Supporting Information

Modulation of Electronic and Redox Properties in Phenolate-rich Cobalt(III) Complexes and their Implications for Catalytic Proton Reduction

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Table of Contents

Figure S1. Synthesis of precursors and ligands

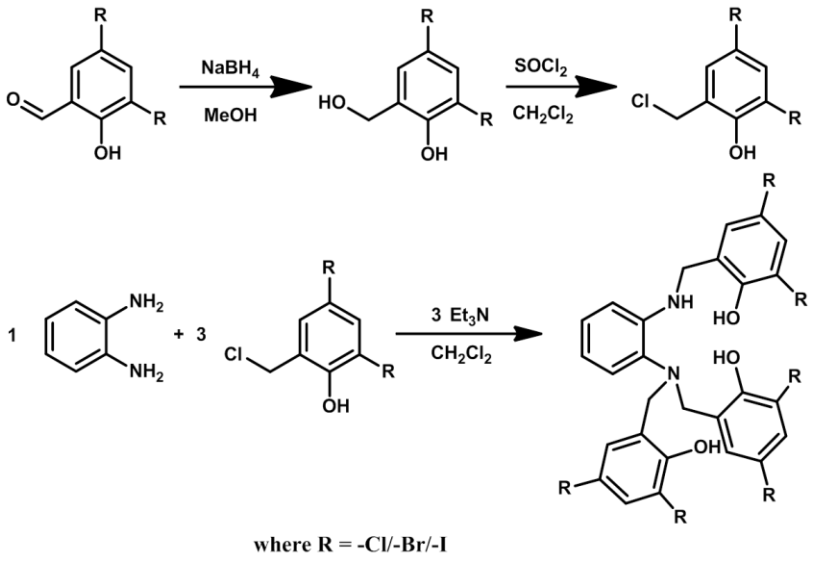


Figure S2. Synthesis of the cobalt(III) complexes

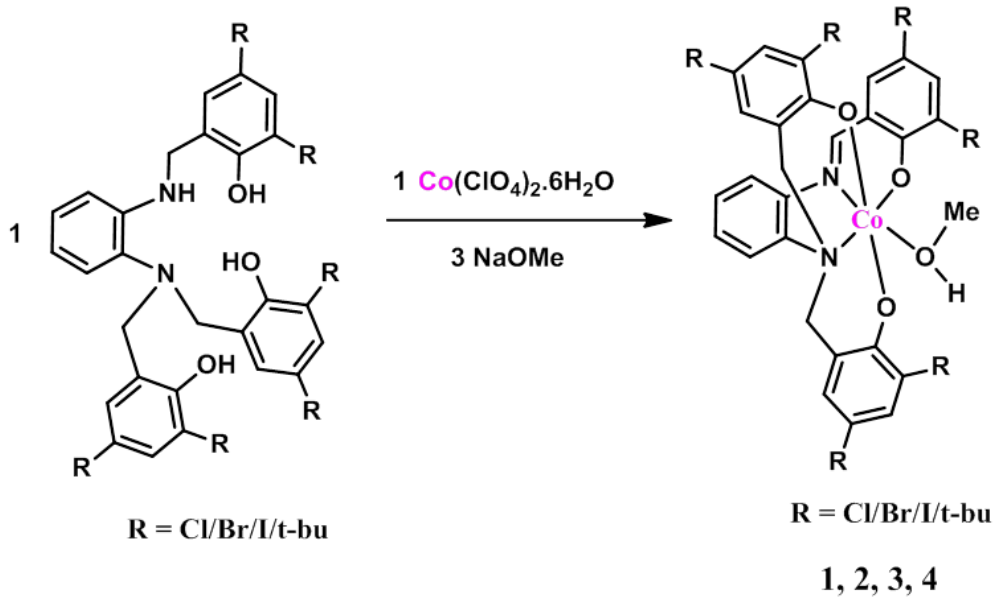


Figure S3. Experimental (bars) and simulated (line) isotopic distribution for the molecular ions of complexes **1**-**3** (left to right)

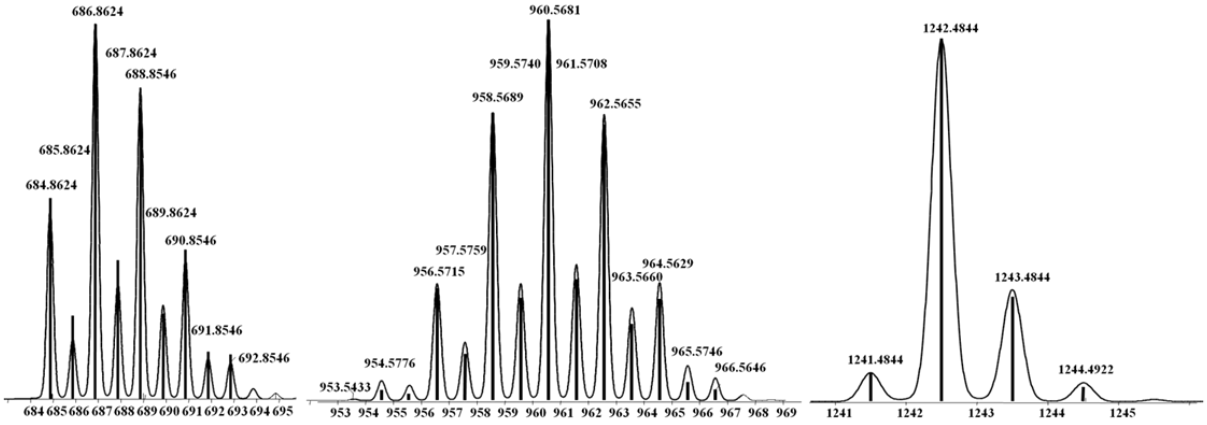


Figure S4. Full scale ^{1}H-NMR spectra of [$Co^{III}L^{Br}$(MeOH)] **(2)** in d_6-DMSO

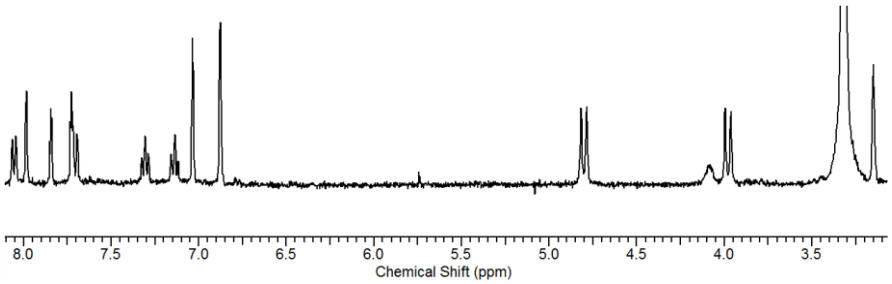


Figure S5. Full scale ^{1}H-NMR spectra of [$Co^{III}L^{I}$(MeOH)] **(3)** in d_6-DMSO

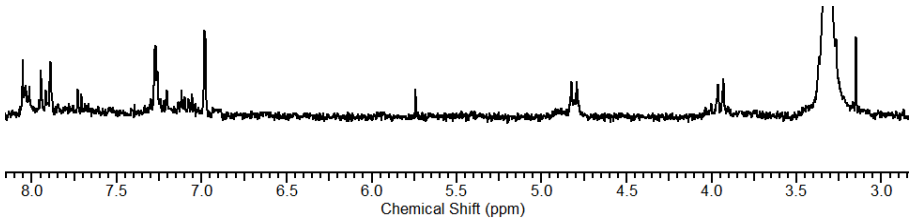
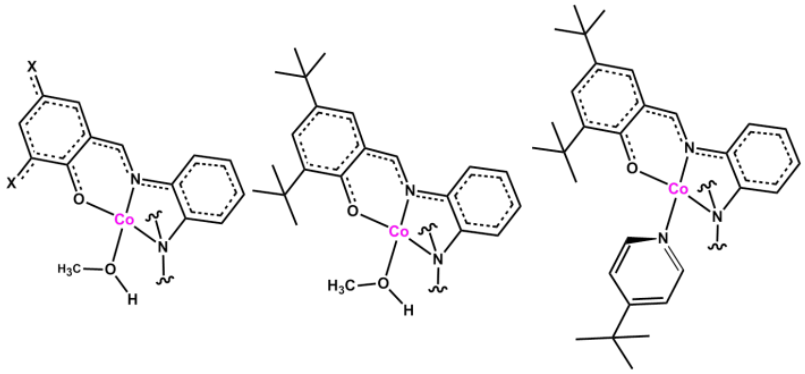


Figure S6. Fully conjugated structure of phelonate-imine-diamino aromatic ring system



Where X = -Cl/-Br/-I; Partial structure used for simplicity

Figure S7. MO ladder for **2**

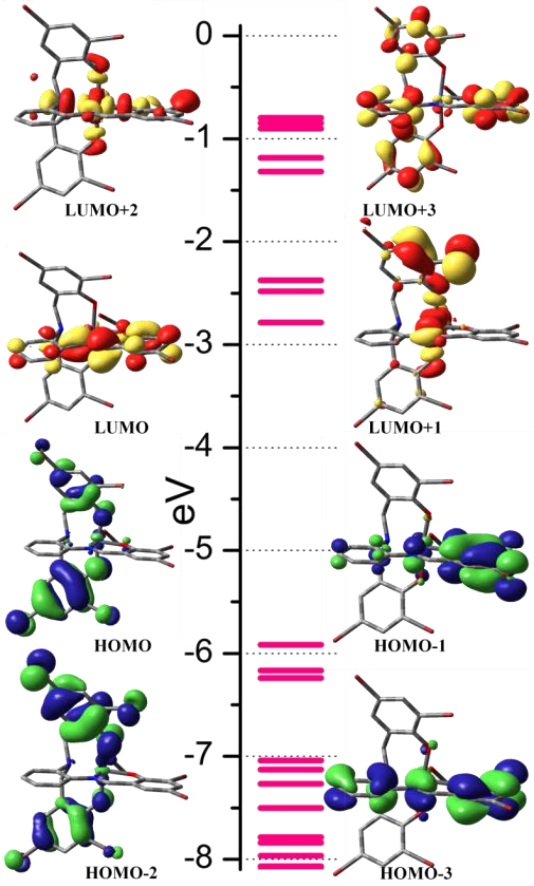


Figure S8. UV-Visible spectra of **1**-**4** ([C] = 1.0 × 10^{-4} M) in dichloromethane

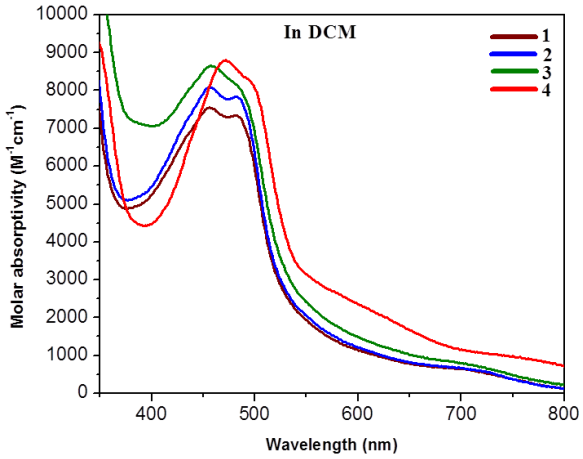


Figure S9. Comparison of UV-Visible spectra for **1** and **4** in different solvents (acetonitrile, dichloromethane, dimethyl formamide and pyridine)

