113378
34.H	-0.096240	9.220218	11.439182

[**4**]$^{2+}$ E = −6598.97 kcal/mol			
1.Co	0.225934	0.048155	0.362324
2.H	-2.114316	-0.727316	-1.573008
3.C	1.002934	-1.078319	-2.425821
4.C	3.007437	-0.849292	1.131444
5.H	0.841295	-2.527154	1.904743
6.H	-0.440469	-4.609507	2.303702
7.S	-0.095386	0.694749	2.456075
8.C	-0.886231	-3.805997	1.722546
9.C	-2.224593	1.407243	1.030650
10.H	-3.302185	1.434723	0.825238
11.H	-1.841954	2.430734	1.008494
12.C	-1.892457	0.794848	2.361932
13.H	-2.362861	-0.181415	2.516533
14.H	-2.232946	1.461732	3.163513
15.C	-0.155582	-2.649756	1.498885
16.N	-0.648650	-1.628100	0.780241
17.N	0.757437	1.827715	-0.178114
18.N	-1.556311	0.671238	-0.103832
19.C	-2.332335	-0.530196	-0.518334
20.H	-3.407678	-0.346257	-0.434178
21.C	-0.164033	2.445102	-0.950101
22.C	0.041414	3.725416	-1.447247
23.H	-0.727646	4.193912	-2.056413
24.C	1.229623	4.382473	-1.150050
25.H	1.414347	5.384718	-1.531755
26.C	2.166701	3.744766	-0.344940
27.H	3.105451	4.220961	-0.072635
28.C	1.893604	2.471621	0.131307
29.H	2.592885	1.952876	0.776176
30.C	-1.379947	1.626550	-1.231420
31.H	-2.274807	2.245917	-1.354842
32.H	-1.236512	1.060269	-2.156173
33.C	-1.902080	-1.709693	0.287000
34.C	-2.693054	-2.834734	0.486530
35.H	-3.702000	-2.860026	0.082239
36.C	-2.174893	-3.903235	1.207342
37.H	-2.774962	-4.795464	1.375419
38.N	1.935529	-0.504262	0.860571
39.C	4.337904	-1.277195	1.468881
40.H	4.766005	-0.591534	2.207952
41.H	4.959583	-1.281077	0.567253
42.H	4.299166	-2.287826	1.889608
43.N	0.614222	-0.616783	-1.436593
44.C	1.479703	-1.647329	-3.657692
45.H	2.308469	-2.330527	-3.443375
46.H	1.827103	-0.846373	-4.318629
47.H	0.668331	-2.199596	-4.143453

Table S4. Bond energies and coordinates of the optimized structures of $[\mathbf{2^*}]^+_{fac}$ and $[\mathbf{2^*}]^+_{mer}$.

