Supporting information for:

Tuning redox potentials of bis(imino)pyridine cobalt complexes: an experimental-theoretical study involving solvent and ligand effects

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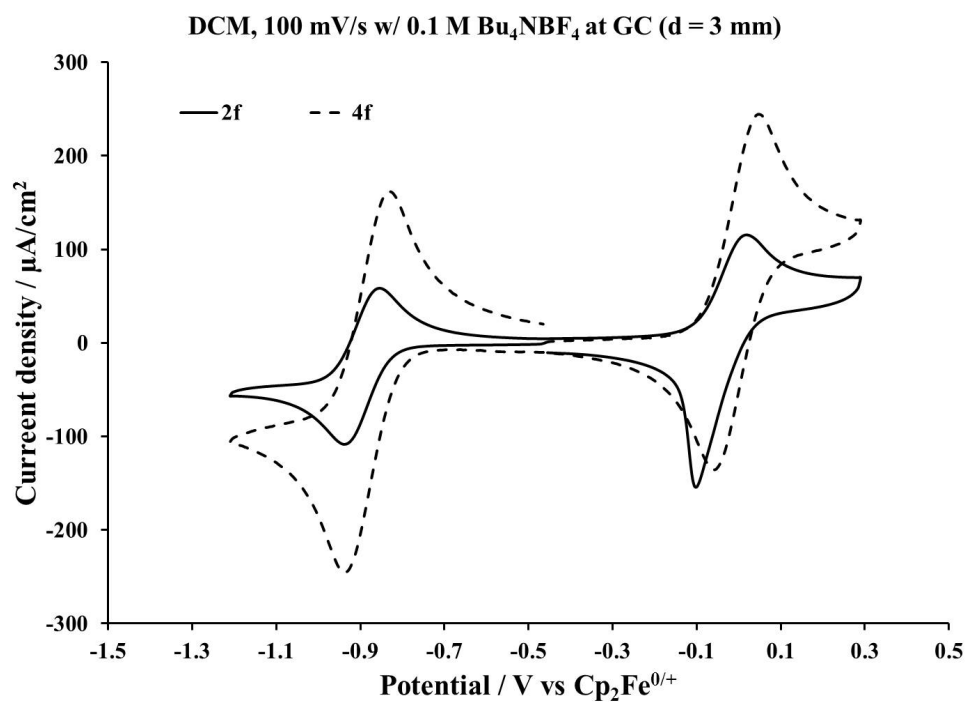**DCM, 100 mV/s w/ 0.1 M Bu$_4$NBF$_4$ at GC (d = 3 mm)**

Figure S1. Cyclic voltammograms of 1 mM solutions of **2f** (—) and **4f** (- -) in dichloromethane with 0.1 M [Bu$_4$N][BF$_4$] as supporting electrolyte and v = 0.1 V/s at a glassy carbon working electrode (d = 3 mm).

Table S1: Electrochemical data for **2a-d**, **f**, **g** and **3a** in acetonitrile and dichloromethane (0.1 M [Bu$_4$N][BF$_4$] supporting electrolyte) vs. Cp$_2$Fe$^{0/+}$ at 0.1 V/s at a glassy carbon working electrode (d = 3 mm).

	CH$_3$CN		CH$_2$Cl$_2$	
	E_{red} (V)[a]	ΔE (mV)	E_{red} (V)[a]	ΔE (mV)
2a	-2.23	76	-1.34[b]	N/A
	-1.50	76		
	-1.01	124		
3a	-0.88	160	+0.31[b]	N/A
	-1.47	75	-1.28[b]	N/A
			-1.65[b]	N/A
			-1.83[b]	N/A
2b	+0.07[b]	N/A	+0.14[b]	N/A
	-0.65	70	-1.18	110
	-1.10	95		
	-1.55	95		
	-1.94[b]	N/A		
2c	+0.13[d]	N/A	+0.03[b]	N/A
	-0.69	70	-1.22	120
	-1.11	120		
2d	-0.88	75	-0.08[b]	N/A
			-1.26	140
2f	-0.94	75	-0.90	85
	-1.95[b]	N/A		
2g	-1.13[b]	N/A	-1.02	75
	-1.37[b]	N/A	-1.28	170
	-1.61[b]	N/A		
	-2.06[b]	N/A		

[a] half wave potentials, $E_{1/2}$, unless otherwise indicated. [b] irreversible reduction, E_{PC}.

Figure S2. ^{1}H NMR spectrum of **2b** in CD$_3$CN at 24°C.
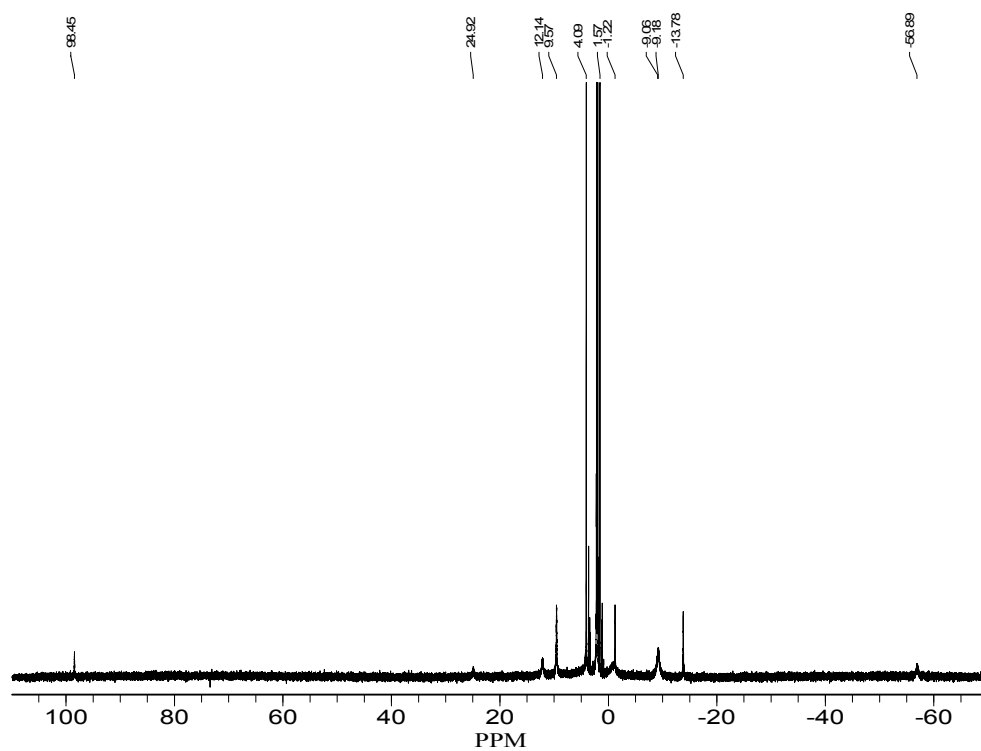
Figure S3. ^{1}H NMR spectrum of **2g** in CD$_3$CN at 24°C.

S 4
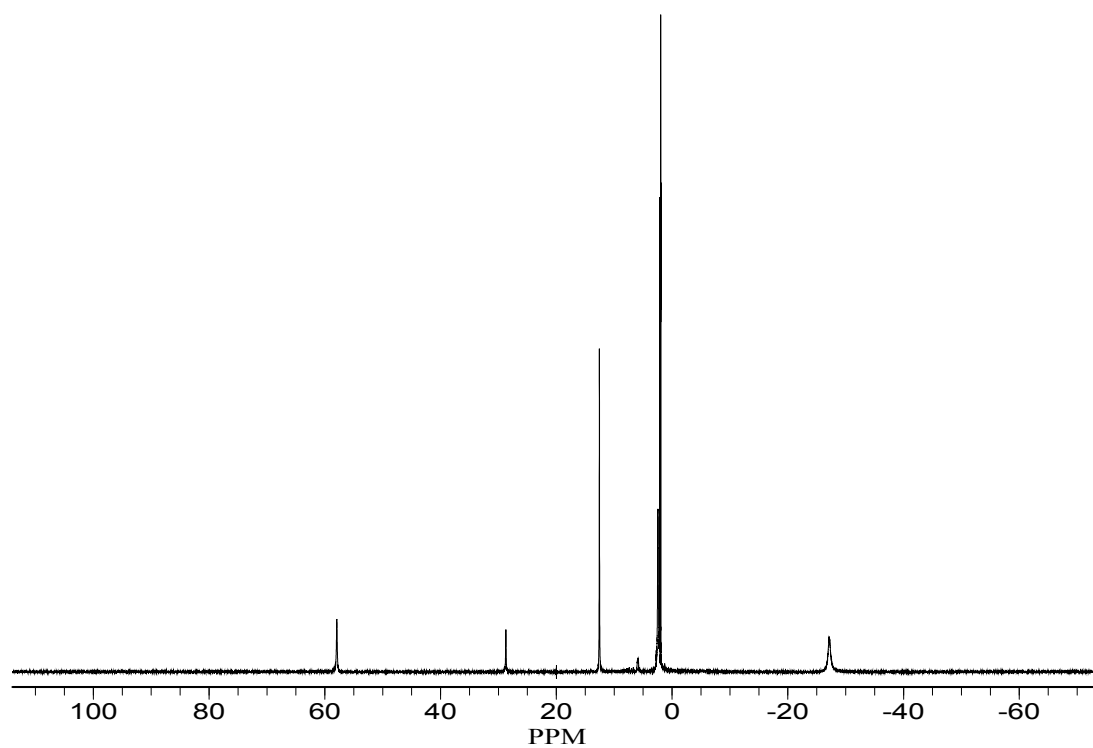
Figure S4. ^{1}H NMR spectrum of **4b** in CD$_3$CN at 24°C.