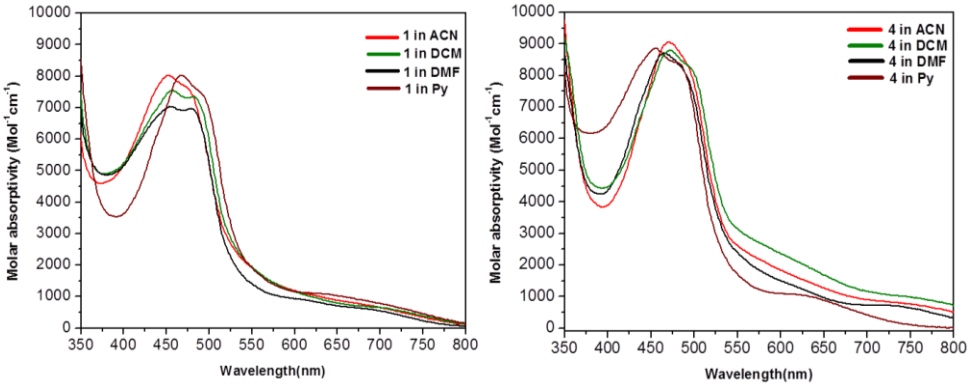


Figure S10. Absorption spectra: calculated vs experimental for **4** (B3PW91/6-311+g(d,p) (acetonitrile))

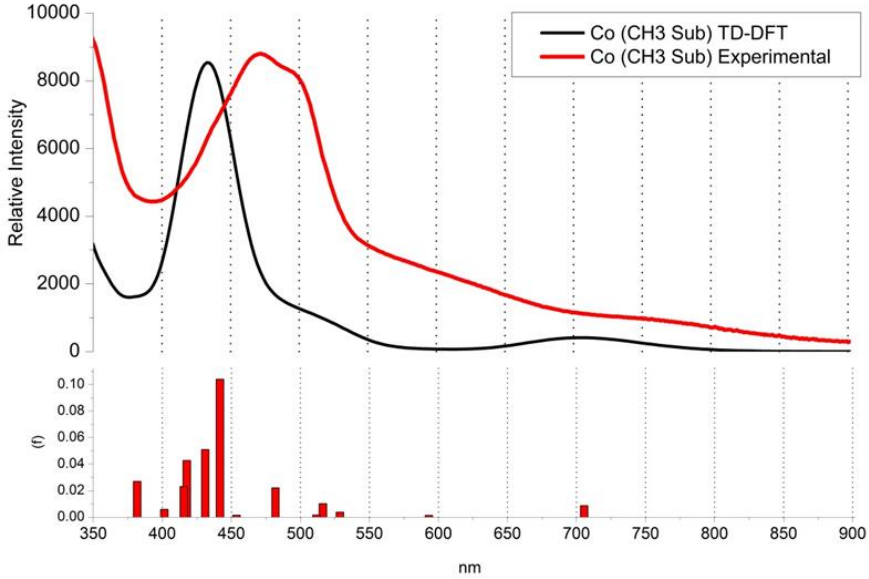


Table S1. TD-DFT calculated transitions and assignments for $[CoL–Cl]^0$ parent complex **(1)**

#	nm	cm-1 (/1000)	(f)	Assignment	Transition Type
1	682.8	14.6	0.0086	H-0->L+1(+33%) H-6->L+1(+14%) H-1->L+1(12%) H-10->L+1(+12%)	Amino-Phenol --> Cobalt (LMCT)
2	584.9	17.1	0.0038	H-6->L+2(+28%) H-1->L+2(26%) H-22->L+2(7%) H-12->L+2(7%)	phenol/cobalt --> Cobalt
3	512.1	19.5	0.0082	H-0->L+2(+21%) H-10->L+2(+8%) H-0->L+0(8%) H-11->L+1(+6%)	Amino-Phenol --> Cobalt (LMCT)
4	506.9	19.7	0.0035	H-0->L+2(+33%) H-0->L+0(16%) H-11->L+2(+8%) H-9->L+2(+7%)	Amino-Phenol --> Cobalt (LMCT)
5	487.2	20.5	0.0157	H-0->L+0(+73%) H-0->L+2(+15%)	Amino-Phenol --> Phenylene Imine (LLCT)
6	471.5	21.2	0.0136	H-1->L+1(+34%) H-0->L+1(+21%) H-1->L+0(+9%) H-0->L+2(8%)	Imino-Phenol --> Cobalt (LMCT)
7	436.6	22.9	0.0991	H-1->L+0(+69%) H-2->L+0(16%)	Imino-Phenol --> Phenylene Imine (LLCT)
8	432.9	23.1	0.0377	H-2->L+0(+79%) H-1->L+0(+15%)	Amino-Phenol --> Phenylene Imine (LLCT)
9	414	24.2	0.027	H-2->L+1(+28%) H-1->L+2(19%) H-10->L+1(+11%) H-0->L+1(10%)	Amino-Phenol --> Cobalt (LMCT)
10	410.8	24.3	0.0338	H-2->L+1(+40%) H-2->L+2(19%) H-1->L+2(+16%)	Amino-Phenol --> Cobalt (LMCT)
11	406.1	24.6	0.0123	H-2->L+2(+63%) H-2->L+1(+18%)	Amino-Phenol --> Cobalt (LMCT)

12	393.9	25.4	0.028	H-1->L+2(+17%) H-10->L+1(+15%) H-0->L+1(12%) H-10->L+2(10%)	Imino-Phenol --> Cobalt (LMCT)
13	375.3	26.6	0.0388	H-6->L+1(+38%) H-1->L+1(+24%)	phenol/cobalt --> Cobalt
				(B3PW91/6-311+g(d,p) (acetonitrile))	

Table S2. TD-DFT calculated transitions and assignments for $[CoL-CH_3]^0$ parent complex **(4)**

-CH3 Sub Parent Compound

#	nm	cm-1 (/1000)	(f)	Assignment	Transition Type
1	705.5	14.2	0.0087	H-0->L+1(+36%) H-10->L+1(11%) H-4->L+1(+8%) H-6->L+1(+7%)	Amino-Phenol --> Cobalt (LMCT)
2	593	16.9	0.0013	H-6->L+2(+25%) H-12->L+2(16%) H-2->L+2(13%) H-1->L+2(+12%)	phenol/cobalt --> Cobalt
3	528.6	18.9	0.0037	H-0->L+0(+67%) H-0->L+2(18%) H-10->L+2(+7%)	Amino-Phenol --> Phenylene Imine (LLCT)
4	516.3	19.4	0.0103	H-0->L+2(+34%) H-0->L+0(+29%) H-10->L+2(11%)	Amino-Phenol --> Cobalt (LMCT)
5	511.6	19.5	0.0017	H-11->L+1(+17%) H-7->L+1(14%) H-13->L+1(+14%) H-0->L+2(+13%)	phenol/cobalt --> Cobalt
6	481.9	20.8	0.0222	H-1->L+1(+28%) H-2->L+1(25%) H-0->L+1(24%) H-6->L+1(+8%)	Imino-Phenol --> Cobalt (LMCT)
7	453.7	22	0.0015	H-1->L+0(+48%)	Imino-Phenol --> Phenylene Imine (LLCT)
8	441.7	22.6	0.1041	H-2->L+0(+47%) H-1->L+0(35%) H-2->L+1(10%)	Phenol --> Phenylene Imine (LMCT)
9	431	23.2	0.0511	H-1->L+1(+39%) H-2->L+1(+29%) H-1->L+0(12%) H-2->L+2(8%)	Imino-Phenol --> Cobalt (LMCT)
10	417.7	23.9	0.0428	H-1->L+2(+22%) H-10->L+1(19%) H-0->L+1(17%) H-0->L+2(8%)	Imino-Phenol --> Cobalt (LMCT)
11	415.5	24.1	0.0231	H-1->L+2(+37%) H-2->L+2(+37%) H-1-	Imino-Phenol --> Cobalt

				>L+1(+10%) H-2->L+1(+5%)	(LMCT)
12	401.4	24.9	0.006	H-2->L+2(+25%) H-10->L+1(17%) H-1->L+2(12%) H-10->L+2(+8%)	Amino-Phenol --> Cobalt (LMCT)
13	381.7	26.2	0.027	H-6->L+1(+41%) H-2->L+1(+21%) H-1->L+1(11%) H-4->L+1(+7%)	phenol/cobalt --> Cobalt
(B3PW91/6-311+g(d,p) (acetonitrile))					

Figure S11. Cyclic voltammograms for **2** in acetonitrile. Conditions: 0.1 M $TBAPF_6$ as supporting electrolyte; scan rate: 100 mVs^{-1}; Glassy carbon (working), platinum wire (counter) and Ag/AgCl (reference) in the three electrode cell

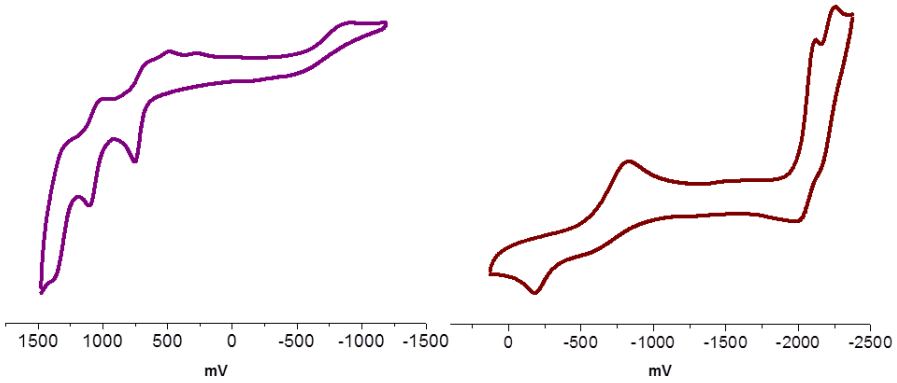


Figure S12. Cyclic voltammogram for **3** in *N*,*N*'-dimethylformamide. Conditions: 0.1 M $TBAPF_6$ as supporting electrolyte; scan rate: 100 mVs^{-1}; Glassy carbon (working), platinum wire (counter) and Ag/AgCl (reference) in the three electrode cell

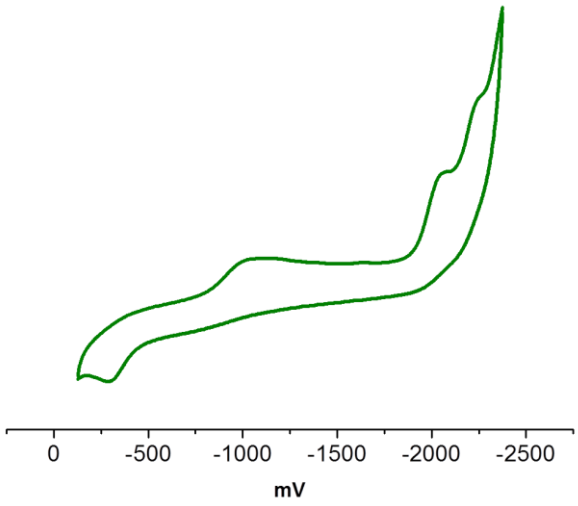


Figure S13. Cyclic voltammetry of **1** and **4** in DCM and ACN. Conditions: [C] = 1×10^{-4} M; 0.1 M $TBAPF_6$ as supporting electrolyte); Glassy carbon (working), Pt wire (counter) and Ag/AgCl (reference); Scan rate: 100 mVs^{-1}