$[\mathbf{2^*}]^+_{fac}$ E = −7754.13 kcal/mol				$[\mathbf{2^*}]^+_{mer}$ E = −7749.08 kcal/mol			
1.Co	-4.705905	-4.191381	7.721768	1.Co	1.027591	-0.388613	-0.031175
2.Cl	-5.855791	-6.008439	8.430441	2.H	-2.122372	-0.740773	-1.540858
3.N	-6.345606	-3.202751	6.677648	3.H	3.360204	-0.763558	1.895706
4.N	-4.250841	-4.905331	5.715097	4.H	-0.449241	-0.863034	-2.976517
5.N	-4.861196	-3.236899	9.600409	5.H	1.280405	-3.310357	0.736888
6.N	-2.945247	-4.800594	8.718999	6.H	-0.170476	-5.166245	1.520492
7.C	-2.675310	-1.519675	7.405107	7.Cl	1.178569	0.168456	2.155637
8.H	-1.852054	-2.172513	7.703687	8.C	-0.616795	-4.251198	1.136424
9.H	-3.143757	-1.124670	8.309402	9.C	-1.692184	1.129464	1.152271
10.C	-4.774843	-1.395976	6.266849	10.H	-2.712741	1.533745	1.052171
11.H	-4.503692	-0.735370	5.428151	11.H	-1.009785	1.929698	1.441771
12.H	-4.951782	-0.736280	7.126774	12.H	5.324458	-2.433315	-2.259971
13.C	-2.998836	-2.842053	5.438769	13.H	6.741920	-2.388297	-0.239710
14.H	-1.987411	-3.141463	5.744026	14.H	4.060648	-2.500192	-3.838912
15.H	-2.865795	-2.075473	4.659036	15.C	0.197553	-3.216883	0.696856
16.C	-6.077903	-2.089215	5.973908	16.N	-0.279560	-2.058093	0.215096
17.C	-6.998372	-1.532939	5.087258	17.N	1.206806	1.586412	-0.858767
18.H	-6.740562	-0.635923	4.526362	18.N	-1.249268	0.525910	-0.114803
19.C	-8.243958	-2.131660	4.936854	19.C	-2.109456	-0.607361	-0.451973
20.H	-8.979257	-1.712161	4.251142	20.H	-3.155706	-0.435067	-0.156522
21.C	-8.526369	-3.275585	5.675993	21.C	0.102223	2.305213	-1.130793
22.H	-9.485956	-3.782868	5.596218	22.C	0.160332	3.666524	-1.419193
23.C	-7.548935	-3.780660	6.523259	23.H	-0.757564	4.215473	-1.622599
24.H	-7.706654	-4.686142	7.107162	24.C	1.391769	4.310979	-1.433678
25.C	-3.656209	-4.062529	4.853087	25.H	1.456298	5.376556	-1.650318
26.C	-3.554439	-4.344141	3.491686	26.C	2.532893	3.568954	-1.151739
27.H	-3.076267	-3.630803	2.822241	27.H	3.521119	4.024245	-1.139748
28.C	-4.061924	-5.543906	3.006254	28.C	2.391425	2.217475	-0.868029
29.H	-3.991066	-5.785066	1.946234	29.H	3.261307	1.610450	-0.629207
30.C	-4.662879	-6.423071	3.900865	30.C	-1.199831	1.548082	-1.159184
31.H	-5.075420	-7.375574	3.573501	31.H	-2.042636	2.253637	-1.091752
32.C	-4.744702	-6.060986	5.238857	32.H	-1.281495	1.065318	-2.140543
33.H	-5.226635	-6.698542	5.978238	33.C	-1.613672	-1.892920	0.159027
34.C	-3.932095	-3.583248	10.519298	34.C	-2.496773	-2.880920	0.587980
35.C	-4.025005	-3.150496	11.845892	35.H	-3.570120	-2.705476	0.538249
36.H	-3.276552	-3.435930	12.578736	36.C	-1.995148	-4.078860	1.083286
37.C	-5.093056	-2.356050	12.235609	37.H	-2.670368	-4.860149	1.429881
38.H	-5.178711	-2.018279	13.267255	38.N	1.422400	-1.190525	-2.175879
39.C	-6.052573	-2.011876	11.288566	39.C	0.551391	-1.225638	-3.190467
40.H	-6.916109	-1.401787	11.545911	40.C	0.849618	-1.690136	-4.464344
41.C	-5.893466	-2.477212	9.991084	41.C	2.138401	-2.152002	-4.706435
42.H	-6.630373	-2.244455	9.225980	42.H	0.086212	-1.687744	-5.240152
43.C	-2.852052	-4.454802	10.022363	43.H	2.426265	-2.525916	-5.687943
44.C	-1.806094	-4.921040	10.825272	44.C	3.053681	-2.133903	-3.665922
45.H	-1.736805	-4.636354	11.870672	45.C	2.668896	-1.651004	-2.407937
46.C	-0.848360	-5.765195	10.283101	46.N	3.057823	-1.164319	-0.094266
47.H	-0.032297	-6.138298	10.900046	47.C	3.583812	-1.629359	-1.250455
48.C	-0.958702	-6.131745	8.945387	48.C	4.909374	-2.070370	-1.325077
49.H	-0.242108	-6.802738	8.475968	49.C	5.708780	-2.046698	-0.191092
50.C	-2.020844	-5.625868	8.209660	50.C	5.160710	-1.581043	0.998129
51.H	-2.150068	-5.899470	7.165182	51.C	3.840692	-1.149859	0.997824
52.N	-3.661985	-2.286870	6.627994	52.H	5.739073	-1.543390	1.919316
53.H	-2.261166	-0.676678	6.829625	53.H	-1.670457	0.382904	1.947165

Table S5. Bond energies and coordinates of the optimized structures of $[\mathbf{3}]^{2+}_{fac}$ and $[\mathbf{3}]^{2+}_{mer}$.