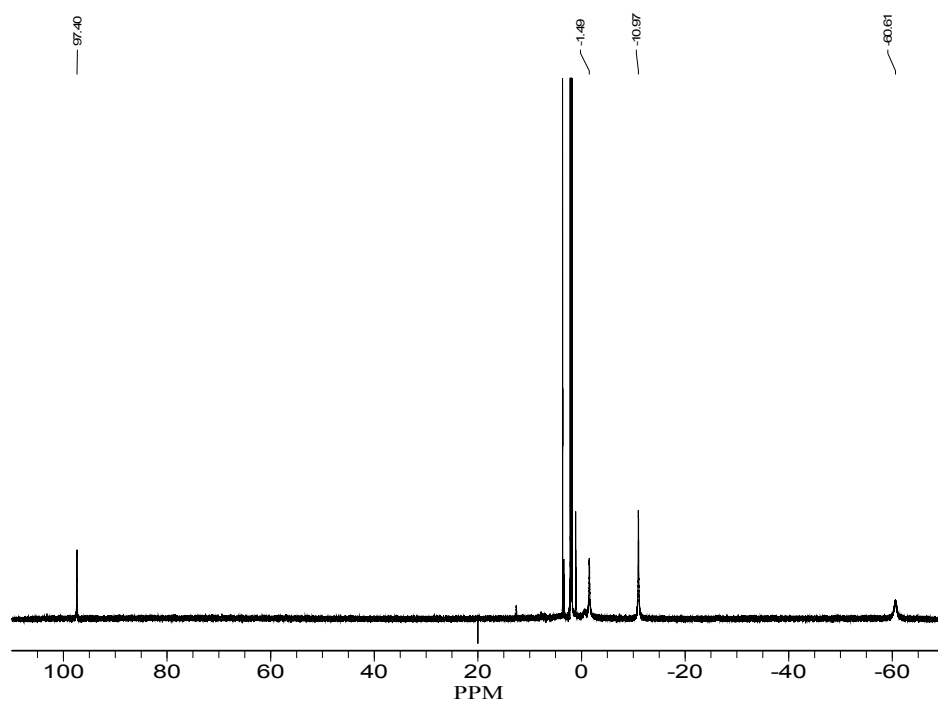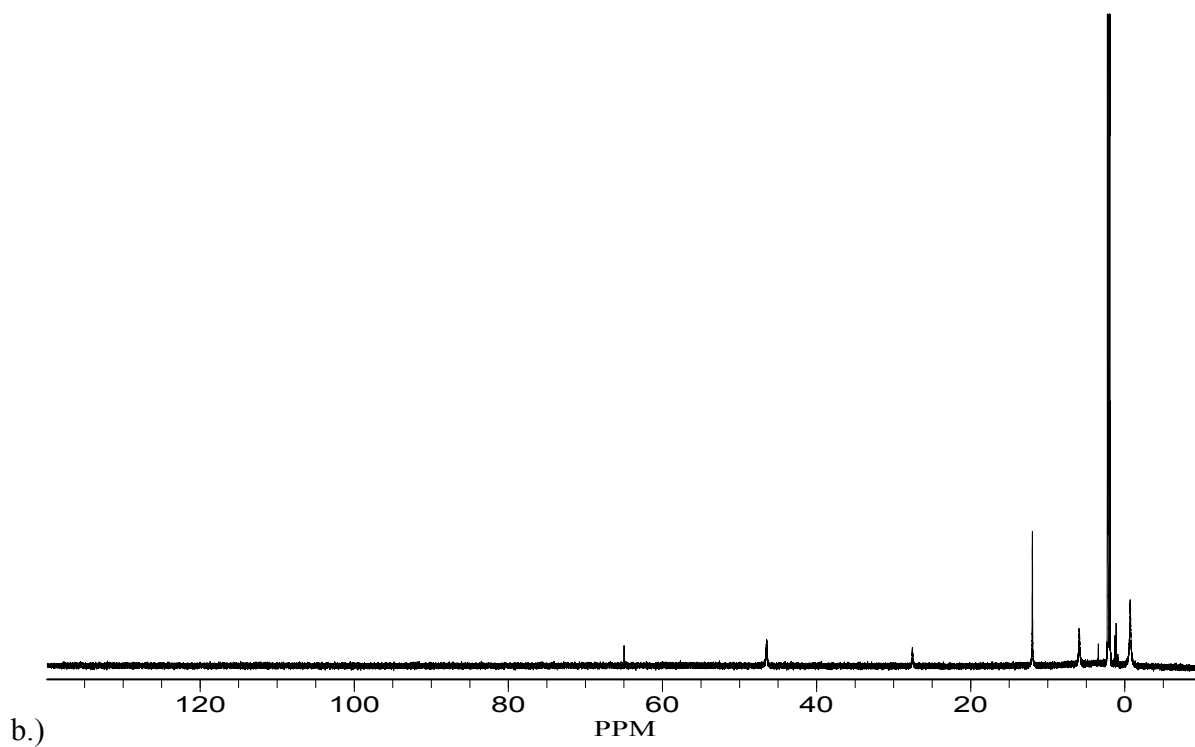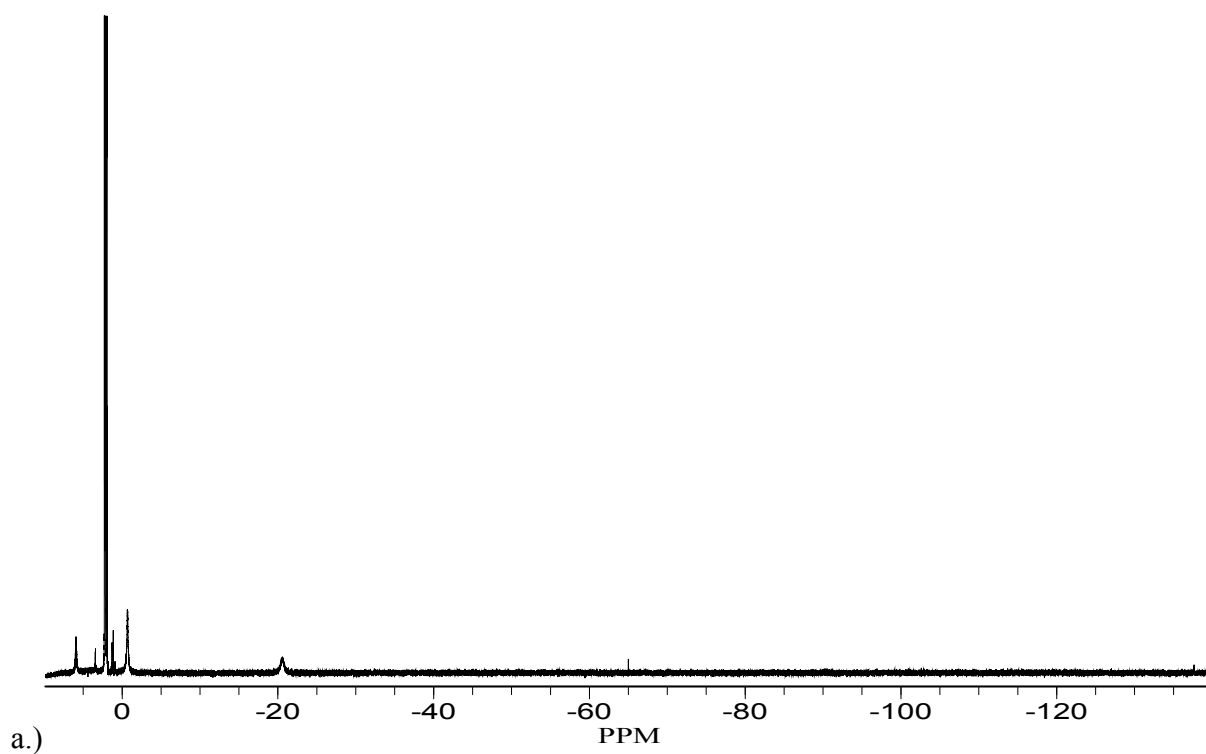Figure S5. a.) High field and b.) low field ^{1}H NMR spectrum of **4c** in CD$_3$CN at 22°C.
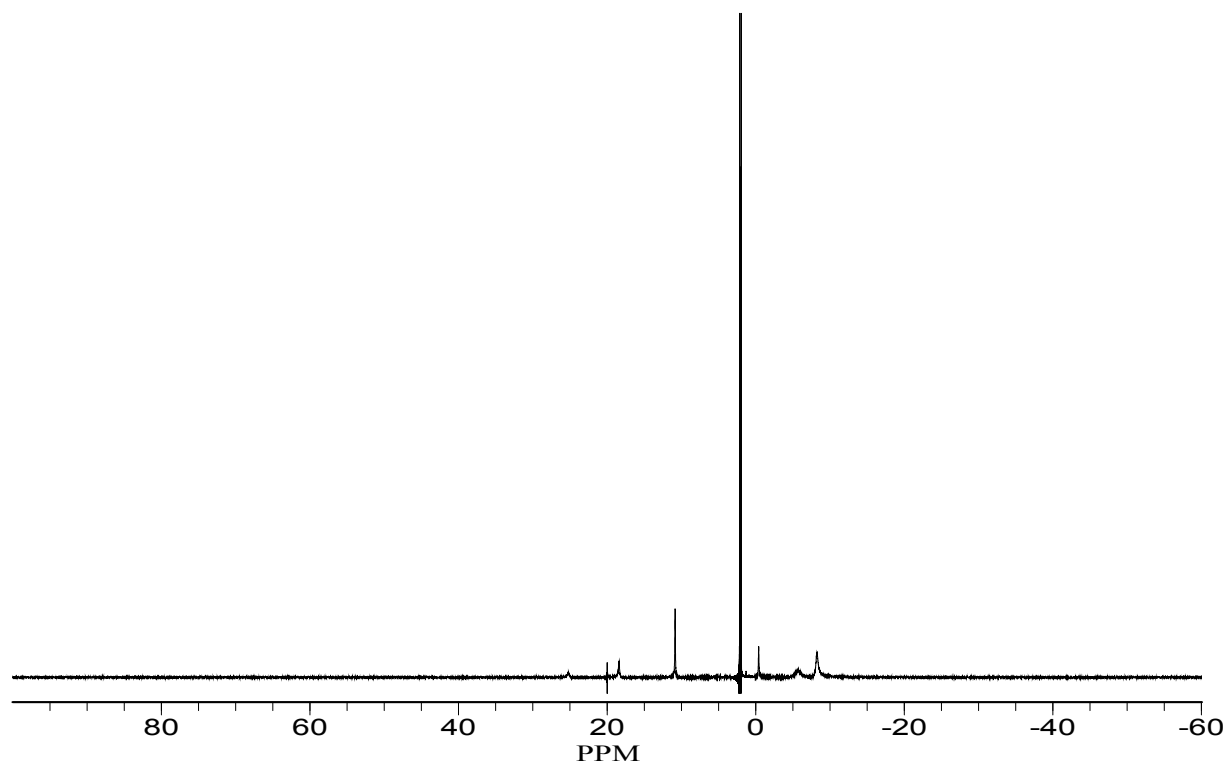
Figure S6. ^{1}H NMR spectrum of **4d** in CD$_3$CN at 24°C.
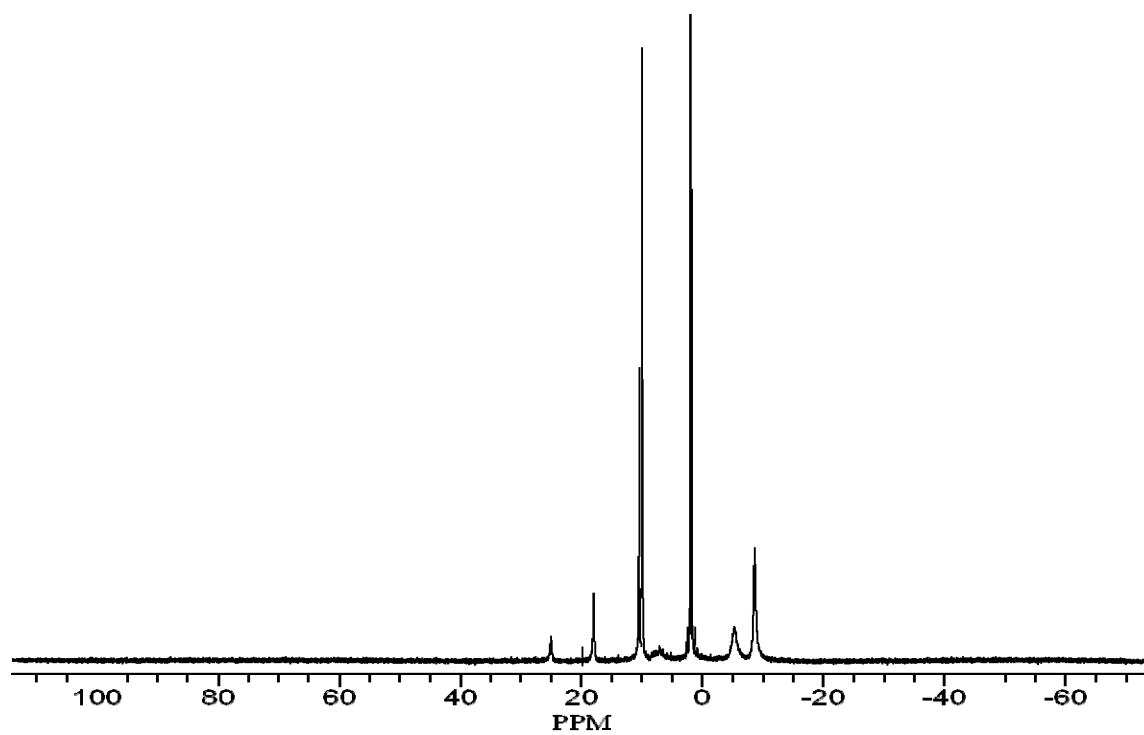
Figure S7. ^{1}H NMR spectrum of **4e** in CD$_3$CN at 24°C.