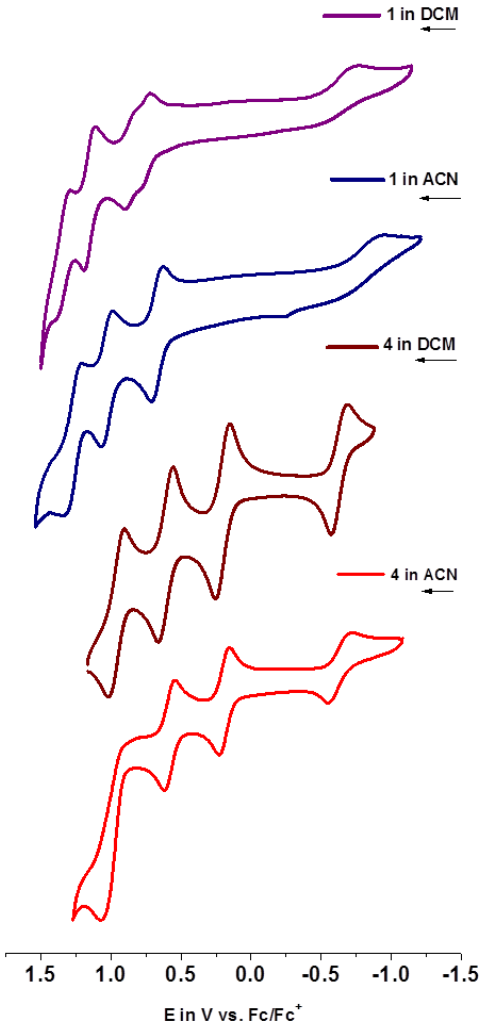


Table S3: Cyclic voltammetry parameters in dichloromethane

	3^{rd} $PhO^-/PhO^\bullet$ $E_{½}$, V (ΔE, V) $\lvert i_{pc}/i_{pa}\rvert$	2^{nd} $PhO^-/PhO^\bullet$ $E_{½}$, V (ΔE, V) $\lvert i_{pc}/i_{pa}\rvert$	1^{st} $PhO^-/PhO^\bullet$ $E_{½}$, V (ΔE, V) $\lvert i_{pc}/i_{pa}\rvert$	Co(III)/Co(II) $E_{½}$, [E_{pc}; E_{pa}], V (ΔE, V) $\lvert i_{pc}/i_{pa}\rvert$	$C{=}N/C^\bullet\text{-}N^-$ $E_{½}$, V (ΔE, V) $\lvert i_{pc}/i_{pa}\rvert$
1	+1.34 (0.10) |0.85|	+1.16 (0.08) |0.81|	+0.75 (0.06) |0.87| +0.87 (0.07) |0.87|	-0.66 [-0.69; -0.64] (0.05) |1.16|	-2.12 (0.04) |1.03|
2	--	--	--	--	--
3	--	--	--	--	--
4	+0.96 (0.11) |1.04|	+0.61 (0.10) |1.08|	+0.21 (0.10) |1.10|	-0.63 [-0.68; -0.57] (0.11) |0.95|	-2.69 (0.03) |1.00|

TableS4. Calculated redox potentials

Phenolato -X	Redox St.	E(SCF)	Thermal	G(sol)	del-G(sol)	Eo(DFT) (ACN)*	Eo(exp) (ACN)	Eo(err)
		Eh	Eh	Eh	eV		vs Fc/Fc+	
Cl-	$[1]^{0}$	-5632.467057	0.346859	-5632.120198	0.000			
	$[1]^{+}$	-5632.259251	0.350422	-5631.908829	-5.752	**0.58**	0.73	0.148
	$[1]^{+2}$	-5632.034370	0.351513	-5631.682857	-6.149	**0.98**	1.09	0.111
	$[1]^{+3}$	-5631.801726	0.352348	-5631.449378	-6.353	**1.18**	1.33	0.147
	$[1]^{-1}$	-5632.629647	0.341108	-5632.288539	-4.581	**-0.59**	-0.78	-0.191
	$[1]^{-2}$	-5632.734023	0.334253	-5632.399770	-3.027	**-2.14**	-2.03	0.113
CH3-	$[4]^{0}$	-3110.926434	0.567177	-3110.359257	0.000			
	$[4]^{+}$	-3110.740331	0.572256	-3110.168075	-5.202	**0.03**	0.19	0.158
	$[4]^{+2}$	-3110.536371	0.573595	-3109.962776	-5.586	**0.42**	0.58	0.164
	$[4]^{+3}$	-3110.318886	0.574495	-3109.744391	-5.943	**0.77**	0.99	0.217
	$[4]^{-1}$	-3111.082231	0.559572	-3110.522659	-4.446	**-0.72**	-0.64	0.084
	$[4]^{-2}$	-3111.166799	0.555438	-3110.611361	-2.414	**-2.76**	-2.55	0.206
CH3- Pyridine	$[5]^{0}$	-3282.778940	0.632068	-3282.146872	0.000			
	$[5]^{+}$	-3282.594460	0.631609	-3281.962851	-5.007	**-0.16**	0.27	0.433
	$[5]^{+2}$	-3282.394376	0.631961	-3281.762415	-5.454	**0.28**	0.65	0.366
	$[5]^{+3}$	-3282.179682	0.632472	-3281.547210	-5.856	**0.69**	1.01	0.324
	$[5]^{-1}$	-3282.918908	0.621929	-3282.296979	-4.085	**-1.09**	NA	NA
	$[5]^{-2}$	-3282.996307	0.614937	-3282.381370	-2.296	**-2.87**	-2.57	0.304

(b3pw91/6-311+g(d,p) (solvent=acetonitrile))

* Calculated Vs. Fc/Fc^{+} (J. Phys. Chem. A 2010, 114, 12299–12304)

Figure S14. Calculated and experimental correlation between redox potentials

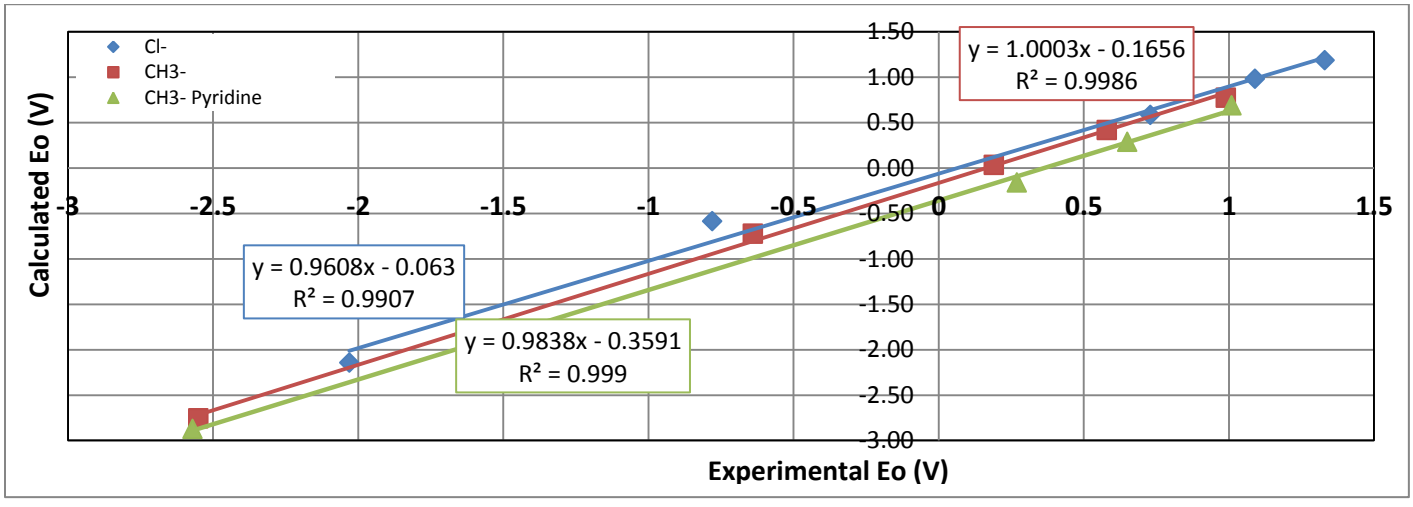


Figure S15. Redox sequence for **4**

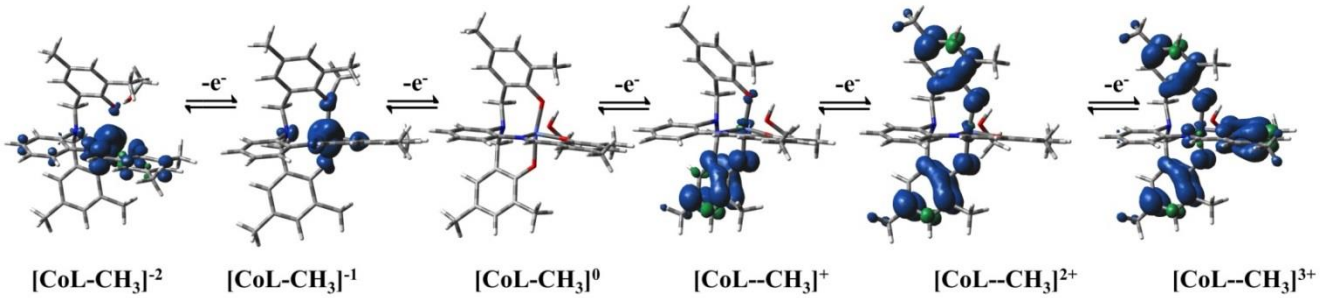


Figure S16. Spectral changes upon electrochemical reduction of complexes **1**, **2** and **4** in acetonitrile and **3** in *N*,*N*'-dimethylformamide. The applied potential was –2.40 V *vs*. Fc^+/Fc over a period of 10 minutes and after 10 minutes (inset – for **1** - **3**). $TBAPF_6$ (0.1 M) was used as supporting electrolyte

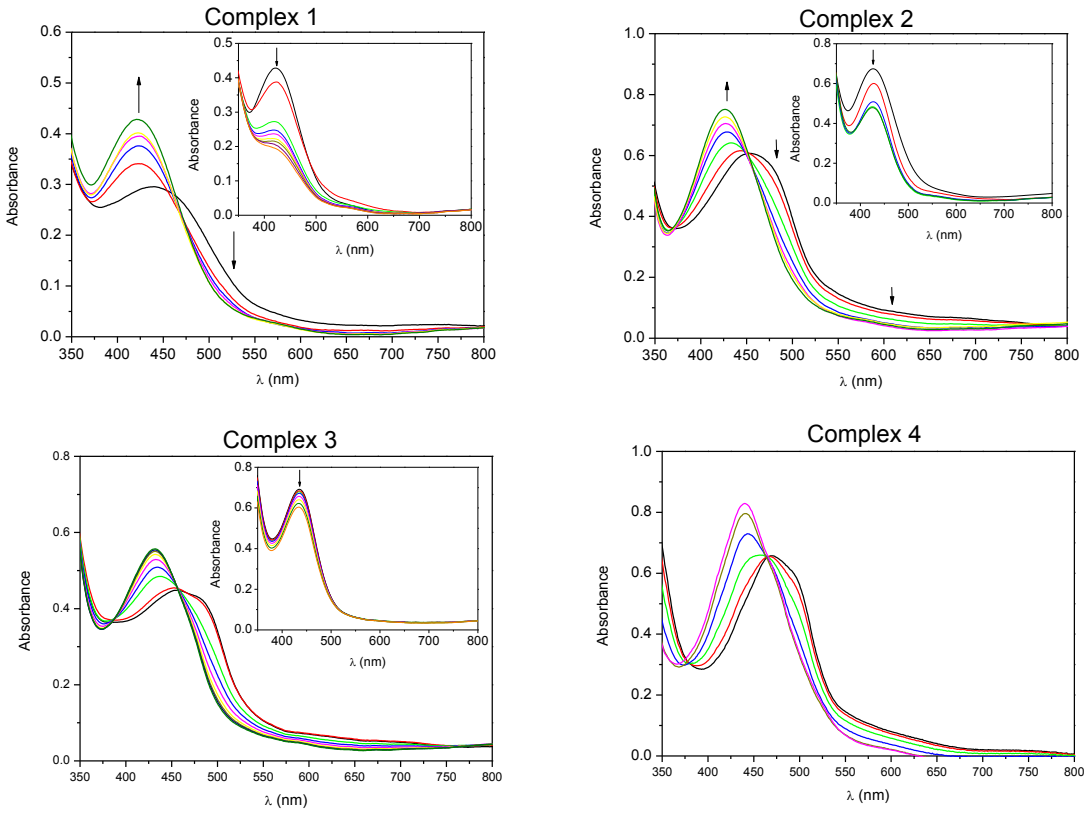


Figure S17. Spectral changes upon electrochemical oxidation of **1**, **2** and **4** in acetonitrile and **3** in *N*, *N'*-dimethylformamide. The applied potential was 0.85 V for **1-3** and 0.30 V for **4** *vs*. Fc^{+}/Fc over a period of 10 minutes. $TBAPF_6$ (0.1 M) was used as supporting electrolyte