$[\mathbf{3}]^{2+}_{fac}$ E = −7880.35 kcal/mol				$[\mathbf{3}]^{2+}_{mer}$ E = −7888.61 kcal/mol			
1.N	-1.257881	-1.556936	-0.933532	1.Co	0.883410	-0.387903	-0.117866
2.C	-1.796961	-0.999977	-2.212091	2.H	-2.169401	-0.784362	-1.395651
3.C	-1.938285	0.468333	-2.100484	3.H	2.966779	-0.903247	2.038423
4.C	-2.877227	1.221295	-2.797532	4.H	-0.812286	-1.096596	-2.814957
5.C	-2.919069	2.595655	-2.604635	5.H	1.585563	-3.156498	0.964154
6.C	-2.045471	3.162100	-1.680932	6.H	0.253872	-5.168991	1.502979
7.C	-1.138599	2.347343	-1.021805	7.S	0.957569	0.187927	2.023461
8.N	-1.045357	1.023313	-1.258463	8.C	-0.244253	-4.276639	1.129375
9.C	-2.346005	-1.712954	0.076091	9.C	-1.265360	1.210287	1.086199
10.C	-2.288864	-0.677590	1.165932	10.H	-2.347751	1.406850	1.080348
11.N	-1.189680	0.100727	1.218419	11.H	-0.739757	2.165911	1.008815
12.C	-1.073286	0.995279	2.216401	12.C	-0.784950	0.499868	2.315528
13.C	-2.044685	1.156119	3.191834	13.H	-1.343051	-0.414836	2.545500
14.C	-3.188805	0.364694	3.133417	14.H	-0.864142	1.167200	3.183278
15.C	-3.310087	-0.563613	2.107043	15.C	0.510840	-3.154910	0.825541
16.C	-0.632944	-2.872204	-1.287997	16.N	-0.037762	-2.019315	0.356449
17.C	0.585630	-2.680497	-2.174924	17.N	1.407109	1.403917	-0.684237
18.S	1.297092	-1.013581	-1.982658	18.N	-0.933226	0.419244	-0.162117
19.Co	0.093407	-0.241353	-0.271347	19.C	-1.923892	-0.676965	-0.334278
20.C	2.288064	-0.683025	1.460969	20.H	-2.867477	-0.422296	0.162464
21.C	3.083559	-1.228888	2.470999	21.C	0.394506	2.111334	-1.238657
22.C	2.692339	-2.395917	3.106657	22.C	0.570231	3.407286	-1.706896
23.C	1.484181	-2.972795	2.733172	23.H	-0.271980	3.946109	-2.137271
24.C	0.740948	-2.374239	1.727543	24.C	1.822547	4.003687	-1.603574
25.N	1.129007	-1.271715	1.065736	25.H	1.983296	5.018744	-1.963952
26.C	2.607449	0.543212	0.746081	26.C	2.851889	3.287223	-1.004788
27.C	3.818939	1.226965	0.851259	27.H	3.842676	3.717246	-0.872166
28.C	4.066162	2.322084	0.037279	28.C	2.604488	1.999946	-0.550054
29.C	3.100865	2.678775	-0.896476	29.H	3.382297	1.431918	-0.053202
30.C	1.913307	1.964374	-0.944779	30.C	-0.916070	1.388920	-1.286984
31.N	1.630181	0.948217	-0.106468	31.H	-1.760847	2.086612	-1.214253
32.H	-1.056419	-1.204446	-2.993100	32.H	-1.018819	0.859130	-2.237167
33.H	-2.736448	-1.498366	-2.479404	33.C	-1.379133	-1.966618	0.199426
34.H	-3.566994	0.727671	-3.479554	34.C	-2.196792	-3.052556	0.494565
35.H	-3.637732	3.210501	-3.144610	35.H	-3.274512	-2.969270	0.365248
36.H	-2.063350	4.227230	-1.458445	36.C	-1.624065	-4.229149	0.961174
37.H	-0.467934	2.764643	-0.278221	37.H	-2.246771	-5.089984	1.200496
38.H	-2.267738	-2.710972	0.524985	38.N	1.123316	-1.091588	-2.071071
39.H	-3.327346	-1.688499	-0.412336	39.C	0.229012	-1.268614	-3.056951
40.H	-0.167524	1.596986	2.225495	40.C	0.555065	-1.667208	-4.345525
41.H	-1.901842	1.894140	3.978692	41.C	1.890490	-1.897500	-4.650812
42.H	-3.976722	0.467923	3.878291	42.H	-0.232538	-1.787976	-5.086709
43.H	-4.189856	-1.201327	2.035915	43.H	2.197544	-2.191131	-5.653367
44.H	-0.348568	-3.370589	-0.362659	44.C	2.824626	-1.772580	-3.634137
45.H	-1.392800	-3.504901	-1.770599	45.C	2.415278	-1.392996	-2.352881
46.H	0.344973	-2.818248	-3.236774	46.N	2.724889	-1.054139	-0.016407
47.H	1.339718	-3.433296	-1.919403	47.C	3.314933	-1.373015	-1.199416
48.H	4.005147	-0.736194	2.765381	48.C	4.665372	-1.723773	-1.267041
49.H	3.308375	-2.835423	3.889533	49.C	5.430021	-1.777050	-0.111038
50.H	1.106545	-3.874101	3.211933	50.C	4.813458	-1.487862	1.099551
51.H	-0.216500	-2.799900	1.457989	51.C	3.473044	-1.130484	1.102936
52.H	4.581502	0.887111	1.545385	52.H	5.351886	-1.529209	2.044471
53.H	5.009767	2.861066	0.105293	53.H	5.121264	-1.966469	-2.221578
54.H	3.259107	3.491737	-1.602218	54.H	6.483217	-2.050537	-0.156795
55.H	1.175673	2.194877	-1.703434	55.H	3.869016	-1.985257	-3.839506

