Supporting Information

Spin Modulation and Electrochemical Behavior of a Five-coordinate Cobalt(III) Salen Complex

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Figure S1. FT-IR spectra of **H₂L** (dark brown), **CoL** (orange), **CoL⁺** (green), and **CoLPy⁺** (dark green) in KBr pellet.

Figure S2. CVs of **CoL⁺** (1 mM) in anhydrous DCM (left) and MeCN (right) at various scan rates using a glassy carbon working electrode. The arrow indicates the initial scan direction.

Figure S3. *Left*: ^1H NMR spectra of **CoL** at (a) 24 (b) 14 and (c) 0 ° C in chloroform- d , showing an inverse dependence the chemical shifts with temperature. *Right*: ^1H NMR Curie plots and linear square fits of chemical shifts (in chloroform- d) for **CoL**.

Figure S4. ^1H NMR spectra of **CoL** in chloroform- d after addition of 0-1 eq. of pyridine.

Figure S5. *Left:* ^1H NMR spectra of CoL^+ at (a) 25 (b) 15 and (c) 0 $^\circ\text{C}$ in chloroform-d, showing an inverse dependence the chemical shifts with temperature. *Right:* ^1H NMR Curie plots and linear square fits of chemical shifts (in chloroform-d) for CoL^{1+} .

Figure S6.

Figure S6. ^1H NMR spectra of CoL^+ in chloroform-d after addition of 0 - 1.1eq. of pyridine.

Figure S7. ^1H NMR spectra of CoLPy^+ in $\text{chloroform-}d$. (*inset*) shows an enlarged view of chemical shifts in the diamagnetic region.

Figure S8. ^1H NMR spectra of $\text{CoL}(\text{ACN})^+$ in acetonitrile- d_3 . (*inset*) shows an enlarged view of chemical shifts in the diamagnetic region.

Figure S9. NIR difference spectra obtained from a 0.5 mM solution of CoL^+ (solid purple line) in anhydrous chloroform-*d* at -10°C , followed by the addition of one equivalent of WCl_6 to generate CoL^{2+} (dash-dotted red line). The sharp peaks in the NIR region are due to imperfect solvent background subtraction.

Figure S10. NIR spectra obtained from a 3.2 mM solution of CoL(ACN)^+ (solid blue line) in anhydrous acetonitrile, followed by electrochemical oxidation to CoL(ACN)^{2+} at $+0.80\text{ V}$ vs $\text{Fc}^{0/+}$ (solid purple line). The potentials listed are referenced to $\text{Fc}^{0/+}$ and correspond directly to the CV in Figure 2b. Pt mesh working electrode, Pt wire counter electrode and Ag wire pseudo-reference electrode. The sharp peaks in the NIR region are due to imperfect solvent background subtraction.

Figure S11. TDDFT predicted UV-vis-NIR spectra for (top) CoL^{2+} in dichloromethane and (bottom) CoL(ACN)^{2+} in acetonitrile. The predicted spectrum of CoL(ACN)^{2+} is compared against the experimental difference spectrum obtained via spectroelectrochemistry.

T: FTMS + p ESI Full ms [100.00-900.00]

Figure S12. High-resolution electrospray ionization (ESI) mass spectrum of **CoL**.

Figure S13. MALDI mass spectrum of **CoL⁺**.

Figure S14. High-resolution ESI mass spectrum of **CoLPy⁺**.

Calculated Minimum Energy Geometries

Geometries were optimized without symmetry constraints in the gas phase at the TPSSh/def2-TZVP level of theory. Frequency calculations were performed to confirm that the geometries are true minima of the ground state potential energy surface.