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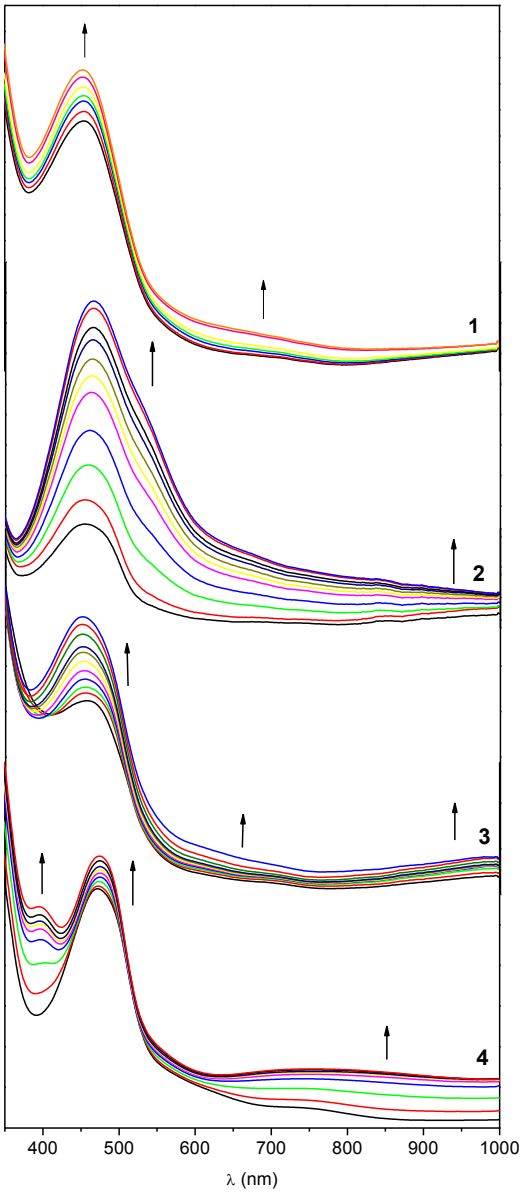

Figure S18. Computed electronic spectra for **1** in the parent state after 1st reduction (top) and after 1st oxidation (bottom)

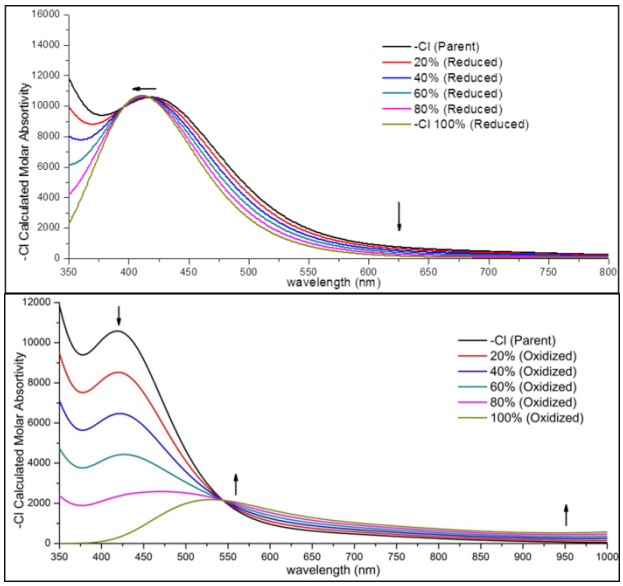

Figure S19. TD-DFT for spectroelectrochemical changes

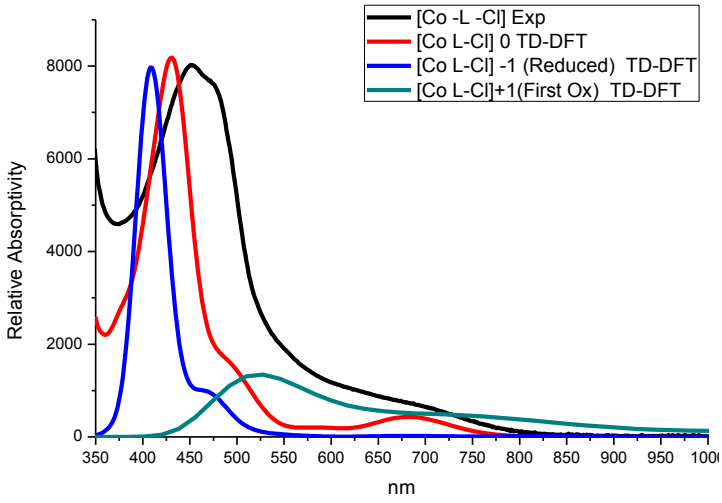

Figure S20: Time-tracked UV-Visible spectral change in acetonitrile/water (90:10 % v/v) for the complexes **1 – 4**. Conditions: $[C]_{final}$ = 1.80 × 10^{-4} M, [AA] = 2.00 × 10^{-2} M and pH ~ 3.0

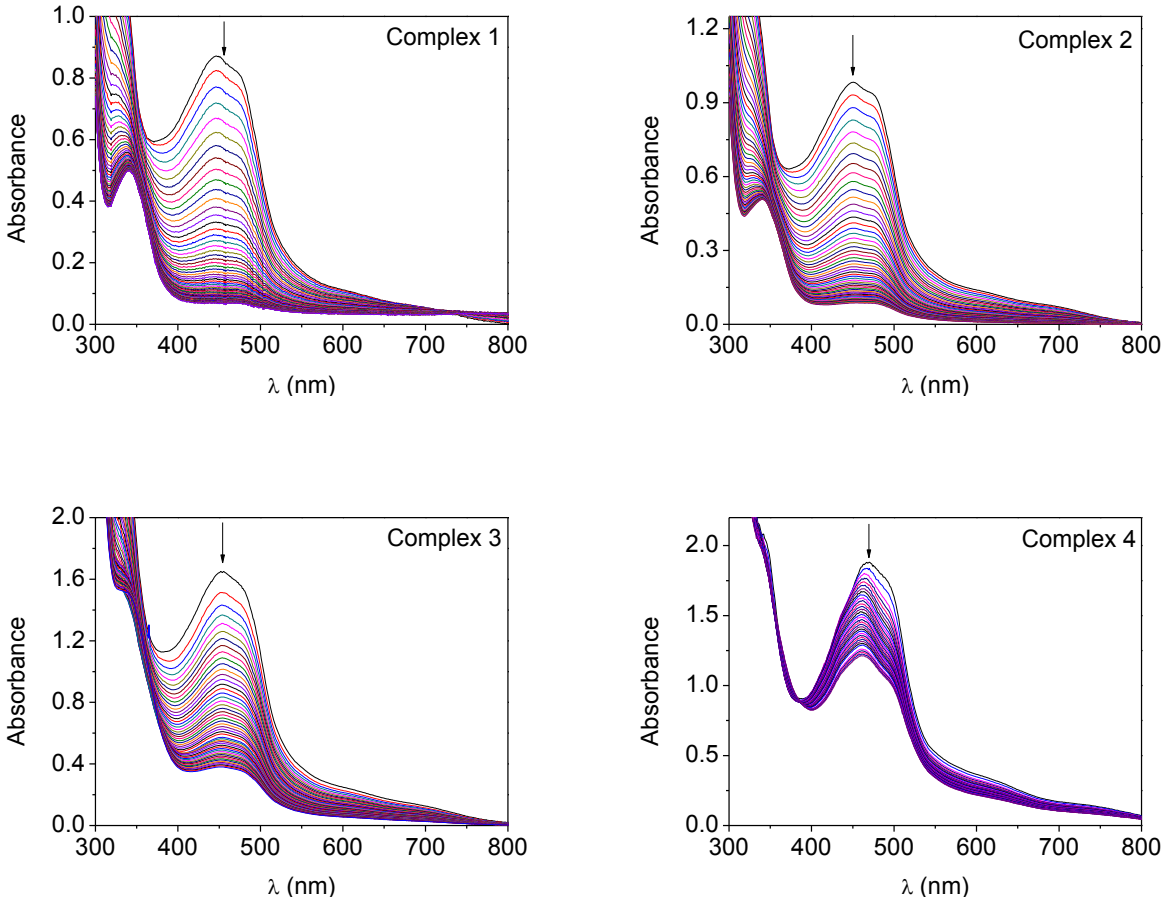

Figure S21. Chemical reduction tests for the complexes **1 – 4** towards the reductant (ascorbic acid). [Complex] (M) *versus* time (s) plot fitted as a first order exponential decaying equation

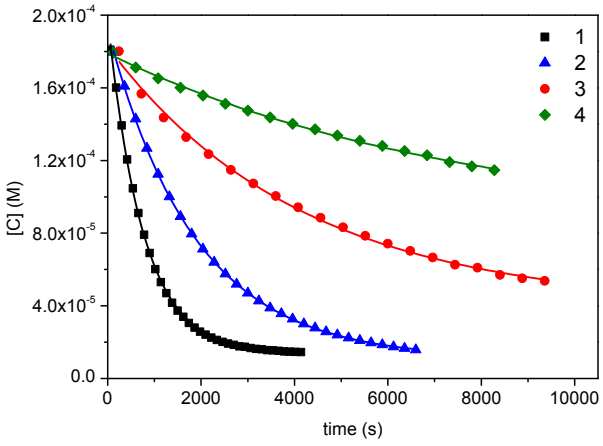

Figure S22. Electrocatalytic activity of **4** towards proton reduction in presence of acetic acid (HOAc)

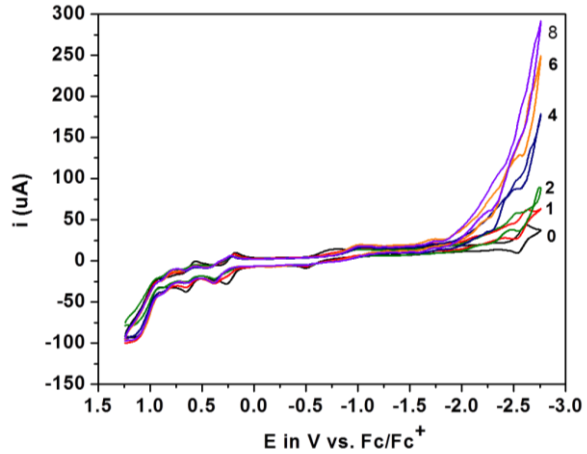

Figure S23. Cyclic voltammogram for blank in the presence of HOAc

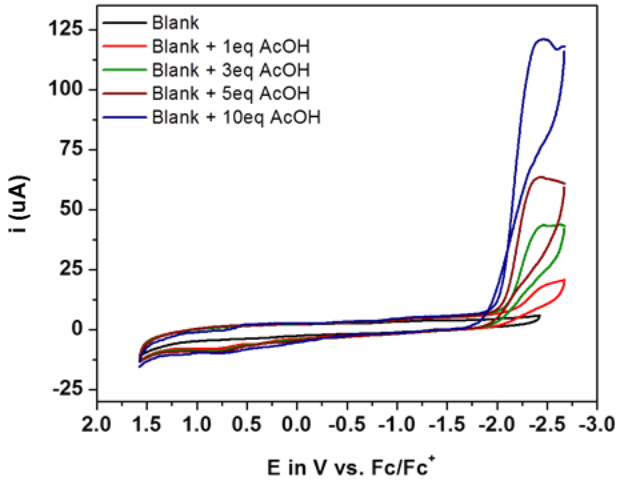

Figure S24. UV-Visible spectra of the solution before and after bulk-electrolysis at -1.8 V *versus* Ag/AgCl in the presence of HOAc