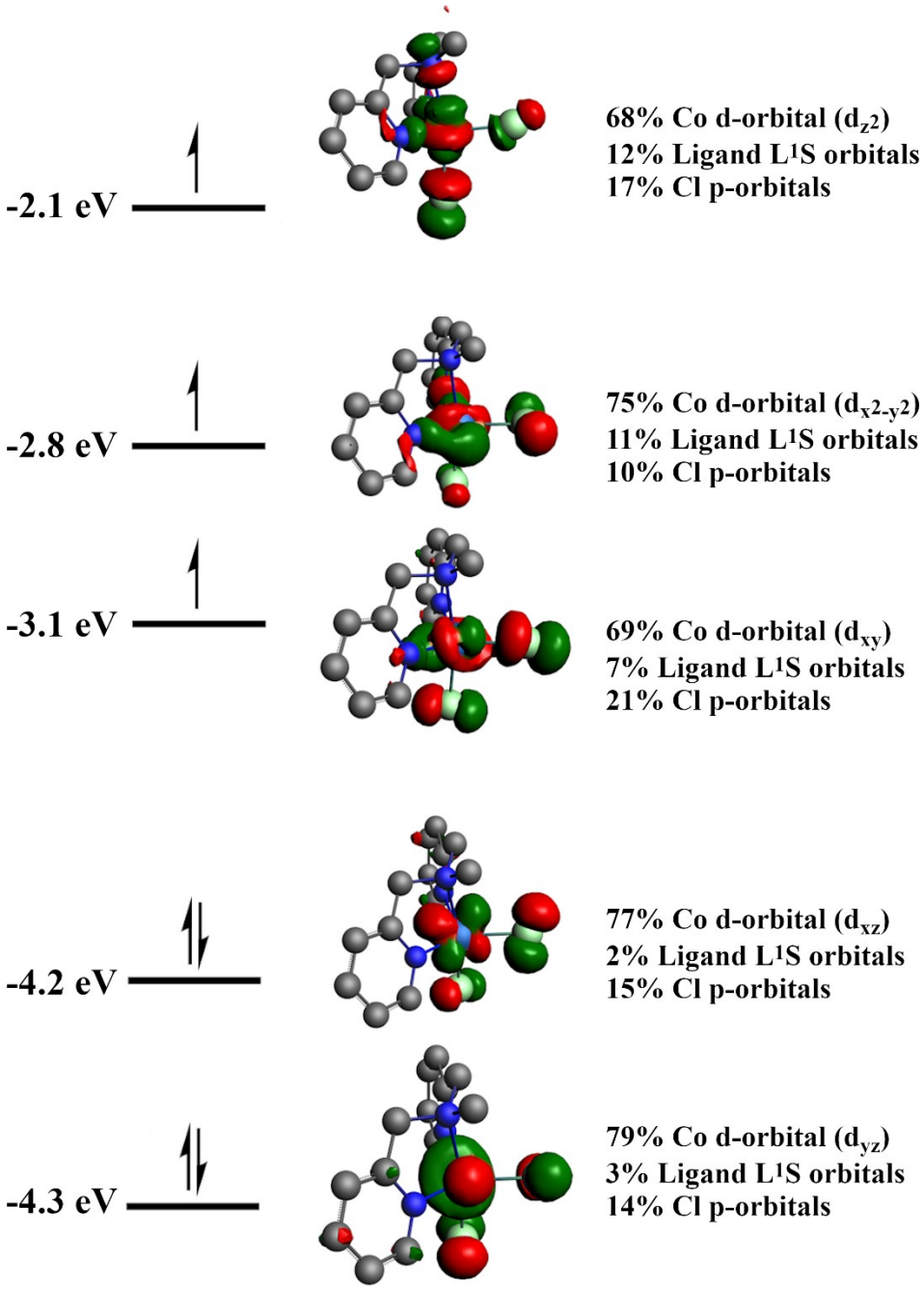

Figure S15. Several frontier orbitals of [**1***] associated with Co d-orbitals along with their energies, orbital visualization, and orbital composition.