S 7
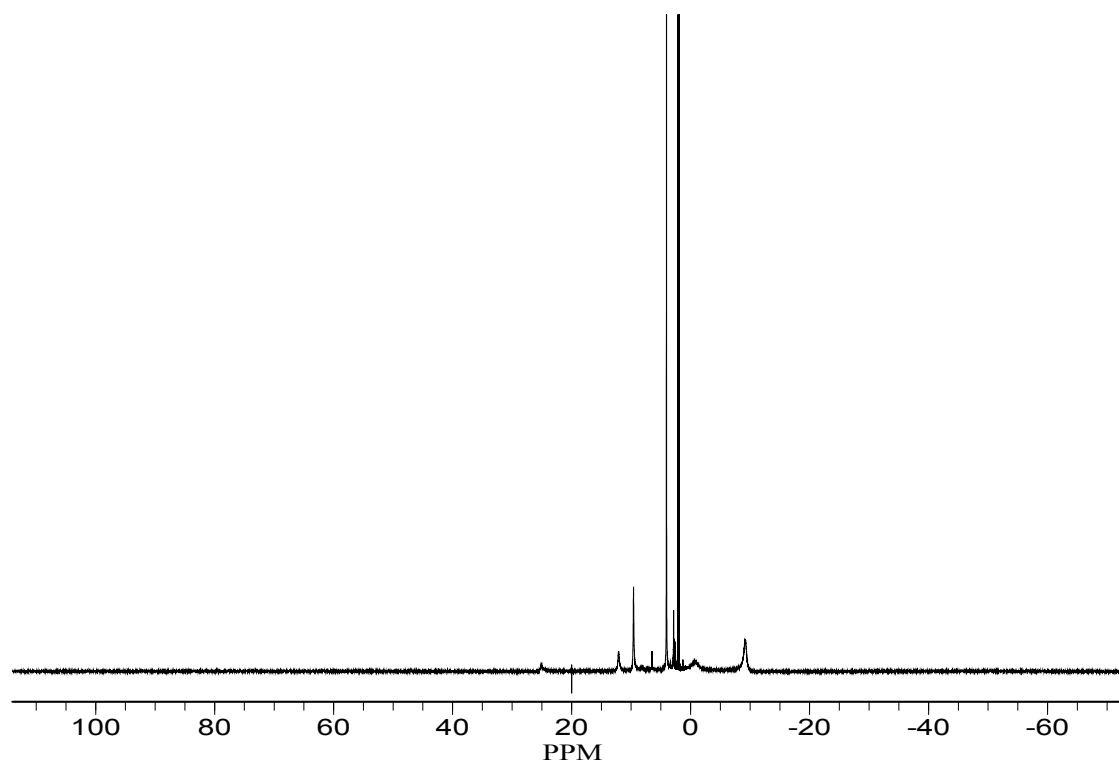
Figure S8. ^{1}H NMR spectrum of **4g** in CD$_3$CN at 24°C.

Table S2. Gas phase zero point energy (ZPE), entropy (S), Enthalpy (H$_g$) and Gibbs free energies (G$_g$) of investigated complexes, molecules and ions, which are relevant for the construction of the diagram in Figure 6.