CoL⁺

Co	-0.00395	1.23384	-0.10955
N	0.89892	1.38638	1.58265
N	0.05996	3.38069	-0.34528
N	-0.89573	1.05921	-1.79895
O	1.52198	0.50412	-0.89813
O	-1.54787	0.70941	0.79242
C	6.18523	-1.92623	2.92945
H	5.31090	-2.29205	3.49138
H	6.33058	-0.85936	3.16367
H	7.06749	-2.46892	3.30159
C	6.03280	-2.16352	1.41711
C	5.87085	-3.68203	1.17240
H	6.74170	-4.22430	1.57392
H	5.79691	-3.91902	0.09960
H	4.96703	-4.06793	1.66962
C	7.31329	-1.66056	0.71047
H	7.45583	-0.58049	0.87270
H	7.28064	-1.84065	-0.37534
H	8.19561	-2.18655	1.10851
C	4.81362	-1.42590	0.84403
C	3.95890	-0.64692	1.61034
H	4.12488	-0.52116	2.68170
C	2.84029	-0.00034	1.03286
C	2.55873	-0.11263	-0.36307
C	3.43779	-0.90428	-1.17722
C	4.51339	-1.52297	-0.53822
H	5.17844	-2.13138	-1.15069
C	3.22645	-1.05336	-2.69549
C	1.81952	-1.62498	-2.99070
H	1.71322	-2.62898	-2.54996
H	1.67700	-1.71843	-4.07965
H	1.02525	-0.98646	-2.58440
C	3.41549	0.32826	-3.36528
H	2.74520	1.08202	-2.92972
H	3.21093	0.26078	-4.44616
H	4.45038	0.68165	-3.23604
C	4.24936	-2.01406	-3.33243

H	5.28483	-1.65681	-3.21865
H	4.04583	-2.08973	-4.41166
H	4.17981	-3.02905	-2.91040
C	2.01513	0.79434	1.89175
H	2.37508	0.91694	2.92435
C	0.24762	2.22346	2.58909
H	0.74979	2.08934	3.56111
H	-0.79068	1.87802	2.68839
C	0.27425	3.69953	2.18992
H	-0.21898	4.27640	2.98876
H	1.31399	4.06295	2.14951
C	-0.47179	4.01741	0.89782
H	-1.52003	3.69375	0.98946
H	-0.47852	5.11326	0.74460
C	-0.84359	3.79860	-1.45504
H	-0.87069	4.90381	-1.49201
H	-1.85091	3.45954	-1.17185
C	1.45396	3.80021	-0.60969
H	1.81453	3.33126	-1.53264
H	2.10450	3.47322	0.20958
H	1.51815	4.89905	-0.70976
C	-0.49591	3.26673	-2.84551
H	-1.35564	3.52251	-3.48511
H	0.36873	3.79797	-3.27237
C	-0.23485	1.74658	-2.90338
H	-0.57961	1.33655	-3.86633
H	0.83702	1.52818	-2.81641
C	-1.99980	0.40758	-2.00914
H	-2.34604	0.32832	-3.05074
C	-2.82721	-0.20873	-1.01622
C	-2.57234	-0.01482	0.37695
C	-3.46695	-0.61891	1.32403
C	-3.28404	-0.43899	2.84246
C	-3.45715	1.05699	3.19690
H	-2.77459	1.69168	2.61532
H	-3.26256	1.22068	4.26931
H	-4.48638	1.38623	2.98458
C	-1.89306	-0.95975	3.27613
H	-1.81069	-2.04021	3.07809
H	-1.75629	-0.80429	4.35874
H	-1.08055	-0.45215	2.74124
C	-4.33437	-1.22355	3.65236
H	-5.36128	-0.88750	3.43934
H	-4.15243	-1.06198	4.72604
H	-4.27396	-2.30748	3.46651
C	-4.52607	-1.37081	0.81332

H	-5.20144	-1.83714	1.53023
C	-3.93016	-0.97570	-1.46170
H	-4.07496	-1.08395	-2.53802
C	-4.79682	-1.57922	-0.56250
C	-5.99960	-2.43517	-0.98611
C	-7.29761	-1.80277	-0.43189
H	-8.16850	-2.41106	-0.72362
H	-7.44181	-0.78519	-0.82801
H	-7.28765	-1.74218	0.66754
C	-5.83576	-3.86253	-0.41362
H	-4.91932	-4.33868	-0.79631
H	-6.69486	-4.48747	-0.70523
H	-5.78442	-3.85983	0.68632
C	-6.11990	-2.53382	-2.51662
H	-5.23138	-3.00418	-2.96757
H	-6.26588	-1.54492	-2.98028
H	-6.99079	-3.15331	-2.77965