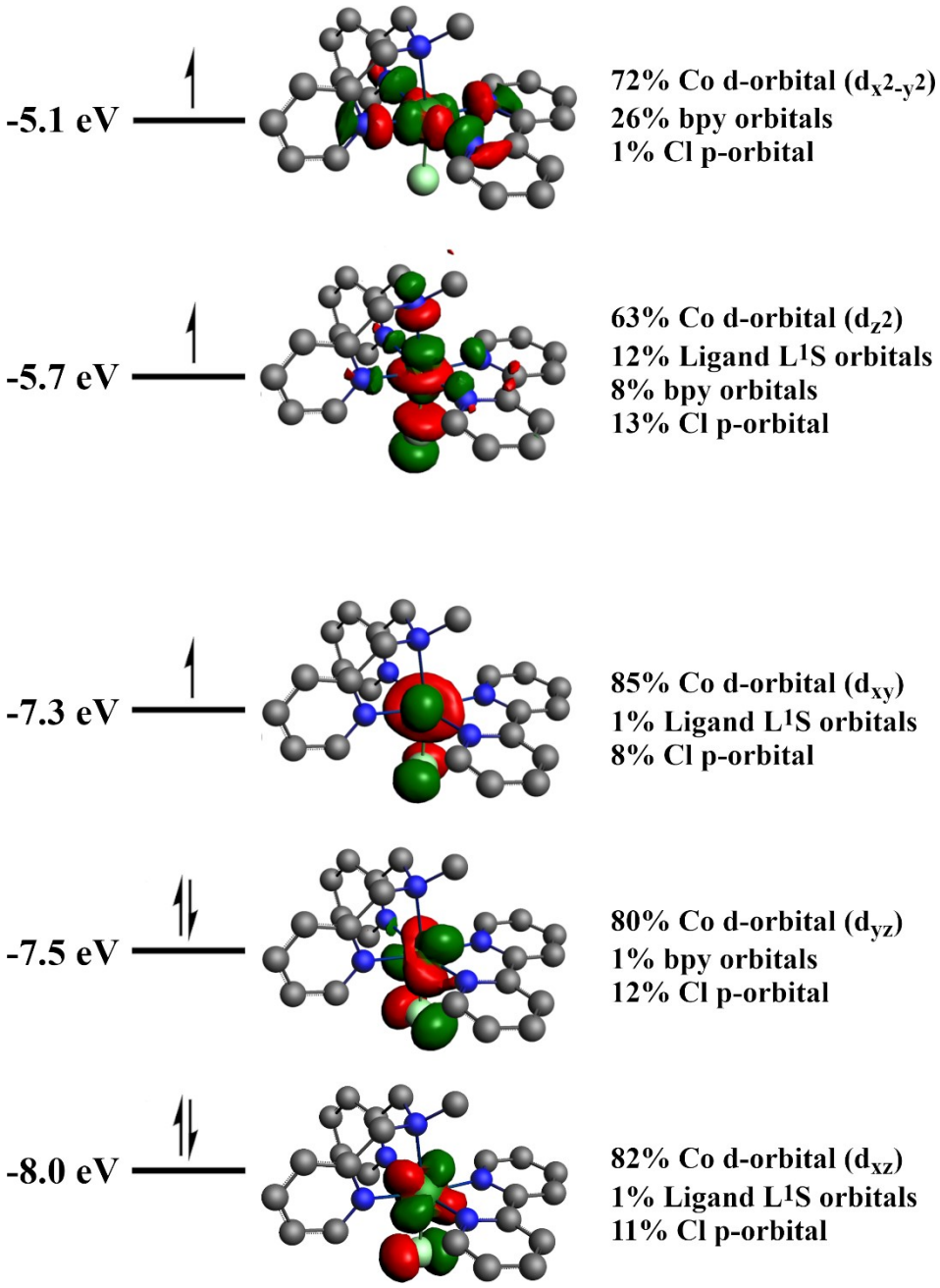

Figure S16. Several frontier orbitals of $[\mathbf{2^*}]^+_{fac}$ associated with Co d-orbitals along with their energies, orbital visualization, and orbital composition.