Complexes/energetics	ZPE (kcal/mol)	S (cal mol^{-1} K^{-1})	H$_g$ (kcal/mol)	G$_g$ (kcal/mol)
2d R=H	224.710	178.947	-1281077.574	-1281130.927
2f R=OCH$_3$	265.347	203.456	-1424810.345	-1424871.014
2b R=CN	222.466	198.542	-1396872.453	-1396931.649
2d(DCM)	243.507	208.338	-1883333.084	-1883395.200
2d(AN)	253.899	201.974	-1364384.744	-1364444.962
2d$^+$	226.578	168.217	-1280921.161	-1280971.315
2d(AN)$^+$	256.539	195.457	-1364250.930	-1364309.205
2d(H$_2$O)$^+$	242.092	182.196	-1328908.713	-1328963.035

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2d(DCM)$^+$	245.498	200.147	-1883181.091	-1883240.765
5d	237.495	183.383	-1040106.89	-1040161.561
6d	236.747	171.456	-751075.102	-751126.221
7d	255.606	183.425	-799056.735	-799111.423
L$_2$Co^{II} – bis NNN				
R=OCH$_3$	529.498	303.821	-1602988.279	-1603078.863
R=H	448.490	252.681	-1315514.876	-1315590.213
R=CN	443.422	294.157	-1547080.848	-1547168.551
L$_2$Co^{III} – R=H	449.261	246.707	-1315252.784	-1315326.34
[CoCl$_4$]$^{2-}$	2.169	94.401	-1246401.121	-1246429.266
[CoCl$_4$]$^-$	2.619	94.254	-1246388.938	-1246417.04
H$_2$O	13.417	45.141	-47962.682	-47976.141
Cl$^-$			-288839.644	-288850.577

Table S3. Total Gibbs free energies of R =H complexes. It is obtained from the sum of the gas phase Gibbs free energy (Table S2) and the solvation energy.

Complex/solvents	Gibbs free energies (kcal/mol)		
	H$_2$O	ACN	DCM
2d	-1281161.19	-1281162.892	-1281158.741
2d R=H	-1281161.190	-1281162.892	-1281158.741
2f R=OCH$_3$	-1424903.300	-1424905.296	-1424899.980
2b R=CN	-1396974.070	-1396975.720	-1396969.631
2d(DCM)			-1883417.894
2d(AN)		-1364478.9572	
2d$^+$	-1281020.962	-1281022.058	-1281016.452
2d(AN)$^+$		-1364359.755	
2d(H$_2$O)$^+$	-1328959.519		
2d(DCM)$^+$			-1883283.899
5d	-1040215.682	-1075549.001	
6d	-751289.350		
7d	-799264.136		
L$_2$Co – bis NNN			
R=OCH$_3$	-1603198.525	-1603200.447	-1603188.159
R=H	-1315711.422	-1315712.398	-1315700.850
R=CN	-1547334.803	-1547333.956	-1547316.073
L$_2$Co^{III} – R=H			
[CoCl$_4$]$^{2-}$	-1246611.737	-1246611.08	-1246594.894
[CoCl$_4$]$^-$	-1246460.914	-1246462.555	

Table S4. Hydration energy of H_2O molecule and the experimental solvation energies of Cl^- in water and acetonitrile.[2]

	Solvation energies (kcal/mol)	
	H_2O	ACN
Cl^-	-72.6	-60.5
H_2O	-2.05	

In Figure S9 (a) we display the optimized structure of **2d** with R=H. The bond lengths and angles display good agreement with the experimental structure, but the *N*-aryl group is rotated with respect to the equivalent one in the crystal structure. This difference may come from the packing in the crystal. We have carried out some constrained optimization forcing the orientation of *N*-aryl group to be closer to the crystal orientation and it was found to give a negligible change in the gas phase free energy, having a more significant effect on the solvation energy (~ 3 kcal/mol). Since the optimized structure more accurately represents the structure in solution we have used the fully optimized structure in our investigation.
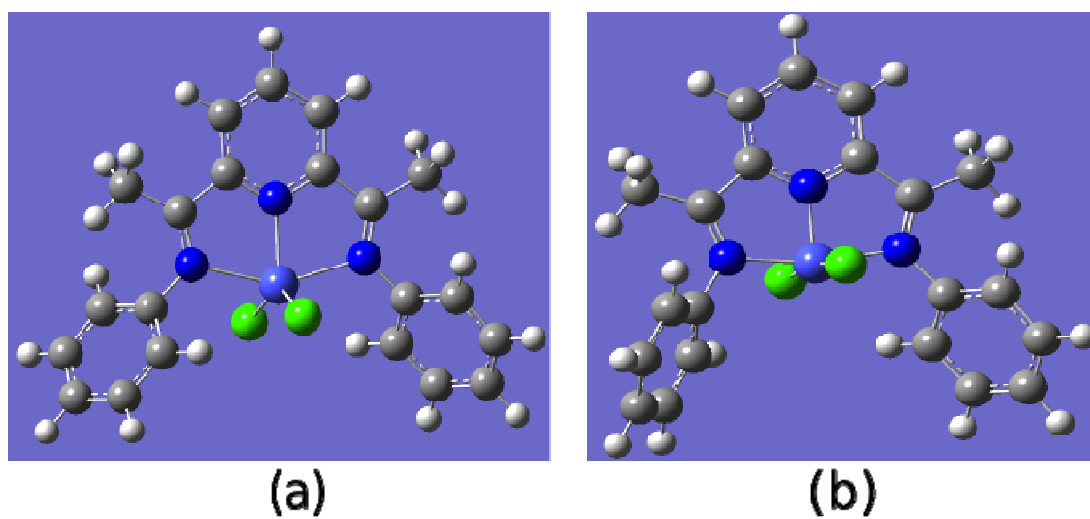
Figure S9. Optimized structures of (a) **2d** and (b) **2d**$^+$ (R=H).
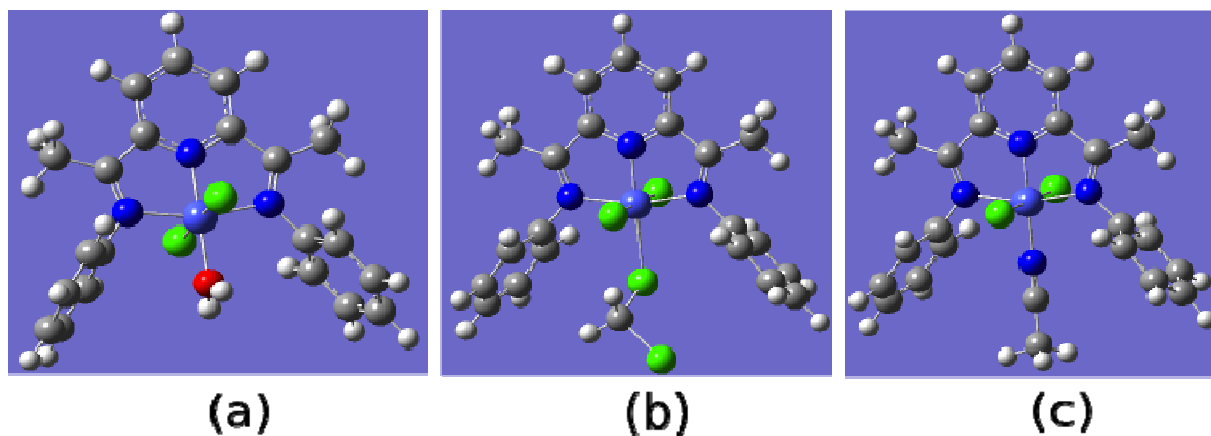
Figure S10. Optimized structures of **2d(solv)**$^{+}$ for (a) H_2O, (b) CH_2Cl_2 and (c) CH_3CN.
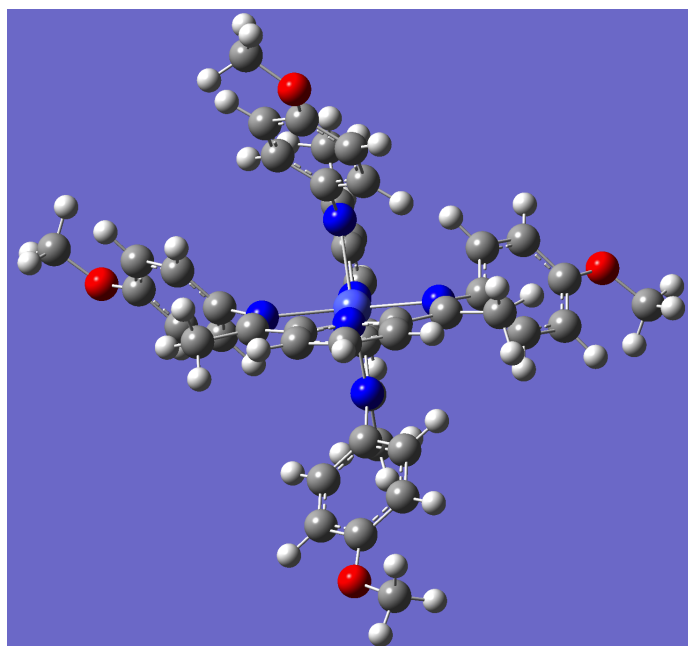
Figure S11. Optimized structure of $[(1f)_2Co]^{2+}$ (R=OCH_3).

References:

1.   B. de Bruin, E. Bill, E. Bothe, T. Weyhermuller and K. Wieghardt, *Inorg. Chem.*, 2000, **39**, 2936-2947.
2.   (a) C. P. Kelly, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2007, **111**, 408-422; (b) J. Sefcik and W. A. Goddard, III, *Geochim. Cosmochim. Acta*, 2001, **65**, 4435-4443.