CoL²⁺

Co	0.01820	1.31269	0.07504
N	0.90768	1.23273	1.76478
N	0.14410	3.43837	0.06792
N	-0.87331	1.32718	-1.63219
O	1.57369	0.72249	-0.80112
O	-1.55002	0.55992	0.88397
C	6.05970	-2.41235	2.65189
H	5.17374	-2.82000	3.16468
H	6.25054	-1.39422	3.02725
H	6.91939	-3.03331	2.94278
C	5.90322	-2.44164	1.12177
C	5.68281	-3.90831	0.67016
H	6.53295	-4.52314	1.00284
H	5.61502	-3.99996	-0.42462
H	4.76442	-4.32619	1.11075
C	7.20285	-1.89356	0.47695
H	7.38573	-0.84989	0.77577
H	7.17163	-1.93912	-0.62232
H	8.05823	-2.50047	0.81075
C	4.72368	-1.59477	0.64656
C	3.89229	-0.88109	1.52263
H	4.07065	-0.91417	2.59831
C	2.81428	-0.12389	1.04445
C	2.54127	-0.03422	-0.36896
C	3.38303	-0.76746	-1.29215

C	4.42682	-1.50572	-0.73942
H	5.06951	-2.05952	-1.42201
C	3.16723	-0.71583	-2.81230
C	1.73097	-1.17697	-3.16110
H	1.57420	-2.22092	-2.84706
H	1.58535	-1.12961	-4.25160
H	0.96773	-0.55266	-2.67897
C	3.42914	0.72776	-3.30962
H	2.78991	1.46143	-2.79889
H	3.23757	0.79073	-4.39213
H	4.47745	1.01370	-3.13484
C	4.14028	-1.64446	-3.56508
H	5.19180	-1.35247	-3.42080
H	3.93097	-1.58085	-4.64316
H	4.02069	-2.69794	-3.26753
C	2.00820	0.58402	2.00184
H	2.37319	0.57227	3.03893
C	0.27973	1.97325	2.86300
H	0.77068	1.70913	3.81286
H	-0.77118	1.65467	2.92239
C	0.36467	3.48119	2.62752
H	-0.10855	3.98468	3.48532
H	1.41725	3.80607	2.62819
C	-0.36536	3.96086	1.37868
H	-1.42782	3.67699	1.43777
H	-0.32674	5.06443	1.33931
C	-0.75564	4.01194	-0.98007
H	-0.74121	5.11277	-0.88875
H	-1.77356	3.68256	-0.72373
C	1.54749	3.86281	-0.15898
H	1.89458	3.49785	-1.13241
H	2.19692	3.43918	0.61554
H	1.62515	4.96375	-0.13449
C	-0.43632	3.63512	-2.42461
H	-1.29590	3.97665	-3.02214
H	0.43538	4.18998	-2.80236
C	-0.20436	2.12807	-2.65938
H	-0.55965	1.83466	-3.65919
H	0.86312	1.88227	-2.59817
C	-1.96948	0.70694	-1.93491
H	-2.31412	0.75919	-2.97791
C	-2.80813	-0.05178	-1.03574
C	-2.55222	-0.07901	0.39388
C	-3.45337	-0.83666	1.25995
C	-3.25994	-0.88540	2.77963
C	-3.44802	0.54304	3.35270

H	-2.75345	1.26329	2.89898
H	-3.27546	0.52862	4.43988
H	-4.47415	0.90077	3.17823
C	-1.85478	-1.44281	3.12277
H	-1.73946	-2.46760	2.73655
H	-1.74043	-1.48276	4.21694
H	-1.04924	-0.82234	2.70982
C	-4.29727	-1.79869	3.46109
H	-5.32868	-1.44428	3.31036
H	-4.11041	-1.80171	4.54488
H	-4.22434	-2.84062	3.11214
C	-4.50750	-1.49813	0.64392
H	-5.18465	-2.07282	1.27350
C	-3.89872	-0.73165	-1.57214
H	-4.07081	-0.68335	-2.64819
C	-4.77470	-1.48093	-0.75355
C	-5.96696	-2.24703	-1.30987
C	-7.26144	-1.69826	-0.64885
H	-8.12596	-2.25328	-1.04341
H	-7.40409	-0.63135	-0.87860
H	-7.25592	-1.82248	0.44441
C	-5.80497	-3.74922	-0.94953
H	-4.89259	-4.16990	-1.39909
H	-6.66952	-4.30552	-1.34217
H	-5.76738	-3.91548	0.13752
C	-6.09270	-2.11209	-2.83711
H	-5.21153	-2.51532	-3.36122
H	-6.24566	-1.06635	-3.14805
H	-6.96607	-2.68433	-3.18146