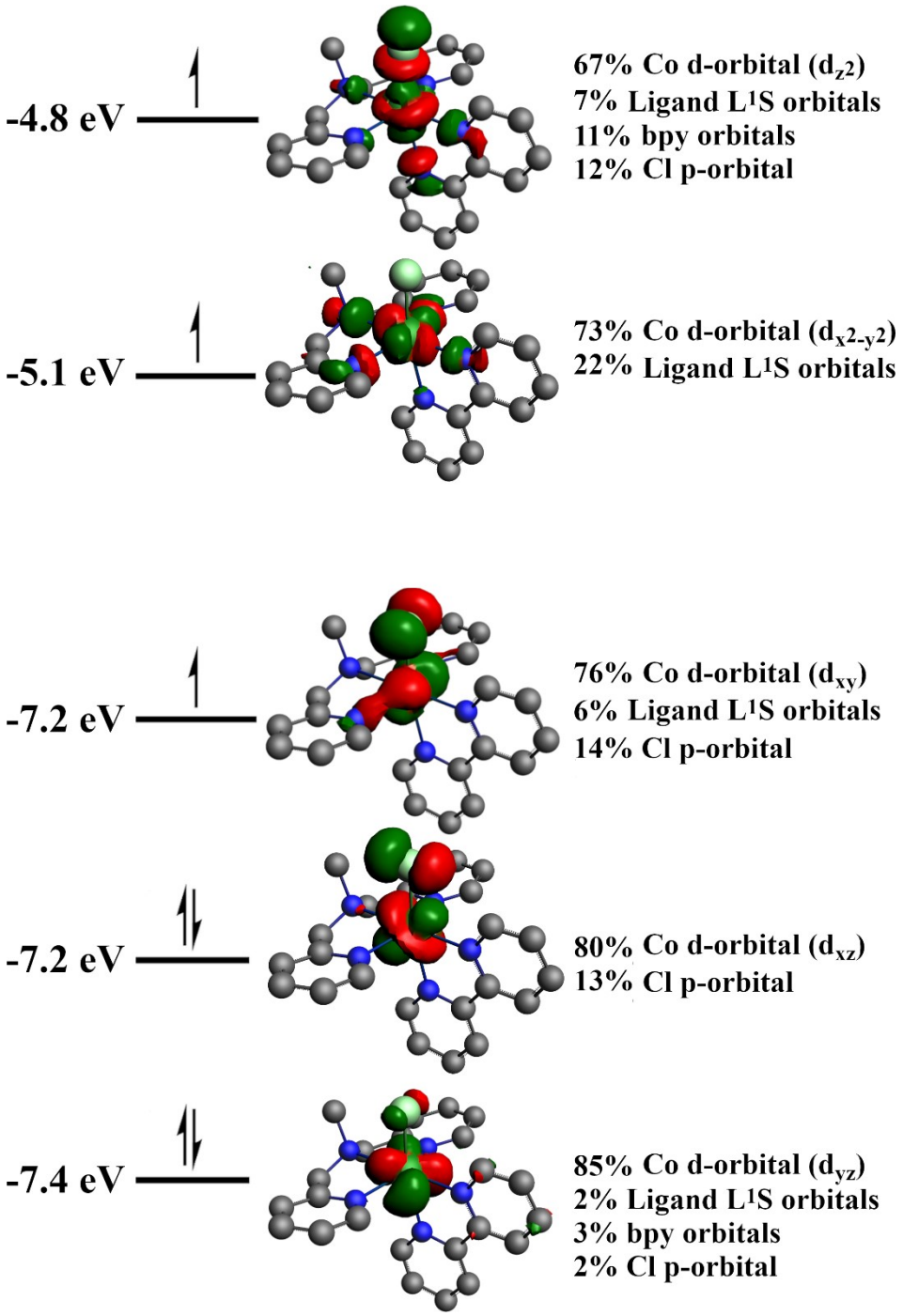

Figure S17. Several frontier orbitals of $[\mathbf{2^*}]^+_{mer}$ associated with Co d-orbitals along with their energies, orbital visualization, and orbital composition.