Appendix: Cartesian coordinates of optimized complexes:

2d

Co	12.8719496076	2.1305201702	4.2779512996
N	14.6072878371	1.3329164244	3.5100584372
N	14.4889599643	3.0941267418	5.4969818054
N	12.1920148482	0.7192955565	2.6745880344
C	15.7823529489	1.7433867415	4.0341708234
C	16.9875171198	1.2488108699	3.5131771402
C	16.9389483434	0.3307391602	2.4581262547
C	15.7082982202	-0.0787962180	1.9381033118
C	14.5317784375	0.4517891069	2.4920671710
C	15.6881315362	2.7345830140	5.1462777322
C	16.9696531663	3.2044300551	5.7888943912
C	13.1538112583	0.1060155054	2.0514331923
C	12.9899500523	-0.8770268366	0.9185517257
C	14.1814087136	4.0911556486	6.4685971515
C	13.2066969521	3.7875877204	7.4357744430
C	12.8448578072	4.7558486517	8.3746035475
C	13.4192446953	6.0333644179	8.3372536969
C	14.3627132971	6.3434189996	7.3502849872
C	14.7511606118	5.3770270187	6.4184868990
C	10.8040094600	0.4584987503	2.4671773646
C	10.2782883158	-0.8415320199	2.5812916925
C	8.9037367086	-1.0483701760	2.4370402237

C	8.0524003141	0.0302282732	2.1684096806
C	8.5798841269	1.3243384189	2.0669971961
C	9.9485851401	1.5484597331	2.2315103578
H	17.9392239403	1.5699940359	3.9142797783
H	17.8596610624	-0.0633311825	2.0427782351
H	15.6658623131	-0.7901923606	1.1244023836
H	16.7661105326	3.7560914959	6.7068739605
H	17.6072210554	2.3478239723	6.0347667509
H	17.5394191262	3.8603360169	5.1185398849
H	11.9560825248	-0.9073737474	0.5744211618
H	13.6265696988	-0.5913010622	0.0731172286
H	13.2764675610	-1.8920695770	1.2215244855
H	12.0981595488	4.5160158983	9.1243491074
H	13.1198729697	6.7867227397	9.0586862092
H	14.7874711517	7.3405431503	7.2958683701
H	8.4985408949	-2.0492025106	2.5473780502
H	6.9854035678	-0.1338812080	2.0571197810
H	7.9227606277	2.1667710300	1.8768040246
H	10.9324365228	-1.6684957393	2.8356403566
H	10.3677396314	2.5475595710	2.1906839822
H	15.4452938349	5.6314954780	5.6250753267
H	12.7428838732	2.8069803844	7.4271967320
Cl	11.8999958554	0.7587538653	5.9248025943
Cl	12.3494079286	4.0793823156	3.0616194836

2d+

Co	13.0710532624	1.9263487756	4.2553978447
N	14.6035127856	1.4366664247	3.4177105655
N	14.2826296396	2.9625526186	5.3912642666
N	12.2253077559	0.8241753243	2.8773294801
C	15.7600526747	1.9229686152	3.9145669466
C	16.9554446032	1.5458022392	3.2904739052
C	16.8923119818	0.6824922314	2.1862038388
C	15.6625888568	0.2032630551	1.7098609214
C	14.4900043154	0.6039346268	2.3618667473
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C	13.4958800461	6.0837841321	7.2800725733
C	14.0779246968	5.2242449758	6.3465093479
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C	8.7699537017	1.1867248582	1.5149450024

C	10.1648282889	1.1662310329	1.5709744796
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H	12.1570998885	6.2585254825	8.9636110143
H	13.7267530784	7.1426649821	7.2490115546
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H	6.9286032099	0.8429277018	2.5866791948
H	8.2758406654	1.4979101772	0.6014338665
H	10.5524851963	0.1400877974	4.8131631593
H	10.7525104257	1.4934258791	0.7210063879
H	14.7280750194	5.6149985157	5.5722521365
H	12.6179802257	2.2920101942	7.3391710086
Cl	13.1155903401	0.1755636886	5.7081449688
Cl	12.6676881328	3.7683706358	3.0157376671

2d(MeCN)$^+$

Co	12.9785254256	1.9393049883	4.2247668839

N	14.5780443427	1.4690582503	3.4199831696
N	14.1936816122	2.9530095064	5.4103889368
N	12.2422613806	0.7868380690	2.7940686982
C	15.7160439909	1.9675049498	3.9403830291
C	16.9390505843	1.6306463370	3.3501740306
C	16.9316324160	0.7831155086	2.2330360239
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C	15.4587975217	2.8368636614	5.1087900745
C	16.5915142713	3.4908776946	5.8380070025
C	13.1441671050	0.2714379899	2.0026164291
C	12.8696494289	-0.6344175352	0.8418261085
C	13.7080616544	3.7602992269	6.5013887067
C	13.4389104213	3.1520784751	7.7364462072
C	12.9381788741	3.9358506222	8.7815927917
C	12.6983513171	5.3034399325	8.5902057761
C	12.9568476865	5.8932299645	7.3459060425
C	13.4610213185	5.1249224493	6.2906699681
C	10.8268440890	0.5699742348	2.6342603804
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C	8.7269971003	1.1592521120	1.5981728701
C	10.1082788284	1.3499865489	1.7161538337
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H	13.6415293085	5.5608362333	5.3145226315
H	13.6097795121	2.0886244730	7.8602022647
Cl	13.1508970513	0.0929437484	5.6291301432
Cl	12.8289148022	3.7758174138	2.8087522316
N	11.3154267891	2.4387167333	5.0519055064
C	10.3063777846	2.7452921853	5.5383169632
C	9.0383827746	3.1265610194	6.1389025734
H	8.2158182033	2.6086926415	5.6354694594
H	9.0244211069	2.8589462580	7.2003449958

H	8.8839358624	4.2063828437	6.0453032075

2d(H$_2$O)$^+$

Co	13.0258547115	1.9043853003	4.2209721207
N	14.6177334718	1.4589668152	3.3970023758
N	14.2369901689	2.9284170630	5.4011126741
N	12.2766114999	0.7592625647	2.7929329674
C	15.7557024376	1.9651638614	3.9118867969
C	16.9753979502	1.6430466883	3.3063331408
C	16.9617967568	0.8045049040	2.1817125772
C	15.7543429703	0.3011871654	1.6757491653
C	14.5620589049	0.6522917979	2.3193211060
C	15.5006016652	2.8264250063	5.0898094176
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C	13.1734107916	0.2624617229	1.9834453381
C	12.8924906423	-0.6290824070	0.8134739068
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C	13.4817660881	3.1073528102	7.7302442758
C	12.9506261922	3.8746627542	8.7727711760
C	12.6660531477	5.2331013516	8.5793108919
C	12.9130284269	5.8306392782	7.3364099025
C	13.4462997081	5.0788809342	6.2834161330
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C	10.1961386514	-0.3163089734	3.5181727287
C	8.8133315894	-0.4806211351	3.3936741756

C	8.0989196721	0.2330576078	2.4217529439
C	8.7706547573	1.1140210435	1.5651156166
C	10.1557050155	1.2821359612	1.6695307632
H	17.9071624198	2.0326428105	3.6953068015
H	17.8950766058	0.5433504704	1.6973481365
H	15.7449451885	-0.3433153289	0.8063730789
H	16.2767695858	4.0466444330	6.6797393837
H	17.3575348138	2.7408492153	6.1542093515
H	17.1586104088	4.1837298744	5.1470793770
H	13.1341061189	-0.1184299385	-0.1274367588
H	13.5075866244	-1.5348329014	0.8673788640
H	11.8435177558	-0.9226348942	0.7818161858
H	12.7618048912	3.4100656130	9.7347113114
H	12.2546558374	5.8219292077	9.3918308516
H	12.6917428284	6.8814093929	7.1832542410
H	8.2951783153	-1.1657084938	4.0560670901
H	7.0256101412	0.1043158677	2.3340352300
H	8.2196989154	1.6728904309	0.8165604760
H	10.7614104015	-0.8507405286	4.2729300995
H	10.6820985923	1.9827849161	1.0311964955
H	13.6204592542	5.5228819278	5.3098196746
H	13.6940227616	2.0522778992	7.8605889720
Cl	13.1630682778	0.0916025126	5.6521272362
Cl	12.7619337181	3.7605072933	2.8671192924
O	11.3559874900	2.3824470239	5.0695281714