CoLPy⁺

Co	0.00273	0.93606	0.23337
N	-0.03355	-0.95883	-0.32621
N	-0.75082	0.48702	1.95086
N	0.79033	1.43614	-1.45989
O	-1.78349	1.13007	-0.48089
O	1.75395	0.61539	0.97398
C	-6.78264	-1.99145	2.20547
H	-6.05825	-1.99949	3.03518
H	-7.59551	-2.68794	2.46704
H	-7.20855	-0.97812	2.13587
C	-5.54347	-3.83396	1.00763
H	-5.07444	-4.16078	0.06581
H	-6.33983	-4.55224	1.26112

H	-4.78181	-3.88456	1.80184
C	-7.21809	-2.43632	-0.21734
H	-7.70065	-1.45365	-0.33979
H	-8.00193	-3.15585	0.06504
H	-6.81645	-2.75062	-1.19398
C	-6.12818	-2.40952	0.86884
C	-4.99156	-1.43002	0.52569
C	-4.97983	-0.63866	-0.64395
H	-5.83465	-0.72597	-1.31018
C	-3.97260	0.26019	-1.01874
C	-4.15802	1.09515	-2.30748
C	-3.96608	2.59724	-2.00479
H	-4.10576	3.19032	-2.92306
H	-2.96365	2.79698	-1.60842
H	-4.70464	2.94082	-1.26329
C	-3.16446	0.63355	-3.39557
H	-3.30095	1.22364	-4.31634
H	-3.32534	-0.42724	-3.64446
H	-2.12305	0.75721	-3.07084
C	-5.57299	0.94316	-2.90425
H	-6.35598	1.23588	-2.18753
H	-5.77813	-0.08300	-3.24678
H	-5.66108	1.60231	-3.78168
C	-3.91924	-1.24712	1.38428
H	-3.87826	-1.76874	2.34492
C	-2.81176	0.35634	-0.17228
C	-2.84716	-0.38325	1.05995
C	-1.88821	-0.12260	2.09112
H	-2.17669	-0.41892	3.11210
C	-0.07020	1.00882	3.13081
H	1.00427	0.86264	2.98491
H	-0.38273	0.44967	4.02784
N	0.03463	2.95475	0.78511
C	-0.39204	2.50914	3.28488
H	0.47170	3.02889	3.72710
H	-1.22776	2.64744	3.98961
C	-0.83685	3.17497	1.98387
H	-1.83495	2.81615	1.69704
H	-0.91295	4.26425	2.15153
C	1.41327	3.42196	1.06433
H	1.39575	4.49657	1.31712
H	2.04743	3.26151	0.18601
H	1.84151	2.85192	1.89253
C	-0.57295	3.80856	-0.28868
H	-0.58223	4.84622	0.09048
H	-1.61342	3.47685	-0.39020