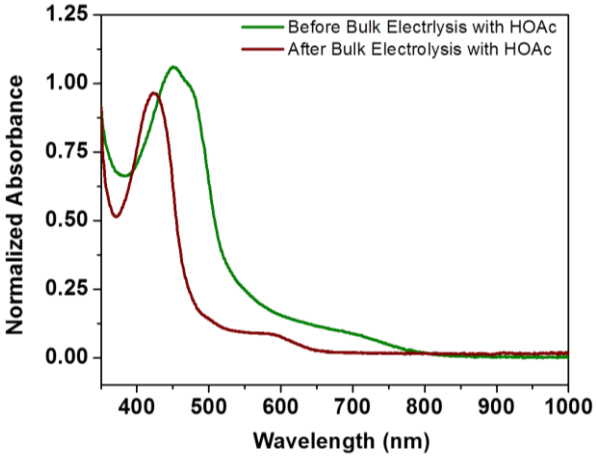

Table S5. Cartesian coordinates for DFT calculations

[CoL –Cl]^{0}

H	-1.89542700	2.17885300	4.42383300
H	-0.32766400	0.49487400	3.60660900
H	2.78275000	-1.95529100	3.05646700
C	-1.78396900	2.03313300	3.35516000
C	-0.89014200	1.08075500	2.89073500
H	-3.23723600	3.53638100	2.83275600
H	1.07907200	-0.52201700	2.66246800
C	2.81848000	-2.26688200	2.01871600
C	-2.53930800	2.79359200	2.46393800
C	3.70804100	-3.22704300	1.61107000
C	1.02191800	-0.70431900	1.59190800
C	-0.73955500	0.88392400	1.51319600
H	-5.15462300	-3.08823900	1.01021400
C	1.93572200	-1.67315100	1.08836800
H	3.81371100	4.46267300	0.44847200
C	-2.40507400	2.59035300	1.09702200
N	0.14530400	-0.03522700	0.90821900
C	3.75062000	-3.63601600	0.27017100
C	-4.64976900	-2.26045700	0.52786000
H	4.45255000	-4.39712100	-0.04822800
C	-5.31708200	-1.07111600	0.26547700
C	2.86952800	4.08930700	0.07203900
C	1.75272600	4.91186700	0.00457700
C	-1.51269800	1.63373800	0.62903400
H	-3.00021300	3.17568200	0.40577000
C	-3.31467000	-2.37093800	0.17109500
C	2.75631400	2.76988700	-0.34187800
C	1.95239500	-2.05328600	-0.28933800
C	-4.66587400	-0.01120700	-0.34928200
C	0.54201300	4.43558600	-0.47994800
H	-0.32043800	5.09049300	-0.53297900
H	-5.19782700	0.91238500	-0.54883700
C	2.89579400	-3.06488100	-0.64306500
C	1.54898800	2.23930700	-0.84290100
C	-2.60709000	-1.32472800	-0.46524100
C	0.44639100	3.11647000	-0.90822000
C	-3.33132600	-0.13904300	-0.71930000
N	-1.33124200	1.36073200	-0.79612500
Co	-0.03267800	-0.13677200	-0.95636400
O	1.46673800	0.99770800	-1.26441800
O	1.18846300	-1.55825300	-1.19032700
O	-1.36032300	-1.48442900	-0.82650300
C	-0.81596800	2.58346100	-1.50747000
H	-1.59652600	3.34880600	-1.49294600
C	-2.63366600	0.97097800	-1.44050600
H	-3.28104000	1.85102600	-1.48540800
H	-0.66175200	2.28161900	-2.54670300
H	-2.38428200	0.69175600	-2.46681400
O	-0.15794800	-0.10612700	-2.95095400
H	0.72273400	0.23778000	-3.16385700
H	0.30885100	-2.07049400	-3.48075100
C	-0.41730600	-1.29597500	-3.72595200
H	-1.41823000	-1.62953900	-3.46544300
H	-0.36992100	-1.03506500	-4.78445000
Cl	4.16153900	1.73840400	-0.26232200
Cl	1.87901500	6.57376500	0.54299000
Cl	2.95515600	-3.58079600	-2.30476100
Cl	4.80595500	-3.96281500	2.75576100
Cl	-2.47703200	-3.86755700	0.50097200
Cl	-6.99984800	-0.90931500	0.72742000

[CoL –Cl]$^{+1}$

H	-1.74507700	2.31677500	4.46936800
H	-0.25795600	0.55338300	3.64463700
H	3.03883300	-1.75825700	2.96261100
C	-1.64768400	2.16193000	3.39983600
C	-0.79734000	1.16805500	2.93323300
H	-3.04447200	3.72238300	2.88226900
H	1.26223100	-0.34975700	2.64687400
C	2.94792500	-2.15727500	1.95777400
C	-2.38114000	2.94905100	2.51014900
C	3.77364400	-3.16998700	1.53195000
C	1.11357400	-0.61358200	1.60177300
C	-0.66716100	0.96251700	1.55369400
H	-5.49939400	-2.75626200	1.04979100
C	1.96821800	-1.62744800	1.08566200
H	4.18711500	4.04356900	0.21060200
C	-2.27652700	2.73084300	1.14010100
N	0.18059100	0.01307200	0.94369800
C	3.64881600	-3.69478100	0.23456900
C	-4.90446800	-1.98148200	0.58174000
H	4.29934900	-4.49660900	-0.09623800
C	-5.48301100	-0.75154300	0.23350100
C	3.19192200	3.75474900	-0.10678700
C	2.15254400	4.68154000	-0.12682100
C	-1.43022900	1.73107300	0.67087800
H	-2.86058100	3.33443000	0.45332400
C	-3.56793900	-2.18162400	0.32160400
C	2.93601700	2.44449100	-0.49220500
C	1.81975700	-2.12533100	-0.24596100
C	-4.73763300	0.27969400	-0.37605000
C	0.87497000	4.31898800	-0.54137000
H	0.07783200	5.05451600	-0.56585500
H	-5.23160000	1.20907700	-0.63772400
C	2.69595500	-3.18543700	-0.62233000
C	1.65261800	2.03166600	-0.91151800
C	-2.76302800	-1.14706700	-0.29608200
C	0.63534200	3.00893800	-0.94539300
C	-3.40302500	0.09577300	-0.64462900
N	-1.28183400	1.42264000	-0.75525400
Co	-0.10128100	-0.16889000	-0.89586600
O	1.43034400	0.79241900	-1.31611900
O	0.94529700	-1.69547400	-1.09217100
O	-1.53417500	-1.37254600	-0.53245300
C	-0.68805800	2.59091600	-1.49814500
H	-1.39777300	3.42249200	-1.46567000
C	-2.60853600	1.12658800	-1.38462300
H	-3.18879500	2.05051100	-1.45733900
H	-0.59594900	2.27006100	-2.54083100
H	-2.40073600	0.79360900	-2.40607600
O	-0.33295800	-0.22094700	-2.85354000

H	0.53841500	0.10878300	-3.13350700
H	0.06973900	-2.22274900	-3.30513300
C	-0.63551200	-1.43787400	-3.57751000
H	-1.64894700	-1.72750100	-3.30736800
H	-0.58779900	-1.21845000	-4.64503900
Cl	4.23947500	1.29204600	-0.47789400
Cl	2.46546600	6.32501700	0.37494200
Cl	2.55077700	-3.84449400	-2.22546100
Cl	4.98941700	-3.82876800	2.59743500
Cl	-2.81299300	-3.66472900	0.73326600
Cl	-7.14739300	-0.49365400	0.55904100

[CoL –Cl]$^{+2}$

H	-1.69642600	2.43630400	4.44813800
H	-0.21508700	0.65005300	3.65369400
H	3.14129200	-1.65399400	2.91506900
C	-1.60387900	2.25591100	3.38219500
C	-0.75748200	1.25211200	2.93337500
H	-2.99955500	3.80603000	2.83428600
H	1.33114400	-0.23964800	2.64441100
C	2.99257000	-2.06854300	1.92355300
C	-2.34048600	3.02215800	2.47581900
C	3.81291000	-3.12583400	1.48865200
C	1.14859300	-0.53180000	1.61330900
C	-0.64395700	1.01911400	1.55650900
H	-5.55910700	-2.67333600	1.09398300
C	2.00133500	-1.56776800	1.09731000
H	4.26407900	3.90845800	0.16070600
C	-2.24962400	2.77616000	1.10772100
N	0.19717500	0.05633700	0.96005700
C	3.64632800	-3.71757400	0.22297100
C	-4.95118200	-1.91331200	0.61736000
H	4.28708400	-4.53556200	-0.08570200
C	-5.51369400	-0.68399600	0.24042500
C	3.26139200	3.64519500	-0.15694100
C	2.24981500	4.60240500	-0.19125600
C	-1.41081900	1.76473000	0.65616700
H	-2.83824000	3.36944100	0.41588200
C	-3.61412300	-2.13157700	0.37590400
C	2.96781400	2.33796000	-0.52662500
C	1.80353300	-2.13931700	-0.22225000
C	-4.74951800	0.33050600	-0.38142300
C	0.96089600	4.27392800	-0.60203300
H	0.18551900	5.03266500	-0.63254400
H	-5.23333300	1.25962900	-0.66371600
C	2.66304400	-3.24646500	-0.61468000
C	1.67483300	1.96677200	-0.94789600
C	-2.79489900	-1.11379700	-0.25292000
C	0.68456200	2.96750600	-0.99332900
C	-3.41591600	0.12869300	-0.63360200
N	-1.26841600	1.42424700	-0.76365000
Co	-0.13100500	-0.17479100	-0.87185200
O	1.41182700	0.72647100	-1.34033200
O	0.92056700	-1.73975300	-1.02677300
O	-1.56300400	-1.35417900	-0.46337700
C	-0.65157200	2.57168100	-1.53125300
H	-1.34734900	3.41468300	-1.50146200
C	-2.60409100	1.13750600	-1.38712100
H	-3.16434200	2.07270100	-1.47071900
H	-0.57930200	2.23259800	-2.56964700
H	-2.40050200	0.79194400	-2.40512600
O	-0.39170500	-0.28889900	-2.80773900
H	0.46857100	0.02694300	-3.14535100
H	-0.05296600	-2.29736300	-3.30668500
C	-0.76980500	-1.50158300	-3.50927800
H	-1.75955600	-1.77883300	-3.15269600
H	-0.80879500	-1.26970800	-4.57451200
Cl	4.22617700	1.13984500	-0.48722800
Cl	2.60994700	6.23921100	0.29137100
Cl	2.42808700	-3.93816800	-2.15825300
Cl	5.03230100	-3.71405700	2.52937000
Cl	-2.87490700	-3.60888300	0.82271100
Cl	-7.17385600	-0.40097600	0.54137800

[CoL –Cl]$^{+3}$

H	-1.57295700	2.32468600	4.62724000
H	-0.33456000	0.40202500	3.75938800
H	2.39026700	-2.55999700	3.04346000
C	-1.46203900	2.20528100	3.55465800
C	-0.75279500	1.11929100	3.06318100
H	-2.59210300	3.97923100	3.07597500
H	0.93770100	-0.79156600	2.77085800
C	2.33815900	-2.79357600	1.98540300
C	-2.03743800	3.13342600	2.68368800
C	3.05531000	-3.90249700	1.48901600
C	0.84242600	-0.91449500	1.69532300
C	-0.61099000	0.96396700	1.67786800
H	-5.72661200	-2.27176700	0.68695900
C	1.57502200	-2.01590900	1.13312800
H	4.78643000	3.70332600	0.19543600
C	-1.91609900	2.97401800	1.30576400
N	0.09951200	-0.07802100	1.04179000
C	3.00605000	-4.26317600	0.13121200
C	-5.04410000	-1.51551400	0.31714800
H	3.55997300	-5.12356100	-0.22621600
C	-5.48209500	-0.19757800	0.11737600
C	3.75655200	3.49598400	-0.07124300
C	2.80727500	4.52908500	-0.10641700
C	-1.20703800	1.88575400	0.81252000
H	-2.37995300	3.69522800	0.64107800
C	-3.73200900	-1.82801700	0.04198800
C	3.35416100	2.21484800	-0.37421700
C	1.50962000	-2.34541700	-0.27599600
C	-4.61727900	0.81574000	-0.37182200
C	1.45244400	4.29404800	-0.46217100
H	0.76521000	5.13202200	-0.50860400
H	-5.01185800	1.81312700	-0.53340300
C	2.24906800	-3.51138400	-0.73782500
C	1.96936500	1.93557900	-0.70460700
C	-2.81403700	-0.80951300	-0.43439000
C	1.03670100	3.02566800	-0.76754800
C	-3.30949800	0.52176500	-0.65288200
N	-1.05646400	1.63048200	-0.62681100
Co	-0.07774000	-0.05657600	-0.83242800
O	1.62325500	0.73019400	-0.94457900
O	0.84633400	-1.67833100	-1.11617900