H	11.0502181889	1.9335534539	5.8757553806
H	10.9128777405	3.2166955993	4.8376072117

2d(DCM)⁺ 2d(DCM)$^+$

Co	-0.16753656	-0.11922382	-0.42058853
N	-0.64775064	0.14338645	-2.18139493
N	1.65718560	-0.08596470	-1.19214741
N	-2.13901402	-0.07095130	-0.16129206
C	0.33942372	0.22845763	-3.09409177
C	0.00286497	0.42607563	-4.43782178
C	-1.35259163	0.52832755	-4.78157595
C	-2.34856911	0.43531602	-3.79895865
C	-1.96053147	0.23716278	-2.46931959
C	1.67982408	0.09259624	-2.48592462
C	2.91101785	0.15292350	-3.33589598
C	-2.81078985	0.11251485	-1.26677945
C	-4.30216049	0.18972447	-1.37902966
C	2.85278975	-0.21729917	-0.39583521
C	3.28236945	-1.49506808	-0.00913438
C	4.42531895	-1.61082268	0.78744161
C	5.11989469	-0.46700215	1.20140982
C	4.67258143	0.80323775	0.81714619
C	3.53428962	0.93781648	0.01567648
C	-2.76727597	-0.17518538	1.13187257
C	-2.89610342	-1.43535202	1.73389568

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C	-3.47568580	-1.52337771	3.00340988
C	-3.90578254	-0.36747253	3.66919712
C	-3.76008634	0.88671522	3.06188811
C	-3.18997401	0.99170144	1.78800619
H	0.77341507	0.49880923	-5.19417524
H	-1.63332184	0.68119092	-5.81670414
H	-3.39524552	0.51537918	-4.06200408
H	3.80858657	-0.03645410	-2.74849224
H	2.85577509	-0.59199926	-4.13881063
H	3.00711272	1.14056569	-3.80421145
H	-4.61286930	1.19030402	-1.70544922
H	-4.66517700	-0.52967849	-2.12249192
H	-4.78490867	-0.02363541	-0.42603748
H	4.76785624	-2.59478828	1.08808812
H	6.00181846	-0.56475923	1.82480965
H	5.20410097	1.69031581	1.14335633
H	-3.58634526	-2.49468489	3.47266700
H	-4.35194217	-0.44382064	4.65474200
H	-4.09244582	1.78295336	3.57451223
H	-2.53542331	-2.31720405	1.21756213
H	-3.05422243	1.95794211	1.31479790
H	3.16314125	1.91601569	-0.26898623
H	2.72019451	-2.36901605	-0.31660549
Cl	-0.25351356	-2.40085035	-0.72228555
Cl	-0.08400168	2.17299389	-0.10948603

Cl	0.47783798	-0.62161733	1.91125813
C	0.49568947	0.92777164	3.03332723
H	0.38736054	1.76565945	2.35215988
H	-0.32505953	0.77701153	3.72516304
Cl	2.06550429	1.05012523	3.95594979

2d(DCM)

Co	12.0217756563	3.6835803070	5.4440532578
N	13.7913157689	2.9289191041	4.7106411831
N	13.6377042244	4.7463331299	6.6401198735
N	11.3843979888	2.2059268665	3.8488610806
C	14.9564397700	3.3698158469	5.2346294547
C	16.1744183113	2.8709214384	4.7464041781
C	16.1517300382	1.9179271050	3.7242722610
C	14.9323410215	1.4770084308	3.2017005204
C	13.7418316826	2.0099000084	3.7201555820
C	14.8445383704	4.3984090007	6.3079983440
C	16.1180133888	4.9111758247	6.9351032709
C	12.3795757729	1.6121567069	3.2617403029
C	12.2723467194	0.6007675518	2.1470406751
C	13.3220420833	5.7838067137	7.5659880291
C	12.3677628597	5.5157072075	8.5622298925
C	12.0000612833	6.5250370961	9.4542376983
C	12.5490428460	7.8081868359	9.3410319097
C	13.4757136234	8.0819198062	8.3277865032

C	13.8701702298	7.0747472175	7.4431961365
C	10.0113363318	1.8917569950	3.6287752415
C	9.5320277088	0.5715940213	3.7247964890
C	8.1659936106	0.3184635469	3.5751804352
C	7.2775631286	1.3696343635	3.3181408452
C	7.7577096262	2.6820838720	3.2322789688
C	9.1168356724	2.9519588812	3.4034734360
H	17.1156138760	3.2169429771	5.1508589058
H	17.0821911612	1.5195241684	3.3355236072
H	14.9096223741	0.7373972271	2.4129523879
H	15.9016722587	5.5029607359	7.8246117567
H	16.7621229634	4.0737705915	7.2268553112
H	16.6874226359	5.5411643254	6.2401774378
H	11.2493777631	0.5397379292	1.7754981539
H	12.9255669829	0.8831153706	1.3134717051
H	12.5719611608	-0.4012134061	2.4788266456
H	11.2610705477	6.3142416325	10.2190175255
H	12.2414018075	8.5941904514	10.0228368789
H	13.8816487749	9.0820792277	8.2157156393
H	7.7958248651	-0.6968967608	3.6735883850
H	6.2169704302	1.1695123488	3.2072729855
H	7.0709523063	3.5033109745	3.0614817497
H	10.2132863021	-0.2358179876	3.9707216220
H	9.4967619443	3.9668206340	3.3808921636
H	14.5514163954	7.2991355245	6.6296205173

H	11.9201937982	4.5299338722	8.6122420358
Cl	10.9702323699	2.5147916462	7.1719211247
Cl	11.2181621082	5.6654872261	4.5040705022
C	8.4025647347	5.2450194855	6.9580125177
H	9.0128010796	5.7592608224	6.2229021018
H	8.8149409274	4.2917793537	7.2718401599
Cl	8.2760473971	6.3391203936	8.4631420529
Cl	6.7327543137	4.9221099592	6.1920648863

2d(MeCN)

Co	12.8369154357	1.5421626133	4.4492293013
N	14.4942559334	1.8978843098	3.2709219638
N	14.1128091418	2.8464982288	5.7125098149
N	12.3989471373	0.5165734071	2.4979258258
C	15.4957211350	2.6332288718	3.7979094231
C	16.6762411455	2.8285998260	3.0687800306
C	16.7895721853	2.2429634970	1.8023002757
C	15.7374253760	1.4848670841	1.2789091186
C	14.5740458768	1.3237420627	2.0527992222
C	15.2338658282	3.1937427335	5.1561986097
C	16.2873065597	4.0675381696	5.7865219853
C	13.3604076330	0.5736867084	1.6260407721
C	13.3567567165	-0.0690032690	0.2617801259
C	13.6506240886	3.3160199767	6.9818856318
C	13.3425206465	2.3616858396	7.9632172336

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C	12.8412712314	2.7883874118	9.1961799015
C	12.6063503431	4.1459423006	9.4367876419
C	12.8751415704	5.0853513831	8.4407555732
C	13.4088469160	4.6786160139	7.2153227590
C	11.1089050903	-0.0374987382	2.2441694283
C	10.5738561236	-0.9393241290	3.1801654762
C	9.2880006488	-1.4460182500	2.9891342641
C	8.5178674424	-1.0393563933	1.8932139987
C	9.0428147775	-0.1190051886	0.9783521266
C	10.3368716962	0.3798480014	1.1447429973
H	17.4865805086	3.4195817009	3.4721762764
H	17.6958946707	2.3790241429	1.2235851741
H	15.8182295433	1.0356980570	0.2978976884
H	16.0323644176	4.3010815600	6.8199781378
H	17.2585846536	3.5608384844	5.7754291215
H	16.4001685939	5.0123895614	5.2421064405
H	13.3264755621	0.6810541806	-0.5382392828
H	14.2660095331	-0.6643124329	0.1224587594
H	12.4952811205	-0.7251222299	0.1419128127
H	12.6148595010	2.0532638030	9.9595692631
H	12.1944062383	4.4654037022	10.3877240363
H	12.6454218695	6.1305516555	8.5981495807
H	8.8810249542	-2.1457891494	3.7110059742
H	7.5115804603	-1.4223268202	1.7623927826
H	8.4412375457	0.2223751048	0.1423528440

H	11.1694735595	-1.2174665323	4.0422085675
H	10.7256537058	1.1295761193	0.4641734342
H	13.5730692813	5.4000675874	6.4249439200
H	13.4850019990	1.3106237927	7.7424219999
Cl	13.1900838314	-0.4883220207	5.6087851556
Cl	11.0264374358	2.9932930758	4.1095127993
N	10.2149587636	6.7669446176	6.4437355214
C	9.4343182547	6.1063342168	5.9415316786
C	8.4621888743	5.2778434271	5.2988704410
H	7.6570490790	5.0712611691	5.9653518396
H	8.0597097200	5.7707040187	4.4061498020
H	8.9258069507	4.3667315477	4.9960828057

2f – R=OCH$_3$

Co	12.8473651152	2.1177870132	4.2238990837
N	14.6469294629	1.5284739400	3.3822679856
N	14.3889872812	3.1501497876	5.3990166567
N	12.2892975041	0.8074791122	2.5483599964
C	15.7988307658	1.9673915633	3.9332563273
C	17.0332079440	1.5433351721	3.4175943286
C	17.0407251586	0.6560500651	2.3367442180
C	15.8347973851	0.2025923943	1.7935262537
C	14.6290112726	0.6593566845	2.3487680233
C	15.6246370243	2.8906906293	5.0797882166
C	16.8470968364	3.3852246214	5.8090530559