C	0.10967	3.78064	-1.65002
H	-0.44243	4.48274	-2.29560
H	1.14300	4.15974	-1.59214
C	0.08970	2.40073	-2.30266
H	-0.94973	2.07218	-2.41870
H	0.56655	2.43998	-3.29603
C	1.94982	0.99978	-1.85640
H	2.25728	1.26816	-2.87926
C	2.90430	0.25007	-1.09959
C	2.80879	0.16321	0.32695
C	3.93774	-0.39462	1.03135
C	4.03208	-0.42550	2.57372
C	3.92869	1.01239	3.13074
H	4.75694	1.63385	2.75603
H	3.98222	1.00041	4.23141
H	2.98483	1.48770	2.83371
C	2.92233	-1.31468	3.17662
H	1.92251	-0.93196	2.93485
H	3.01492	-1.34624	4.27426
H	3.00488	-2.34704	2.80095
C	5.37704	-0.99899	3.06413
H	5.51777	-2.04891	2.76274
H	5.39841	-0.96774	4.16445
H	6.23463	-0.41240	2.69985
C	4.98666	-0.90459	0.26434
H	5.82439	-1.35072	0.79948
C	5.06890	-0.88368	-1.15071
C	4.02085	-0.26695	-1.80761
H	4.02488	-0.15809	-2.89403
C	6.28678	-1.49431	-1.86142
C	6.37874	-2.99805	-1.51402
H	5.47727	-3.53561	-1.84881
H	6.48889	-3.16093	-0.43030
H	7.25234	-3.45153	-2.00938
C	7.57398	-0.77852	-1.39115
H	8.45495	-1.21151	-1.89168
H	7.72607	-0.87989	-0.30517
H	7.53705	0.29602	-1.63023
C	6.18266	-1.35309	-3.38974
H	5.29061	-1.86366	-3.78708
H	7.06489	-1.80795	-3.86583
H	6.14702	-0.29670	-3.70096
C	0.42451	-1.92834	0.48727
H	0.81573	-1.60026	1.44753
C	0.41596	-3.27188	0.11910
H	0.80044	-4.01914	0.81469

C	-0.08012	-3.62926	-1.13626
H	-0.09819	-4.67423	-1.45312
C	-0.55229	-2.61941	-1.97750
H	-0.95347	-2.84164	-2.96731
C	-0.51396	-1.29888	-1.53683
H	-0.88576	-0.48120	-2.15029

CoLPy²⁺

Co	0.00204	0.89832	0.30701
N	-0.02869	-0.96034	-0.41729
N	-0.74439	0.30796	1.98592
N	0.78206	1.55545	-1.33872
O	-1.77102	1.11275	-0.40137
O	1.74496	0.49759	0.99733
C	-6.81135	-2.04774	2.03850
H	-6.09770	-2.11550	2.87443
H	-7.63418	-2.74843	2.24791
H	-7.22614	-1.02824	2.01927
C	-5.57930	-3.84633	0.75733
H	-5.10756	-4.13511	-0.19492
H	-6.39133	-4.55946	0.96670
H	-4.83186	-3.94920	1.55969
C	-7.23667	-2.37026	-0.41419
H	-7.71649	-1.38146	-0.48488
H	-8.02496	-3.09907	-0.17542
H	-6.83080	-2.63689	-1.40299
C	-6.15687	-2.41037	0.68083
C	-5.01179	-1.43369	0.40543
C	-4.98996	-0.56406	-0.70941
H	-5.84665	-0.59545	-1.37732
C	-3.97159	0.34185	-1.01990
C	-4.13828	1.26693	-2.24322
C	-3.93961	2.74283	-1.82912
H	-4.08701	3.39674	-2.70235
H	-2.93335	2.92073	-1.43102
H	-4.67309	3.03575	-1.06194
C	-3.13575	0.87083	-3.35149
H	-3.26966	1.52289	-4.22850
H	-3.29952	-0.16879	-3.67478
H	-2.09465	0.96982	-3.01643
C	-5.54984	1.16374	-2.85882
H	-6.33723	1.41717	-2.13244
H	-5.75804	0.16526	-3.27281
H	-5.62464	1.87999	-3.69030