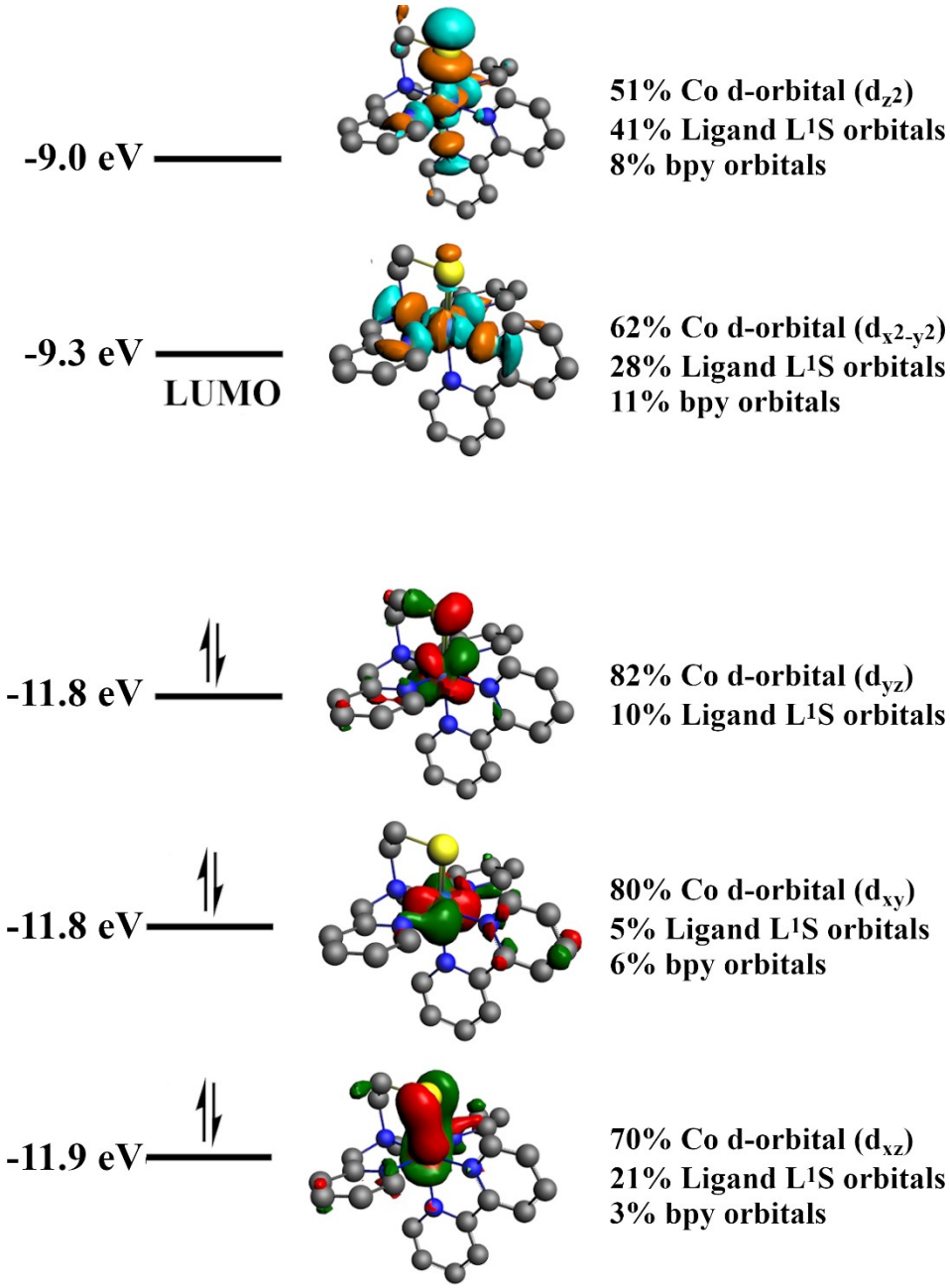

Figure S18. Several frontier orbitals of $[\mathbf{3}]^{2+}_{mer}$ associated with Co d-orbitals along with their energies, orbital visualization, and orbital composition.