C	13.2756445736	0.2626080888	1.8940354403
C	13.1479327062	-0.7624663282	0.7966330526
C	13.9877983764	4.0410028588	6.4378501841
C	13.0246612307	3.5931168187	7.3653110764
C	12.5759405849	4.4485447777	8.3621241499
C	13.0452075211	5.7715276033	8.4265350958
C	13.9798835314	6.2344473383	7.4903980926
C	14.4538453532	5.3630230671	6.5039053621
C	10.9084340914	0.6118370413	2.2584838772
C	10.0385739596	0.3593500344	3.3321051551
C	8.6691410144	0.2145402835	3.1090563811
C	8.1540154983	0.3601372854	1.8124553388
C	9.0151653463	0.6377091217	0.7383638706
C	10.3832325536	0.7569936084	0.9575242489
H	17.9621092508	1.8965815421	3.8455191257
H	17.9828991995	0.3174880387	1.9206149340
H	15.8334910358	-0.4858618608	0.9590541115
H	16.5732513836	3.8458556752	6.7587223099
H	17.5279947102	2.5513288355	6.0130939601
H	17.3997001444	4.1273780039	5.2187191547
H	13.3942868811	-0.3407106098	-0.1863153691
H	13.8324095072	-1.5981901349	0.9789224872
H	12.1320707634	-1.1561867287	0.7488168682
H	11.8434985862	4.1235196423	9.0908706051
H	14.3320145615	7.2582352933	7.5071429114

H	8.0195429120	0.0119429630	3.9509216782
H	8.5868453398	0.7725138654	-0.2475275011
H	10.4503284450	0.2666832077	4.3314847521
H	11.0375175755	1.0162820274	0.1323016474
H	15.1468902366	5.7322239244	5.7552803139
H	12.6539435915	2.5764979188	7.2887911175
Cl	12.6860213065	0.2940319378	5.8386834311
Cl	11.1874350578	3.7148900492	4.1566387386
O	12.5155305936	6.5430973057	9.4510655441
O	6.8100373411	0.2573211222	1.4868608293
C	5.8411876621	0.0713741502	2.5552850491
H	4.8710988936	0.0618879950	2.0598456972
H	6.0012627429	-0.8803065917	3.0748394615
H	5.8845785211	0.8968465955	3.2744586684
C	12.8867262656	7.9435165490	9.5427612918
H	12.3285190652	8.3304017610	10.3944868358
H	13.9620954966	8.0595654600	9.7225177429
H	12.6028813666	8.4884604476	8.6350355399

2b – R=CN

Co	12.9410716189	2.0879411465	4.2244952500
N	14.6958042197	1.4954878619	3.2924808878
N	14.5358005763	3.0997278846	5.3194819085
N	12.3052451305	0.7857090839	2.5931087241
C	15.8750134074	1.9168375051	3.7953263179

C	17.0807740217	1.4717872669	3.2347397146
C	17.0322919695	0.5803767633	2.1576279319
C	15.7980186780	0.1423113448	1.6658105685
C	14.6252423311	0.6215300831	2.2666793680
C	15.7550355130	2.8362424289	4.9548559880
C	17.0038825846	3.3241135081	5.6395948119
C	13.2441113873	0.2335796629	1.8841047384
C	13.0403752731	-0.7810096044	0.7907534824
C	14.1733867508	3.9733630206	6.3875650515
C	13.3548685936	3.4649925371	7.4101429502
C	12.9369834497	4.3078653175	8.4356763421
C	13.3091516218	5.6674759353	8.4366325286
C	14.1076424599	6.1741627919	7.3932080656
C	14.5420854125	5.3292165596	6.3745697525
C	10.9066382648	0.5852669308	2.3954023412
C	10.1427437263	0.1309485314	3.4835906526
C	8.7665596798	-0.0181034798	3.3397957760
C	8.1381975762	0.3083940119	2.1209731695
C	8.9085117318	0.7879031495	1.0440821205
C	10.2884763786	0.9215977663	1.1791052344
H	18.0310854627	1.8077014983	3.6285829036
H	17.9517125563	0.2237941781	1.7080478772
H	15.7511660352	-0.5555451344	0.8400684389
H	16.7660454228	3.8596419008	6.5587554011
H	17.6510197576	2.4765340029	5.8930234858

H	17.5775935661	3.9975930526	4.9906568216
H	13.3448673801	-0.3822798932	-0.1850458901
H	13.6443094134	-1.6743599659	0.9871774544
H	11.9951586666	-1.0829183422	0.7227889318
H	12.3083388255	3.9233332067	9.2303361198
H	14.3740752460	7.2247360045	7.3827746429
H	8.1701228964	-0.3710691936	4.1729748949
H	8.4213329765	1.0602471134	0.1149415683
H	10.6394501570	-0.0877545966	4.4229590053
H	10.8777782033	1.3251378957	0.3632010234
H	15.1264748219	5.7256586957	5.5517040439
H	13.0548057883	2.4229125458	7.3778185873
Cl	12.9177786148	0.2390457376	5.8165383771
Cl	11.2665482038	3.6509716083	4.2699598482
C	12.8741594915	6.5327062173	9.4878640081
N	12.5258947699	7.2427268201	10.3552739882
C	6.7238227721	0.1605802697	1.9774649395
N	5.5637209667	0.0307699025	1.8545595904

L$_2$Co^{II} – R=H

Co	11.8590481763	2.7228254930	5.7278446279
N	9.9607534386	2.6847382437	5.3619043356
N	11.4552641948	4.8361628981	5.0216954676
N	11.3203034882	0.6237724010	6.2811419198
C	9.3327349978	3.8091318006	4.9273328079

C	7.9573021382	3.7936736342	4.6524988208
C	7.2406849965	2.6053723776	4.8108531449
C	7.9032167791	1.4566953905	5.2506688119
C	9.2746464041	1.5227332222	5.5316994537
C	10.1883159915	5.0126805575	4.7685960111
C	9.5524957257	6.2905895935	4.2854386158
C	10.0671180576	0.3700462028	6.0298951087
C	9.3779445631	-0.9513319155	6.2447638790
C	12.4202408217	5.8941909410	4.9801389434
C	13.5638726096	5.7293906770	4.1794045868
C	14.5335418166	6.7349997542	4.1329288870
C	14.3875688335	7.8954214424	4.9052432007
C	13.2588901611	8.0509364448	5.7192717189
C	12.2722286470	7.0597962370	5.7553830352
C	12.2514437889	-0.3702266153	6.7295951350
C	12.5691072985	-1.4879303724	5.9364221960
C	13.5217717688	-2.4107894746	6.3834917642
C	14.1502287732	-2.2342119080	7.6224056560
C	13.8277182869	-1.1231563996	8.4136012568
C	12.8931078025	-0.1846601214	7.9664180802
H	7.4557747639	4.6915201376	4.3183719971
H	6.1793077311	2.5747298890	4.5947478796
H	7.3627587150	0.5282744842	5.3753287130
H	10.3026430036	7.0413609036	4.0391813299
H	8.9512827261	6.1035178998	3.3886742266

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H	8.8837077179	6.7170012715	5.0433882793
H	10.0329764873	-1.6656396884	6.7426654153
H	8.4811858326	-0.8229934378	6.8615111112
H	9.0582738488	-1.3920341128	5.2922517253
H	15.3996929468	6.6179178501	3.4904001622
H	15.1430430701	8.6721624917	4.8689383122
H	13.1399279197	8.9476599649	6.3177318764
H	13.7628204878	-3.2722468545	5.7698311293
H	14.8774452147	-2.9584478849	7.9717440564
H	14.2984366273	-0.9931079433	9.3824258543
H	12.0744825437	-1.6329046184	4.9815193623
H	12.6298711941	0.6686563711	8.5812969409
H	11.3970055911	7.1849946540	6.3837474758
H	13.6655210691	4.8358321041	3.5742279771
N	13.7221765037	2.7251358251	6.0803738886
C	14.1698888823	3.1738664317	7.2782733000
C	15.5416808823	3.1816668752	7.5631315253
C	16.4363760795	2.6998067400	6.6012965500
C	15.9528227536	2.2284388222	5.3754428443
C	14.5732468925	2.2598533625	5.1332986669
C	13.0922939680	3.6120251585	8.1902643921
H	15.9044525357	3.5519628230	8.5128757689
H	17.5005929425	2.6913158306	6.8051390036
H	16.6347751414	1.8481012037	4.6263402863
C	13.9017671571	1.8372247011	3.8856021535

C	14.7275103175	1.3168991574	2.7433156859
H	14.1367891600	1.2038634267	1.8351799407
H	15.5586299417	1.9992093000	2.5310212920
H	15.1641392908	0.3400740619	2.9876330046
C	13.4465144572	4.1358344860	9.5535336042
H	12.5658814658	4.2460729957	10.1852531911
H	14.1467879968	3.4571392022	10.0554498948
H	13.9373968442	5.1149265698	9.4835699869
N	12.6034463386	2.0083810646	3.8836238710
N	11.8823857078	3.4600078958	7.7120768112
C	10.2000897735	0.9407229497	0.5555267813
C	10.3381588940	2.2843615160	0.9287106535
C	11.1236068165	2.6352409750	2.0314238306
C	11.7933611221	1.6342438228	2.7527992107
C	11.6622771427	0.2858915196	2.3794600302
C	10.8607240770	-0.0558474933	1.2844430722
H	9.5921685532	0.6740865475	-0.3016133702
H	9.8444977910	3.0599863169	0.3531087393
H	11.2502653532	3.6745073836	2.3121339859
H	12.1888147435	-0.4826761922	2.9354816874
H	10.7650279460	-1.0963786027	0.9935294158
C	8.4137469417	4.6557816287	9.8387967773
C	8.6236571243	3.3057708964	9.5267633671
C	9.7654894397	2.9120775313	8.8218172791
C	10.7158787113	3.8744720037	8.4455855802