C	-3.93106	-1.32991	1.29162
H	-3.91745	-1.91854	2.21219
C	-2.80766	0.35400	-0.15088
C	-2.85247	-0.47244	1.03686
C	-1.88285	-0.30246	2.08477
H	-2.17457	-0.67344	3.07899
C	-0.05576	0.72264	3.20870
H	1.01766	0.58543	3.05073
H	-0.36826	0.08485	4.05022
N	0.02842	2.85968	1.03361
C	-0.37645	2.20398	3.49300
H	0.49093	2.68190	3.97217
H	-1.20437	2.27952	4.21537
C	-0.83193	2.97957	2.25942
H	-1.83806	2.65923	1.95499
H	-0.89664	4.05020	2.51833
C	1.41206	3.30131	1.34360
H	1.39413	4.34577	1.69738
H	2.03854	3.23334	0.44778
H	1.84703	2.66084	2.11555
C	-0.58765	3.80702	0.04107
H	-0.59584	4.80419	0.51374
H	-1.63104	3.49021	-0.08135
C	0.08939	3.90568	-1.31841
H	-0.46913	4.65758	-1.89816
H	1.11920	4.28744	-1.23276
C	0.07461	2.59173	-2.09531
H	-0.96089	2.26757	-2.24713
H	0.55461	2.72008	-3.07828
C	1.94323	1.17283	-1.77434
H	2.25458	1.54164	-2.76300
C	2.90805	0.36105	-1.08567
C	2.80601	0.12669	0.33443
C	3.93623	-0.49414	1.00529
C	4.02084	-0.67085	2.53519
C	3.91720	0.71092	3.22325
H	4.74009	1.36880	2.90440
H	3.98424	0.59066	4.31551
H	2.96852	1.21319	2.99101
C	2.90737	-1.61589	3.04177
H	1.90578	-1.21284	2.84303
H	3.00379	-1.75419	4.12970
H	2.99080	-2.60687	2.56870
C	5.36513	-1.28915	2.97094
H	5.50772	-2.30484	2.57051
H	5.38029	-1.36624	4.06813

H	6.22371	-0.66756	2.67414
C	4.99192	-0.91641	0.20043
H	5.83099	-1.40595	0.69172
C	5.08007	-0.75239	-1.20734
C	4.02480	-0.07218	-1.82091
H	4.05369	0.14070	-2.89063
C	6.29919	-1.27632	-1.96628
C	6.40239	-2.80759	-1.75072
H	5.51090	-3.32400	-2.13967
H	6.51776	-3.06914	-0.68758
H	7.28301	-3.19522	-2.28545
C	7.57452	-0.59189	-1.41111
H	8.45662	-0.96827	-1.95139
H	7.72595	-0.80225	-0.34132
H	7.52994	0.49981	-1.54604
C	6.20457	-0.99421	-3.47554
H	5.32328	-1.47535	-3.92950
H	7.09454	-1.39762	-3.98026
H	6.16868	0.08564	-3.69103
C	0.38417	-2.00192	0.33270
H	0.73755	-1.76603	1.33430
C	0.37710	-3.31061	-0.14440
H	0.72191	-4.11781	0.50365
C	-0.06878	-3.55851	-1.44487
H	-0.08411	-4.57397	-1.84655
C	-0.49404	-2.47660	-2.21995
H	-0.85273	-2.61258	-3.24135
C	-0.46084	-1.19649	-1.67245
H	-0.79715	-0.33055	-2.23911

CoLACN⁺

Co	0.03174	1.11061	0.29807
N	-0.68886	0.64583	2.03676
N	0.78360	1.61779	-1.41998
O	-1.76202	1.28893	-0.37179
O	1.79559	0.75931	0.97364
C	-6.78484	-1.69722	2.30335
H	-6.09113	-1.63502	3.15664
H	-7.61656	-2.35749	2.59749
H	-7.19338	-0.69037	2.12360
C	-5.53120	-3.65746	1.32873
H	-5.03438	-4.07661	0.43886
H	-6.34752	-4.33948	1.61637
H	-4.80080	-3.64493	2.15330