O	-1.60107600	-1.13409100	-0.65678700
C	-0.33193400	2.75762000	-1.30982400
H	-0.94175600	3.66045900	-1.23171300
C	-2.40166200	1.52444100	-1.29352800
H	-2.87510600	2.50920700	-1.28481300
H	-0.27553100	2.49377900	-2.37098600
H	-2.21508200	1.26844200	-2.34090600
O	-0.19933400	0.05324300	-2.77614600
H	0.69782000	0.22154000	-3.11777300
H	-0.26296200	-1.95213400	-3.39407800
C	-0.78173200	-1.01279000	-3.58373700
H	-1.83071700	-1.08840700	-3.30882900
H	-0.68939900	-0.71402900	-4.62831400
Cl	4.45826700	0.91486400	-0.33824200
Cl	3.28838000	6.11821800	0.27521700
Cl	2.16308100	-3.91238100	-2.39206000
Cl	3.99621000	-4.82786900	2.56706400
Cl	-3.13933700	-3.41146200	0.27399500
Cl	-7.10148700	0.20514300	0.46655900

[CoL –Cl]$^{-1}$

H	-1.96089100	2.15667400	4.50544400
H	-0.43407600	0.44178500	3.65342100
H	2.85084600	-1.57698700	3.22508900
C	-1.84127300	2.03499500	3.43237300
C	-0.96590800	1.07127000	2.94693100
H	-3.25604700	3.58571500	2.92489200
H	1.19520000	-0.25410500	2.71587200
C	2.89280400	-2.02196600	2.23467400
C	-2.57139100	2.83077400	2.54911900
C	3.82435300	-2.99543000	1.96028100
C	1.04206900	-0.58423800	1.68478200
C	-0.79150900	0.89051300	1.56469200
H	-5.40067600	-3.03919700	0.86138000
C	1.97264300	-1.58969400	1.25029600
H	3.94060200	4.35956300	0.16619100
C	-2.43348500	2.63568000	1.17797400
N	0.08355100	-0.05122000	0.98554900
C	3.88412600	-3.58272900	0.68689500
C	-4.86390000	-2.20215200	0.42752300
H	4.61708500	-4.35221300	0.46848400
C	-5.42789600	-0.93056200	0.39352900
C	2.96235000	4.00482400	-0.14046700
C	1.83722500	4.81397700	-0.01910300
C	-1.56254300	1.66746600	0.67843700
H	-3.01780000	3.24065300	0.49015800
C	-3.59368800	-2.38312500	-0.10488400
C	2.81205600	2.72575500	-0.66301300
C	1.99917800	-2.15494100	-0.08101900
C	-4.73407200	0.13841400	-0.16604400
C	0.58623700	4.35594500	-0.42134900
H	-0.28296200	5.00192000	-0.33410000
H	-5.18832400	1.12512300	-0.19309800
C	3.00037000	-3.16777900	-0.28453500
C	1.56103700	2.19619300	-1.07551900
C	-2.83073500	-1.33186000	-0.68398000
C	0.44792100	3.07441000	-0.94798200
C	-3.46382100	-0.05446600	-0.70197200
N	-1.43344800	1.42205200	-0.74491500
Co	-0.08983900	-0.30484800	-1.02095400
O	1.43366100	0.99613100	-1.56349300
O	1.22314900	-1.82083700	-1.03764700
O	-1.65791800	-1.52593900	-1.19935600
C	-0.87819300	2.60200400	-1.46762100
H	-1.60254300	3.42925500	-1.43976000
C	-2.74173100	1.07542100	-1.37539600
H	-3.39124000	1.96231500	-1.40822700
H	-0.77966400	2.28951900	-2.51426500
H	-2.50402700	0.80681700	-2.41175900
O	0.00296300	-0.17605700	-3.33920500
H	0.79391900	0.37208200	-3.15517500
H	1.13896000	-1.88855700	-3.71243300
C	0.35745900	-1.27466600	-4.17198000
H	-0.53997800	-1.88382600	-4.30082500
H	0.69170500	-0.92886000	-5.15849100
Cl	4.23825100	1.72009100	-0.82385100
Cl	2.00524600	6.43248300	0.64306600
Cl	3.09159900	-3.90532900	-1.86693000
Cl	4.95060500	-3.52277700	3.19638900
Cl	-2.89343500	-3.99057100	-0.06535000
Cl	-7.03274200	-0.67879200	1.06492800

[CoL –Cl]$^{-2}$

H	-1.80416000	-1.79163800	-4.93990500
C	-1.68879100	-1.80001100	-3.85760100
C	-0.92782100	-0.80702800	-3.25333900
C	-2.30863700	-2.79388800	-3.09830800
H	-0.48669900	-0.03939700	-3.88082300
C	-0.74459400	-0.76404900	-1.84501000
H	-2.90271000	-3.57184500	-3.56969600
C	-2.15706400	-2.75979600	-1.70881600
N	0.00113200	0.16838600	-1.16232600
C	-1.40440300	-1.77137200	-1.08536900
H	-2.64268700	-3.52269400	-1.10346000
C	0.75845200	1.07747600	-1.82606500
N	-1.26261900	-1.73381800	0.36342700
H	0.83183500	0.98986200	-2.91066400
C	1.51865000	2.13937000	-1.27603000
C	2.24429900	2.95307700	-2.19696100
C	1.60421300	2.45789400	0.14670000
H	2.18610100	2.71824600	-3.25681500
C	3.00548500	4.02487200	-1.77432700
C	2.40091400	3.57454600	0.48303400
O	0.99317700	1.77938900	1.07072500
C	3.10640700	4.36967000	-0.42775600
Cl	3.87788600	4.99393100	-2.96791000
Cl	2.52720400	4.00414900	2.18928600
H	3.70226600	5.21078700	-0.09375200
C	-0.56315400	-2.94160900	0.87527400
C	0.86280300	-3.05362500	0.42558600
H	-1.11861900	-3.84939900	0.59650900
H	-0.58175100	-2.86658900	1.96948100
C	1.29715600	-4.11371300	-0.36374400
C	1.76480900	-2.06620600	0.90635700
C	2.64733900	-4.23384200	-0.68353600
H	0.58390200	-4.85177500	-0.71997200

C	3.12729100	-2.25131500	0.56762100
O	1.34986500	-1.06407300	1.64070400
C	3.57527000	-3.30881300	-0.21769900
Cl	3.19281500	-5.57361900	-1.68183600
Cl	4.30309400	-1.09691000	1.16292900
H	4.62850300	-3.40392600	-0.45939300
C	-2.57859500	-1.66110800	1.05322800
C	-3.40267400	-0.46700500	0.67860800
H	-3.15496900	-2.58178100	0.87758500
H	-2.35289200	-1.62044100	2.12637800
C	-4.65295300	-0.61396800	0.08615900
C	-2.88500000	0.81393600	1.02917500
C	-5.44321600	0.50469300	-0.16409900
H	-5.01651600	-1.60549100	-0.16971700
C	-3.74534000	1.91358700	0.76161900
O	-1.72450600	0.95305200	1.59311900
C	-4.99805000	1.77828900	0.17477500
Cl	-7.02363500	0.31246800	-0.91178000
Cl	-3.19931000	3.52450600	1.19249300
H	-5.61144900	2.65289000	-0.01471300
H	0.69066300	-1.44474300	3.21586100
O	0.24445000	-1.64239300	4.07248600
C	1.21919300	-2.13975300	4.96392900
H	2.01807600	-1.40973600	5.16728500
H	0.72257800	-2.36631400	5.91351300
H	1.69120100	-3.06635700	4.60126100
Co	-0.06574100	0.14858400	0.82490900

[CoL –CH_3]^0

H	-2.06340000	1.81687800	4.48678500
H	-0.26507100	0.38093700	3.67482700
H	3.01352000	-1.80419400	3.16775200
C	-1.93472500	1.68236500	3.41825500
C	-0.91093100	0.86930200	2.95594600
H	-3.59642000	2.95131700	2.89189900
H	1.19417300	-0.54866400	2.74848100
C	3.14575000	-2.06655000	2.12103700
C	-2.79615200	2.31830900	2.52551200
C	4.17748600	-2.89151700	1.74715000
C	1.19466000	-0.69885800	1.67067400
C	-0.73341900	0.68482900	1.57846700
H	-4.46585600	-3.95151600	0.94537100
C	2.22811400	-1.53275600	1.17620800
H	3.20399600	4.96514300	0.46636600
C	-2.63000600	2.13200400	1.15932300
N	0.26547800	-0.10628900	0.97685200
C	4.29398500	-3.19675300	0.36877900
C	-4.09236800	-3.03686600	0.48801100
H	5.10530200	-3.84876800	0.05072300
C	-4.98115200	-1.97494700	0.27382300
C	2.32410200	4.44021600	0.09877700
C	1.10320400	5.12434300	0.04115300
C	-1.60601300	1.31686100	0.69272800
H	-3.30274900	2.62002300	0.46332300
C	-2.74431300	-2.97295500	0.15180300
C	2.46375500	3.10979600	-0.28702400
C	2.36007700	-1.84988400	-0.20973400
C	-4.46636000	-0.82124300	-0.31113000
C	-0.00236600	4.42513200	-0.43787100
H	-0.96660500	4.92432800	-0.50359500
H	-5.12445300	0.02545600	-0.49511900
C	3.43627700	-2.71333100	-0.59566200
C	1.32818100	2.41728600	-0.77156300
C	-2.23772900	-1.79062800	-0.44855400
C	0.10117100	3.09623400	-0.84951200
C	-3.12376200	-0.72347900	-0.68065500
N	-1.38237100	1.07834200	-0.73023000
Co	0.13618800	-0.20287200	-0.89003200
O	1.44517100	1.16038100	-1.18376900
O	1.57187900	-1.40983600	-1.13023800
O	-0.96691100	-1.74412700	-0.80792100
C	-1.06325100	2.36800000	-1.43839200
H	-1.95525600	3.00181400	-1.42048000
C	-2.60740600	0.49439800	-1.37745100
H	-3.38343300	1.26563000	-1.41068100
H	-0.87457300	2.08844700	-2.47866900
H	-2.31330200	0.27782100	-2.40781300
O	0.04122700	-0.14354400	-2.89673600
H	0.87319500	0.33602100	-3.03583500
H	0.82073700	-2.00267000	-3.42641900
C	0.00558400	-1.33441900	-3.70314300
H	-0.94852500	-1.81788700	-3.50786600
H	0.07402900	-1.04901800	-4.75477700
C	3.78931100	2.40798400	-0.22004000
H	3.72002800	1.48540500	0.36395600
H	4.13841000	2.11744400	-1.21687600
H	4.54921200	3.04966400	0.23196600
C	0.99329600	6.55567800	0.49717700
H	1.10260800	6.64105100	1.58437100
H	1.77044500	7.18165500	0.04731500
H	0.02339500	6.98206800	0.22965600
C	3.59646900	-3.06300000	-2.04501100
H	2.70947400	-3.57757100	-2.42830200
H	3.72528200	-2.16475100	-2.65735600
H	4.46213600	-3.71124300	-2.19571100
C	5.15545700	-3.46027200	2.73833500
H	5.13913700	-4.55536200	2.73223800
H	6.18134200	-3.15373000	2.50781600
H	4.92704400	-3.12779100	3.75343000
C	-1.82058400	-4.13141000	0.39423800
H	-1.41667800	-4.52558800	-0.54464700
H	-0.95857700	-3.83252900	0.99890500
H	-2.33956500	-4.94390800	0.90840200
C	-6.43020800	-2.08211300	0.67061500
H	-6.92296200	-2.92517900	0.17429200
H	-6.54321200	-2.23620500	1.74950300
H	-6.97940000	-1.17488100	0.40696100