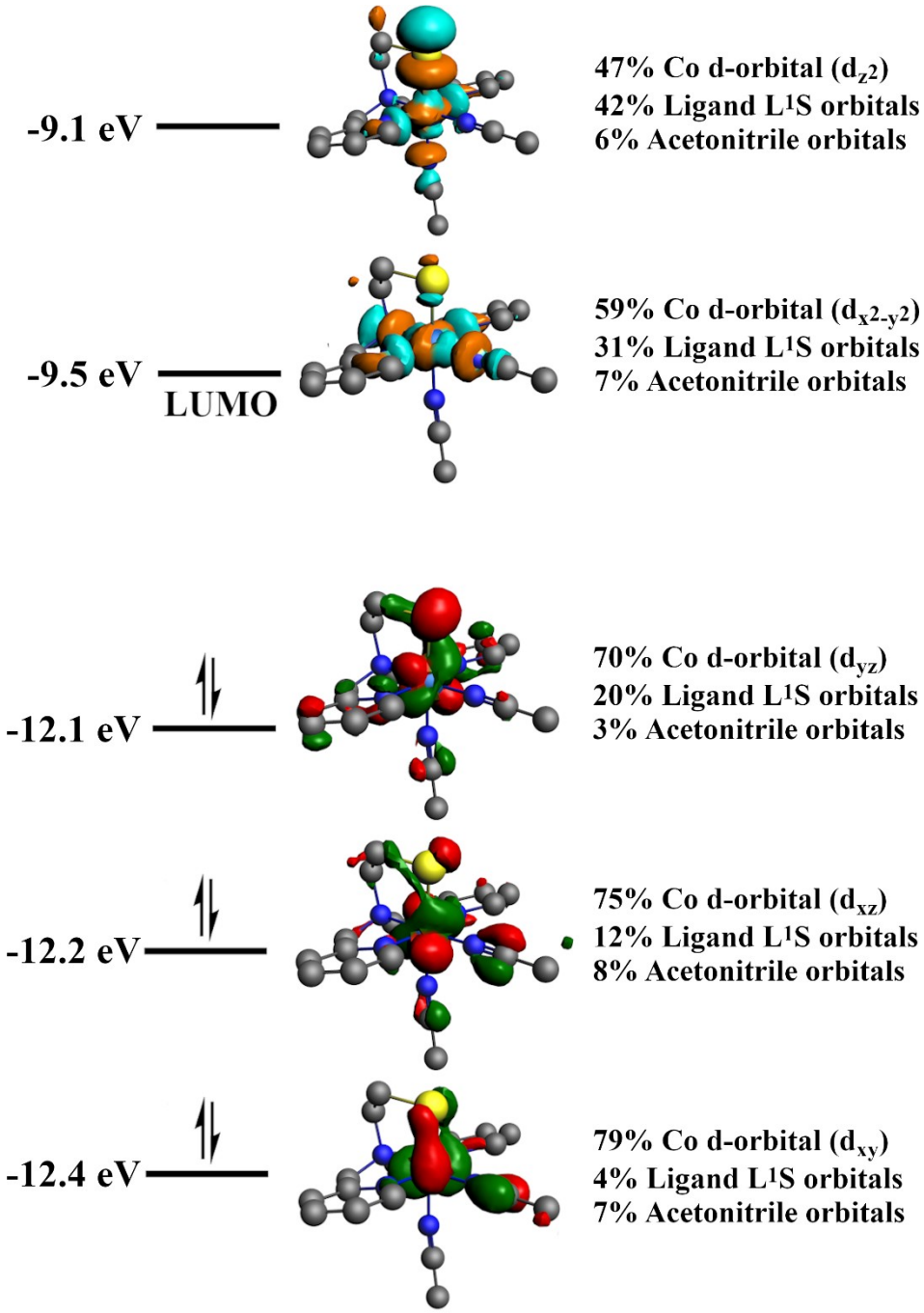

Figure S19. Several frontier orbitals of [**4**]$^{2+}$ associated with Co d-orbitals along with their energies, orbital visualization, and orbital composition.