C	-7.13729	-2.35930	-0.08288
H	-7.59397	-1.38489	-0.31804
H	-7.94560	-3.03451	0.23745
H	-6.70741	-2.77405	-1.00867
C	-6.08773	-2.24498	1.03681
C	-4.92654	-1.31118	0.65000
C	-4.85246	-0.64602	-0.59428
H	-5.66041	-0.81605	-1.30251
C	-3.82408	0.21482	-0.99691
C	-3.85435	0.84561	-2.40287
C	-3.80816	2.38737	-2.30225
H	-3.79078	2.83470	-3.30954
H	-2.92556	2.72931	-1.74821
H	-4.70301	2.76284	-1.78106
C	-2.65901	0.29296	-3.21568
H	-2.58073	0.80465	-4.18907
H	-2.80221	-0.78198	-3.41151
H	-1.71030	0.41474	-2.67629
C	-5.13523	0.49173	-3.18397
H	-6.04272	0.85252	-2.67488
H	-5.23654	-0.59180	-3.35296
H	-5.09599	0.97495	-4.17265
C	-3.88182	-1.06744	1.53015
H	-3.87138	-1.52731	2.52276
C	-2.74222	0.44895	-0.08117
C	-2.80178	-0.22143	1.18606
C	-1.83157	0.05547	2.20362
H	-2.10436	-0.22646	3.23272
C	0.03977	1.13431	3.20142
H	1.10340	0.94402	3.03037
H	-0.27312	0.58045	4.10114
N	0.08640	3.09688	0.85244
C	-0.22579	2.64456	3.36913
H	0.67541	3.14109	3.75971
H	-1.01643	2.80974	4.11862
C	-0.72534	3.31995	2.09374
H	-1.74006	2.97487	1.85229
H	-0.77851	4.40934	2.26593
C	1.48160	3.55332	1.06980
H	1.47996	4.62587	1.33017
H	2.07224	3.39491	0.16181
H	1.94297	2.97268	1.87320
C	-0.57527	3.95106	-0.19291
H	-0.59297	4.98216	0.20187
H	-1.61093	3.59488	-0.26514
C	0.06728	3.95458	-1.57344

H	-0.52008	4.65090	-2.19350
H	1.09212	4.35878	-1.53986
C	0.05869	2.58266	-2.24166
H	-0.97436	2.23553	-2.35344
H	0.52465	2.63955	-3.23906
C	1.92814	1.17600	-1.84966
H	2.21762	1.46380	-2.87231
C	2.87535	0.37713	-1.13375
C	2.77836	0.21683	0.28452
C	3.82711	-0.51794	0.94347
C	3.81580	-0.75519	2.46580
C	3.87531	0.60124	3.20619
H	4.82847	1.11057	2.99435
H	3.80699	0.44729	4.29545
H	3.06123	1.26825	2.89363
C	2.54656	-1.55245	2.85036
H	1.63302	-1.06318	2.48880
H	2.47991	-1.66268	3.94524
H	2.59063	-2.56384	2.41428
C	5.02836	-1.57837	2.94215
H	5.05692	-2.57934	2.48330
H	4.96163	-1.71752	4.03242
H	5.98269	-1.07037	2.73246
C	4.85870	-1.02591	0.15311
H	5.64451	-1.58800	0.65805
C	4.97397	-0.87276	-1.25203
C	3.96641	-0.15378	-1.87030
H	3.98464	0.02482	-2.94739
C	6.17353	-1.47959	-1.99693
C	6.18478	-3.01179	-1.79070
H	5.26616	-3.46997	-2.19109
H	6.26315	-3.28087	-0.72561
H	7.04580	-3.46082	-2.31142
C	7.48346	-0.87681	-1.43883
H	8.35346	-1.30736	-1.96024
H	7.60386	-1.08374	-0.36395
H	7.50526	0.21543	-1.57891
C	6.11103	-1.19230	-3.50692
H	5.20693	-1.62180	-3.96805
H	6.98287	-1.64149	-4.00690
H	6.12929	-0.11104	-3.71785
N	-0.02240	-0.71482	-0.24209
C	-0.04814	-1.82362	-0.56543
C	-0.08526	-3.22029	-0.96572
H	-1.02933	-3.67366	-0.62893
H	-0.01716	-3.29547	-2.06089

H	0.76072	-3.75700	-0.51169
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CoLACN²⁺