[CoL –CH_3]$^{+1}$

H	-1.74711900	2.19347400	4.48653100
H	-0.13074800	0.53829500	3.68176700
H	3.26115000	-1.60723500	3.03648100
C	-1.65117100	2.02102700	3.41867400
C	-0.72781500	1.08832200	2.96260700
H	-3.18049000	3.44788600	2.88425000
H	1.41947300	-0.30731400	2.69323200

C	3.20713500	-2.03713400	2.03793800
C	-2.45855100	2.72290800	2.52165200
C	4.10294800	-3.00954900	1.65786900
C	1.28470900	-0.60186400	1.65348000
C	-0.59615700	0.85625300	1.58618600
H	-5.15668800	-3.23165400	1.10696600
C	2.19318700	-1.56869500	1.15786700
H	4.00691100	4.21454600	0.16397400
C	-2.34773000	2.48067500	1.15568700
N	0.30779000	-0.04395000	0.98875800
C	3.97129200	-3.53678900	0.34833600
C	-4.61845900	-2.41549500	0.63180100
H	4.67058700	-4.30955500	0.03047500
C	-5.32636300	-1.24739300	0.28488800
C	3.02650100	3.85348900	-0.14513900
C	1.94689100	4.75051800	-0.15178800
C	-1.42676000	1.54405100	0.69641700
H	-2.98446900	3.01927800	0.46064200
C	-3.26578500	-2.55308900	0.39388700
C	2.90143600	2.51454000	-0.50882900
C	2.08433300	-2.10446500	-0.16181900
C	-4.62771100	-0.17907600	-0.33203500
C	0.70421300	4.26585500	-0.55995900
H	-0.15363300	4.93573600	-0.58955400
H	-5.17807100	0.71663900	-0.60970300
C	3.00705700	-3.12435200	-0.55119400
C	1.62887000	2.04345100	-0.91178800
C	-2.56325100	-1.45144600	-0.23109300
C	0.54327400	2.93566300	-0.95168500
C	-3.28248800	-0.25904100	-0.59773700
N	-1.26331300	1.22408400	-0.72332700
Co	0.03207900	-0.28319600	-0.84307600
O	1.48544400	0.77596200	-1.30816300
O	1.18374100	-1.73500300	-1.02214700
O	-1.31129100	-1.58318100	-0.45731100
C	-0.75329700	2.42206500	-1.48432800
H	-1.52100100	3.20303200	-1.45438300
C	-2.56723700	0.82503400	-1.34176300
H	-3.21546500	1.70431600	-1.41467400
H	-0.65657400	2.08900100	-2.52402300
H	-2.33552100	0.50963900	-2.36434100
O	-0.19946300	-0.36973400	-2.80798000
H	0.66448700	0.01250100	-3.05780800
H	0.33130600	-2.34498800	-3.23469600
C	-0.41439600	-1.60417400	-3.52445000
H	-1.41324800	-1.95082000	-3.26373800
H	-0.36441400	-1.39430300	-4.59498300
C	4.08223100	1.58519500	-0.50115200
H	3.89919600	0.71070400	0.13297900
H	4.29602200	1.20243600	-1.50679100
H	4.97870700	2.09547300	-0.13580800
C	2.13440600	6.18606400	0.26502700
H	2.50520100	6.26052300	1.29497400
H	2.86513500	6.69780700	-0.37381900
H	1.19415000	6.74335900	0.20799200
C	2.90246400	-3.71283700	-1.92853000
H	1.92792500	-4.19177800	-2.08387500
H	2.99840200	-2.93933600	-2.70005500
H	3.68167700	-4.46254500	-2.09406800
C	5.18408500	-3.51285300	2.57658700
H	5.09409000	-4.59285100	2.74729800
H	6.18163000	-3.33843800	2.15431000
H	5.14157900	-3.01517400	3.55025500
C	-2.50174900	-3.78188900	0.76636900
H	-2.02648200	-4.22849500	-0.11472700
H	-1.69499000	-3.54221400	1.46878100
H	-3.15741700	-4.52502300	1.22605200
C	-6.79348700	-1.12561900	0.54448500
H	-7.34694100	-1.09183000	-0.40361400
H	-7.17423800	-1.96419100	1.13205300
H	-7.02081200	-0.19201600	1.07268400

[CoL –CH_3]$^{+2}$

H	-1.76867600	1.99685200	4.63558200
H	-0.29355400	0.24509500	3.76800900
H	2.94316000	-2.12934700	3.08318600
C	-1.64131600	1.89477200	3.56222900
C	-0.79767200	0.90617000	3.07193200
H	-2.98819400	3.51257200	3.08401200
H	1.22014100	-0.66812100	2.77609500
C	2.91831000	-2.45605000	2.04560800
C	-2.32922700	2.74402400	2.69320800
C	3.76988200	-3.44531500	1.61260800
C	1.12047000	-0.85918000	1.70910800
C	-0.62580100	0.76643200	1.68791200
H	-5.34850000	-3.01275000	0.76114300
C	1.98726200	-1.83623400	1.16671900
H	4.42006200	4.08000100	0.05521400
C	-2.18436200	2.59293400	1.31770700
N	0.22170600	-0.16635300	1.05783500
C	3.67872700	-3.83150400	0.25137900
C	-4.75320900	-2.19035100	0.37411200
H	4.34367100	-4.61600800	-0.10753100
C	-5.38300700	-0.95505500	0.12531600
C	3.41114200	3.75054800	-0.17729000
C	2.36781100	4.69669100	-0.16064300
C	-1.34209400	1.60064700	0.82518700
H	-2.73531800	3.24255600	0.64471800
C	-3.40612200	-2.38606100	0.14794400
C	3.19130500	2.42040300	-0.47263400
C	1.92254400	-2.23267800	-0.20298400
C	-4.60865800	0.12516600	-0.38351000
C	1.04563100	4.27507900	-0.48395600
H	0.25290400	5.01805900	-0.51548800
H	-5.10396100	1.06989500	-0.59265900
C	2.79551500	-3.26857700	-0.65051000
C	1.83069400	2.00070900	-0.74995800
C	-2.62860200	-1.26990500	-0.35682800
C	0.76625100	2.96813400	-0.78320000
C	-3.26722800	-0.00905300	-0.62875300
N	-1.16127800	1.35604600	-0.61036600
Co	0.02792200	-0.22799700	-0.79904200
O	1.62216900	0.75703000	-0.97759800
O	1.09866900	-1.71537100	-1.07039300
O	-1.37994900	-1.45996800	-0.56247000
C	-0.57431000	2.55007400	-1.29926500

H	-1.27489600	3.38607500	-1.21640900
C	-2.47601700	1.08253800	-1.27845300
H	-3.06672500	2.00348300	-1.29367600
H	-0.50171600	2.28944800	-2.36101200
H	-2.24767800	0.83212400	-2.31933800
O	-0.12563900	-0.16893500	-2.76819700
H	0.77799400	0.01745100	-3.07808400
H	-0.07192700	-2.20869300	-3.22949800
C	-0.61639100	-1.30990600	-3.51918900
H	-1.67498500	-1.41160400	-3.28950100
H	-0.48765600	-1.09440700	-4.58094400
C	4.28263200	1.40315600	-0.48624100
H	4.09314500	0.61781500	0.25451600
H	4.33800500	0.90559300	-1.46154500
H	5.24824000	1.86503900	-0.27047000
C	2.62328500	6.12699800	0.17500700
H	2.06480400	6.41131900	1.07679500
H	3.68349200	6.32462300	0.34515100
H	2.26515200	6.78157700	-0.62957900
C	2.72992100	-3.71057400	-2.08375200
H	1.73992900	-4.11333600	-2.32998100
H	2.90750500	-2.87160000	-2.76694500
H	3.47439000	-4.48524900	-2.28772200
C	4.76384600	-4.11005300	2.52631500
H	4.58730600	-5.19085800	2.58867000
H	5.79044700	-3.97385900	2.16466600
H	4.70758400	-3.70120300	3.53953300
C	-2.72050400	-3.68452000	0.41607000
H	-2.24300700	-4.06775300	-0.49315800
H	-1.92365000	-3.55821900	1.15825900
H	-3.42812800	-4.43046600	0.78398300
C	-6.83985900	-0.76050800	0.38234200
H	-7.35386100	-0.45156200	-0.53694000
H	-7.31386100	-1.66853600	0.76053900
H	-6.99561300	0.04631700	1.11029900

$[CoL–CH_3]^{+3}$

H	-1.53087500	2.21302400	4.63610800
H	-0.20809800	0.34201400	3.78926000
H	2.33906900	-2.73557400	3.12782300
C	-1.43086500	2.07726600	3.56421600
C	-0.67665000	1.01709200	3.08304700
H	-2.65021200	3.78689600	3.06847300
H	0.93961000	-0.95542500	2.82091200
C	2.38287000	-2.93367300	2.06063200
C	-2.06096800	2.96064400	2.68469000
C	3.16379500	-4.01807900	1.59874200
C	0.90439400	-1.04555900	1.73833200
C	-0.54605400	0.83769600	1.69909700
H	-5.40722500	-2.77160900	0.62484800
C	1.67461500	-2.12277100	1.18839200
H	4.63648000	3.91821500	0.24390200
C	-1.94238100	2.78283400	1.30963500
N	0.19324700	-0.19051800	1.07148600
C	3.21522800	-4.27533900	0.20867500
C	-4.77664100	-1.96077200	0.27147600
H	3.81892100	-5.10799800	-0.14224800
C	-5.34307100	-0.68125000	0.10840500
C	3.62424600	3.64010200	-0.03542700
C	2.63793400	4.64393500	-0.09943100
C	-1.18731000	1.72024200	0.82601700
H	-2.44177000	3.47031600	0.63508100
C	-3.44687400	-2.21465800	0.00447500
C	3.34360000	2.31683600	-0.30706800
C	1.72993500	-2.39911800	-0.23284900
C	-4.52215500	0.38512800	-0.36342500
C	1.30836400	4.28719000	-0.47439900
H	0.56040500	5.07106300	-0.55640000
H	-4.97177900	1.36291600	-0.51364900
C	2.53243900	-3.51410000	-0.71381800
C	1.97865200	1.97081700	-0.65429000
C	-2.62287500	-1.11019900	-0.44866300
C	0.97112000	2.99049700	-0.75439400
C	-3.19691100	0.19240000	-0.64735100
N	-1.02564000	1.46075400	-0.60951400
Co	0.06382400	-0.16029400	-0.80467000
O	1.71313100	0.73464900	-0.87924100
O	1.10353300	-1.70904500	-1.09220900
O	-1.38236000	-1.34641900	-0.67481900
C	-0.37385400	2.62782600	-1.29812400
H	-1.04331500	3.48852800	-1.22446600
C	-2.36109500	1.26379700	-1.27311700
H	-2.90295300	2.21338100	-1.25498800
H	-0.30218900	2.36141400	-2.35743800
H	-2.15310800	1.03549600	-2.32295900
O	-0.02251500	-0.03741600	-2.75517000
H	0.88339600	0.13989900	-3.06599500
H	-0.08005100	-2.04538000	-3.36058500
C	-0.57511000	-1.09996100	-3.58133100
H	-1.63731900	-1.16130300	-3.35786800
H	-0.43052100	-0.81440100	-4.62379800
C	4.36829800	1.23646900	-0.22483400
H	4.08530800	0.49253700	0.52907500
H	4.44909200	0.70247100	-1.17868600
H	5.34634700	1.64629000	0.03481600
C	2.95634100	6.06580600	0.21054500
H	2.35391100	6.41284300	1.06062300
H	4.01226700	6.20752200	0.44820400
H	2.69273600	6.71134500	-0.63705900
C	2.58311600	-3.78599200	-2.17917100
H	1.58953500	-4.05636800	-2.55662000
H	2.90112900	-2.89515400	-2.73220700
H	3.27160300	-4.60419600	-2.39837900
C	3.91708900	-4.88259200	2.55069600
H	3.53806900	-5.91218900	2.50446000
H	4.97624000	-4.92956300	2.26923100
H	3.83913900	-4.52895300	3.58043700
C	-2.82482700	-3.55863900	0.18321200
H	-2.39742300	-3.91744200	-0.76044900
H	-2.00000600	-3.51191200	0.90373500
H	-3.55985300	-4.28509500	0.53542800
C	-6.77884700	-0.42105700	0.41101000
H	-7.29585300	-0.05048000	-0.48385700
H	-7.29271400	-1.31539600	0.76828500
H	-6.87206600	0.36750800	1.16910500