Co	0.03150	1.04841	0.27930
N	-0.67966	0.58279	2.02104
N	0.77450	1.56248	-1.44291
O	-1.75308	1.19004	-0.40287
O	1.79018	0.67473	0.94002
C	-6.82885	-1.51488	2.34302
H	-6.12822	-1.46257	3.19102
H	-7.68167	-2.13696	2.65535
H	-7.20191	-0.49947	2.13929
C	-5.65838	-3.55531	1.41545
H	-5.18822	-4.02347	0.53632
H	-6.50270	-4.18881	1.72764
H	-4.92706	-3.54891	2.23897
C	-7.23689	-2.23958	-0.02507
H	-7.66653	-1.25813	-0.28008
H	-8.06233	-2.87719	0.32374
H	-6.83379	-2.69713	-0.94249
C	-6.17323	-2.13254	1.08117
C	-4.98686	-1.25967	0.66554
C	-4.90567	-0.61704	-0.59173
H	-5.73038	-0.76805	-1.28383
C	-3.85145	0.19464	-1.01918
C	-3.87502	0.81108	-2.42715
C	-3.80488	2.35443	-2.33595
H	-3.79723	2.78784	-3.34815
H	-2.90994	2.69704	-1.80194
H	-4.68753	2.74813	-1.80875
C	-2.69285	0.22883	-3.24200
H	-2.62873	0.72611	-4.22258
H	-2.85014	-0.84633	-3.42218
H	-1.73190	0.34924	-2.72386
C	-5.16699	0.46926	-3.19590
H	-6.06483	0.85910	-2.69203
H	-5.28949	-0.61412	-3.34892
H	-5.12109	0.93564	-4.19127
C	-3.91399	-1.04819	1.54476
H	-3.92526	-1.49880	2.54030
C	-2.74989	0.39938	-0.09928
C	-2.81468	-0.25583	1.18728
C	-1.82511	0.00535	2.19796
H	-2.09778	-0.26982	3.22783

C	0.05565	1.06627	3.18932
H	1.11818	0.87035	3.02139
H	-0.26020	0.50914	4.08475
N	0.08198	3.02936	0.83593
C	-0.20756	2.57693	3.35864
H	0.69694	3.07045	3.74373
H	-0.99003	2.74125	4.11604
C	-0.71764	3.25533	2.08978
H	-1.73989	2.92485	1.85940
H	-0.75847	4.34411	2.26112
C	1.48143	3.48657	1.04379
H	1.47899	4.55730	1.30689
H	2.06572	3.33818	0.12997
H	1.94768	2.91107	1.84856
C	-0.58820	3.88691	-0.20674
H	-0.60190	4.91520	0.19220
H	-1.62752	3.53894	-0.26965
C	0.04635	3.89629	-1.58996
H	-0.54744	4.58971	-2.20626
H	1.06788	4.30779	-1.56351
C	0.04107	2.52767	-2.26551
H	-0.98812	2.17247	-2.38173
H	0.50843	2.58782	-3.26078
C	1.92388	1.14432	-1.87465
H	2.21532	1.44337	-2.89236
C	2.89105	0.35963	-1.15637
C	2.78823	0.17229	0.26960
C	3.85254	-0.54717	0.94572
C	3.83400	-0.80263	2.46148
C	3.87474	0.54937	3.21510
H	4.81945	1.07539	3.00948
H	3.81409	0.37625	4.30077
H	3.05009	1.21270	2.92159
C	2.57440	-1.62489	2.83021
H	1.64787	-1.14331	2.49161
H	2.52201	-1.75880	3.92205
H	2.62917	-2.62662	2.37467
C	5.05762	-1.61478	2.92997
H	5.10472	-2.60748	2.45565
H	4.98449	-1.77374	4.01613
H	6.00483	-1.08680	2.74051
C	4.90826	-1.00453	0.16128
H	5.70838	-1.54663	0.66322
C	5.03142	-0.82152	-1.24175
C	3.99794	-0.12197	-1.87522
H	4.03921	0.06637	-2.94919

C	6.25320	-1.36623	-1.98174
C	6.31991	-2.90197	-1.78381
H	5.42688	-3.39492	-2.19903
H	6.40762	-3.18002	-0.72230
H	7.20338	-3.30091	-2.30526
C	7.52964	-0.71612	-1.38853
H	8.41594	-1.10604	-1.91208
H	7.65002	-0.94145	-0.31785
H	7.51207	0.37767	-1.51201
C	6.19949	-1.06352	-3.48901
H	5.32260	-1.52496	-3.97115
H	7.09500	-1.47475	-3.97728
H	6.18558	0.01941	-3.69098
N	-0.01972	-0.79839	-0.26835
C	-0.04220	-1.90782	-0.59486
C	-0.07325	-3.30274	-1.00117
H	-1.04631	-3.74233	-0.73530
H	0.07293	-3.37696	-2.08915
H	0.72713	-3.85567	-0.48708