[CoL –CH_3]$^{-1}$

H	1.93922900	1.33117700	-4.95884800
H	0.39687800	-0.22960900	-3.87089500
H	-2.93264100	-2.10476200	-3.18985800
C	1.81235600	1.37136000	-3.88017600
C	0.92738300	0.49603800	-3.26234100
H	3.23860400	2.96888400	-3.59672900
H	-1.24666400	-0.75463100	-2.86015500
C	-2.95429600	-2.45954500	-2.15944500
C	2.54451400	2.28286800	-3.11915900
C	-3.87660600	-3.41331100	-1.79218500
C	-1.09403800	-0.96037500	-1.79650400
C	0.74209500	0.52087900	-1.86912800
H	5.27924000	-3.37296000	-0.05461100
C	-2.00794000	-1.91216900	-1.24864500
H	-4.30771200	3.63357500	-0.51055900
C	2.39468900	2.29227600	-1.73503500
N	-0.13448400	-0.32992600	-1.16948700
C	-3.85487300	-3.84578800	-0.44240500
C	4.74761900	-2.44013300	0.13953000
H	-4.57472400	-4.60233300	-0.12831600
C	5.37116500	-1.22562200	-0.18448000
C	-3.26464200	3.43128800	-0.26393200
C	-2.27746500	4.31275900	-0.72588800
C	1.51410000	1.41524000	-1.10013500
H	2.97855300	2.98863600	-1.13927900
C	3.47481600	-2.50898500	0.70174500
C	-2.97239100	2.30228600	0.50222300
C	-2.00443600	-2.35208700	0.12454400
C	4.66268600	-0.05416900	0.08723800
C	-0.95502800	4.03118400	-0.37671500
H	-0.15937300	4.70250500	-0.70063300
H	5.11949100	0.91070300	-0.13541400
C	-2.96860500	-3.35462600	0.49401700
C	-1.62245100	2.02016900	0.83187500
C	2.75575300	-1.30812500	0.96062300
C	-0.62157600	2.91511500	0.39308600
C	3.38539900	-0.07773000	0.65317200
N	1.37126300	1.39303800	0.34154400
Co	0.01670500	-0.35267000	0.83320800
O	-1.30811700	0.95338000	1.56226400
O	-1.19800100	-1.90838600	1.02753100
O	1.55803200	-1.35087400	1.50779000
C	0.78152500	2.66360000	0.85304000
H	1.43045500	3.51157500	0.58488400
C	2.67785400	1.18663200	1.03169100
H	3.33599500	2.05313400	0.86476500
H	0.79311600	2.57228300	1.94596600
H	2.43354900	1.17015700	2.10158900
O	-0.19266000	1.34433800	4.00661600
H	-0.64150900	1.23964100	3.13106600
H	-1.99845700	1.17217100	5.05926700
C	-1.13925200	1.84780100	4.92286600
H	-0.64472900	1.95899300	5.89411700
H	-1.52947000	2.83549400	4.62981300
C	-4.06081200	1.38383000	0.98537700
H	-3.94527200	0.37291500	0.57519400
H	-4.04154000	1.27685600	2.07701500
H	-5.04932700	1.75617400	0.69609000
C	-2.63241700	5.50562900	-1.57781600
H	-2.82515300	5.22116500	-2.62172800
H	-3.53680000	6.00807900	-1.21406200
H	-1.82215000	6.24290700	-1.58850700
C	-2.97605300	-3.83610500	1.91682700
H	-2.01371500	-4.28627000	2.19113300
H	-3.13618100	-3.00685200	2.61692500
H	-3.76195100	-4.58111600	2.07754200
C	-4.87137700	-3.98895500	-2.76591500
H	-4.75960500	-5.07670200	-2.86417300
H	-5.90532900	-3.80489300	-2.44584900
H	-4.74989000	-3.55171700	-3.76238000
C	2.84009400	-3.82851900	1.04349200
H	2.58825200	-3.89053800	2.11006200
H	1.89837000	-3.97485200	0.49893300
H	3.50649300	-4.66375000	0.80209100
C	6.74321400	-1.19477000	-0.80999400
H	7.45629700	-1.82302600	-0.26108300
H	6.73195200	-1.56144900	-1.84585400
H	7.14716200	-0.17656700	-0.83082500

[CoL –CH_3]$^{-2}$

H	-1.88397700	-1.49818500	-4.97158800
C	-1.76152000	-1.52240000	-3.88953200
C	-0.93816900	-0.58067900	-3.28432600
C	-2.43428200	-2.48479100	-3.13426700
H	-0.45890000	0.16625100	-3.90928600
C	-0.73933900	-0.55725800	-1.87321700
H	-3.07679100	-3.22316900	-3.60659600
C	-2.26868400	-2.46773000	-1.74294500
N	0.06542900	0.32040300	-1.19581600
C	-1.45427500	-1.53379600	-1.11610000
H	-2.79372600	-3.20412100	-1.13711700
C	0.87474000	1.18899000	-1.86238200
N	-1.30002800	-1.51954700	0.33062000
H	0.93429600	1.10263600	-2.94900200
C	1.71290500	2.19506700	-1.30681600
C	2.48289700	2.97238600	-2.22383200
C	1.84168000	2.50319100	0.10518600
H	2.38949100	2.73498800	-3.28549400
C	3.32628600	4.00449300	-1.84166500
C	2.70057100	3.56916400	0.48380000
O	1.19511800	1.85026700	1.04383900
C	3.42139900	4.29656000	-0.46903600
C	4.12121500	4.78777700	-2.85772500
C	2.82398700	3.90056700	1.94754100
H	4.07155300	5.10617400	-0.13471500
H	3.92296300	5.86641900	-2.79178300
H	5.20443900	4.66126100	-2.72026900
H	3.88307200	4.47187400	-3.87980100
H	1.84888300	4.13020600	2.39746100
H	3.23065500	3.05996300	2.52627300
H	3.48153600	4.76396700	2.10244100
C	-0.68223900	-2.77482600	0.83461200
C	0.71378200	-3.01086900	0.34328700
H	-1.32115500	-3.63842800	0.58841000
H	-0.66598500	-2.68285200	1.92814700

C	1.04148700	-4.11844000	-0.44006700
C	1.71590200	-2.10272700	0.75659200
C	2.35575900	-4.37797100	-0.83714300
H	0.24585800	-4.80065100	-0.74127700
C	3.05657900	-2.35575700	0.36568600
O	1.41628900	-1.05400800	1.51169400
C	3.34252800	-3.47700900	-0.41430500
C	2.69890100	-5.56368400	-1.70421200
C	4.14073800	-1.40695800	0.79772000
H	4.37882600	-3.65602700	-0.70490900
H	2.80753600	-5.28350500	-2.76163900
H	3.64556100	-6.02694200	-1.40062500
H	1.92014300	-6.33307000	-1.65436100
H	3.97351500	-0.39849500	0.39717400
H	4.17395200	-1.30174200	1.88951600
H	5.12456700	-1.74818200	0.45752100
C	-2.60308900	-1.34547200	1.02530700
C	-3.29869900	-0.05392000	0.72471100
H	-3.26957500	-2.19476500	0.80399100
H	-2.37180900	-1.38976100	2.09797400
C	-4.55813700	-0.02097000	0.12430400
C	-2.66861100	1.14314900	1.15160700
C	-5.25424800	1.17509700	-0.06980200
H	-5.01178900	-0.96116100	-0.19229800
C	-3.38192300	2.36480600	0.98340300
O	-1.48614800	1.12593800	1.72342200
C	-4.63863800	2.35245900	0.38011200
C	-6.59969100	1.20554500	-0.75105400
C	-2.75740000	3.64323000	1.47028500
H	-5.16346500	3.30133100	0.25527500
H	-7.28060900	1.92190800	-0.27473900
H	-6.52295600	1.49774900	-1.80841400
H	-7.08201100	0.22162800	-0.72550000
H	-2.56548300	3.61129900	2.55108500
H	-1.78399200	3.82356800	0.99616300
H	-3.40276000	4.50483900	1.26595500
H	0.85881100	-1.34182400	3.09514000
O	0.49117900	-1.44855400	4.01052100
C	1.53808400	-1.87832700	4.84941500
H	2.37311800	-1.16060100	4.89048700
H	1.13988100	-1.98349400	5.86504600
H	1.95015400	-2.85568300	4.54940500
Co	0.05866200	0.27141000	0.79932000

[CoL –Br]^{0}

H	1.62394100	2.61117800	-4.40206300
H	0.36553600	0.69825700	-3.55837100
H	-2.11609500	-2.36066700	-2.98263700
C	1.54019600	2.46320400	-3.33119400
C	0.82180600	1.37924600	-2.85129700
H	2.71894700	4.19781000	-2.83422900
H	-0.76536600	-0.59954500	-2.60269500
C	-2.13233000	-2.63698200	-1.93458300
C	2.15644400	3.35337900	-2.45294400
C	-2.83139600	-3.73910200	-1.51307900
C	-0.70296800	-0.73001000	-1.52491300
C	0.70820200	1.17807600	-1.47084900
H	5.75527600	-1.98219900	-0.82149700
C	-1.41995100	-1.84544700	-1.00538200
H	-4.41773100	3.98029600	-0.41548100
C	2.05562900	3.15235300	-1.08291600
N	0.00405300	0.12305500	-0.84964400
C	-2.84569300	-4.09760200	-0.15664900
C	5.10835800	-1.24038600	-0.37059600
H	-3.39730400	-4.96907400	0.17367600
C	5.55827100	0.05266800	-0.13475600
C	-3.42040300	3.77237500	-0.04901200
C	-2.45525800	4.77043600	0.00187300
C	1.33653200	2.06606400	-0.59966500
H	2.54141300	3.84033600	-0.40059000
C	3.80491500	-1.56753900	-0.02689300
C	-3.08272900	2.49290300	0.37062700
C	-1.41096100	-2.17309100	0.38720500
C	4.72443200	1.00208800	0.44019100
C	-1.17744600	4.50576000	0.47720800
H	-0.43475500	5.29422000	0.52356500
H	5.08415600	2.00871800	0.62207100
C	-2.15405500	-3.33491200	0.75581400
C	-1.79924000	2.17341700	0.86132700
C	2.91833000	-0.64235000	0.57102500
C	-0.85830500	3.22469900	0.91231800
C	3.42544100	0.65760700	0.79785100
N	1.19586400	1.79375800	0.83019600
Co	0.17243300	0.10128800	1.01834600
O	-1.50517900	0.96814100	1.29018500
O	-0.79015900	-1.50272700	1.28371700
O	1.71224700	-1.00038200	0.92598300
C	0.47633900	2.92367900	1.51596000
H	1.11433600	3.81067700	1.48306300
C	2.54056200	1.64849700	1.48676400
H	3.02506800	2.62847000	1.51214200
H	0.37559100	2.62109000	2.56143900
H	2.33599400	1.35499800	2.51887800
O	0.27173300	0.20086700	3.01116500
H	-0.65857500	0.38301400	3.21200800
H	0.16955200	-1.80060000	3.59613400
C	0.73961000	-0.89935100	3.82008800
H	1.78657500	-1.05083100	3.57106800
H	0.63825300	-0.62188100	4.87054100
Br	-2.89704600	6.52853000	-0.59004800
Br	-4.40758600	1.13005100	0.31257900
Br	-2.18283300	-3.83328000	2.58728500
Br	-3.79327800	-4.80781900	-2.76092100
Br	3.19244200	-3.34028400	-0.34772200
Br	7.34387100	0.52331600	-0.61362300