C	10.5122337158	5.2289731480	8.7614768263
C	9.3582010175	5.6146933071	9.4521800632
H	7.5270354119	4.9561185860	10.3855388779
H	7.9029087475	2.5587923539	9.8415583352
H	9.9411327302	1.8673825261	8.5931291278
H	11.2491573512	5.9686220943	8.4670186795
H	9.2042114279	6.6598311910	9.6981132832

L$_2$Co^{II} – R=OCH$_3$

C	-6.2381812904	-9.4116348152	10.7474483873
C	-8.0730199580	-8.4309733878	12.0534004365
C	-9.1698980098	-7.5454745937	12.0512649202
C	-9.9087148008	-7.3428482657	13.2087551726
C	-9.5506508795	-7.9978233801	14.4046583673
C	-8.4539211524	-8.8762115684	14.4048016450
C	-7.7199486791	-9.1022540652	13.2360690189
C	-9.8355108450	-7.3594166718	16.7058110747
C	-8.4195895179	-6.8948010069	16.9104174325
C	-10.7856614107	-7.3108913129	17.8353914684
C	-10.4898336712	-6.8547764542	19.1269968813
C	-11.4956349287	-6.8691115791	20.0988979483
C	-12.7694206807	-7.3446061721	19.7733062633
C	-13.0146471912	-7.8002418688	18.4698945023
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C  -15.4936560426  -10.3731975078   15.3838447530
C  -20.1439796567   -9.8763324821   13.9953356422
C   -9.3116281988  -12.9965313657   21.4138096574
C  -10.7318788885  -12.5535224195   19.4597832657
C   -9.9304178335  -11.4980710439   18.9924849979
C  -10.2818039182  -10.8293844957   17.8152901057
C  -11.4083109957  -11.2194023966   17.0766873952
C  -12.2054674111  -12.2836323912   17.5528980385
C  -11.8762802637  -12.9357251356   18.7341831549
C  -11.8926760533  -11.0959329096   14.7287165110
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C  -12.4363860008  -10.2531216148   13.6377214259
C  -12.6648744147  -10.7144753370   12.3338446830
C  -13.2413370017   -9.8530073848   11.3967107092
C  -13.5767958226   -8.5506021109   11.7730835169
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C  -13.6227471663   -6.7681859460   13.5912766611
C  -14.2679146321   -5.7735080643   12.6621522362
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C	-15.1193410342	-3.6696180332	16.3786949241
C	-14.8560351681	-4.8217331488	15.6309146847
C	-15.5050013406	-1.2236214276	17.9127554654
Co	-12.4030557557	-8.3718283889	15.7761703959
H	-9.4064396768	-7.0275125856	11.1297226577
H	-10.7397473522	-6.6479663913	13.2111943480
H	-8.1831593976	-9.4064357942	15.3120731096
H	-6.8848581999	-9.7908531631	13.2587629496
H	-9.4986315443	-6.4953684076	19.3694721867
H	-11.2881619646	-6.5134763529	21.1012116674
H	-13.5551745997	-7.3589469446	20.5164949864
H	-16.6726855984	-7.3825979419	16.5261237423
H	-18.6900816473	-8.1592104379	15.3469153743
H	-15.8742201440	-7.4665051197	19.1917873239
H	-15.1191599650	-8.9097045533	19.8755489703
H	-16.2566273477	-9.0601234629	18.5273329334
H	-5.9204597812	-9.3195039341	9.7110499785
H	-6.4803158557	-10.4556237340	10.9722391300
H	-5.4482030856	-9.0512528069	11.4139187193
H	-16.6581971333	-11.7850232214	14.2321668890
H	-14.6062023057	-10.9917614737	15.4179472698
H	-9.0380547545	-11.1997478984	19.5284498623
H	-9.6551473325	-10.0252165677	17.4491285822

H   -13.0933345263   -12.5821150441   17.0052163634

H   -12.4806421762   -13.7486302030   19.1179903204

H   -12.4081108852   -11.7284893715   12.0588327844

H   -13.4312672477   -10.1947736193   10.3861176913

H   -14.0346019702   -7.8780522841   11.0607333906

H   -11.4841542620   -5.0208590188   16.0758455883

H   -11.9499890487   -2.9392342812   17.3808535504

H   -16.1368241141   -3.3076882399   16.4565309060

H   -15.6776827320   -5.3450444857   15.1532180517

H   -20.7996316587   -10.5287398961   13.4225108949

H   -20.0529405890   -8.9066316088   13.4952031640

H   -20.5369815410   -9.7480103159   15.0088486224

H   -9.3594600259   -13.7117135305   22.2323963817

H   -9.3382782809   -11.9755014142   21.8095121615

H   -8.3972625827   -13.1560226370   20.8328778735

H   -10.8593724207   -12.5577254303   13.5441510523

H   -12.3870933855   -13.1422088401   14.2108514236

H   -10.9769903450   -12.9722413667   15.2624127321

H   -15.3128689449   -6.0344026278   12.4525510594

H   -13.7404529138   -5.7479707713   11.7022199276

H   -14.2506517488   -4.7689062661   13.0845778572

H   -15.3226493206   -0.3465741860   18.5301316505

H   -16.2093189694   -1.8943941725   18.4161431338

H   -15.8988397636   -0.9189218753   16.9379236062

H   -7.8442588520   -7.6034987202   17.5197067473

H	-8.4075606455	-5.9333083981	17.4347824451
H	-7.9003004847	-6.7738852814	15.9597421891
N	-10.3458257977	-7.7920003624	15.5784861943
N	-12.0293696718	-7.7678244193	17.5375691967
N	-14.3065736213	-8.6958612175	16.7205221292
N	-11.7760290208	-10.5070712361	15.8888136164
N	-12.7598345317	-8.9791113753	13.9852519301
N	-13.2566937702	-6.5371565406	14.8245052566
O	-7.4284028079	-8.5673381900	10.8500751398
O	-18.8570786412	-10.5710072449	14.0229218347
O	-10.4965091539	-13.2732480300	20.6055842902
O	-14.1952520990	-1.8579399247	17.7683307940

L_2Co^{II} – R=CN

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N	11.1591143834	0.7372265575	6.1740092763
C	9.1964713539	3.8426539162	4.8509092784
C	7.8227863287	3.8626082476	4.5731195133
C	7.0793125643	2.6885279393	4.7401045680
C	7.7132114534	1.5228591695	5.1868154493
C	9.0858823553	1.5616923588	5.4633774451
C	10.1251500939	4.9835675347	4.7153433784
C	9.6021273372	6.3128192487	4.2506695462

C	9.9008317837	0.4375183841	5.9666512694
C	9.2589764043	-0.8946601261	6.2275194884
C	12.3940356904	5.7112641694	4.9961912499
C	13.4664194170	5.6046824580	4.0971294087
C	14.4745632619	6.5676429820	4.1015655538
C	14.4318106823	7.6367265944	5.0197145131
C	13.3542848176	7.7371755178	5.9213853232
C	12.3387339264	6.7817976069	5.9055060865
C	12.0942852266	-0.2498298717	6.6383007979
C	12.5024908416	-1.2913796053	5.7890967756
C	13.4268970138	-2.2332212637	6.2396189851
C	13.9417655289	-2.1444270250	7.5472619521
C	13.5184210649	-1.1033421028	8.3977755790
C	12.6055406499	-0.1539966443	7.9417114661
H	7.3421573730	4.7710216533	4.2343030172
H	6.0172090895	2.6820129844	4.5254812812
H	7.1504744698	0.6076681460	5.3176090578
H	10.4072146535	7.0096348626	4.0202782510
H	8.9882496912	6.1888730859	3.3513913472
H	8.9640769341	6.7743670329	5.0153794213
H	9.9366082634	-1.5815564936	6.7329851041
H	8.3643494084	-0.7754539958	6.8498069445
H	8.9377463875	-1.3647069228	5.2889969038
H	15.2930845557	6.5057377139	3.3937628130
C	15.4778559075	8.6103355673	5.0379358840

H	13.3148993681	8.5657074575	6.6192385981
H	13.7434051012	-3.0437597229	5.5930592195
C	14.8900626765	-3.1051800345	8.0113555174
H	13.8992127044	-1.0545151737	9.4115791943
H	12.0897179166	-1.3678754525	4.7893661760
H	12.2637379803	0.6367713947	8.5990412620
H	11.5068123476	6.8624617697	6.5962114280
H	13.4901772871	4.7919335541	3.3813472173
N	13.5850031502	2.6863437827	5.9911901927
C	14.0622220027	3.0754824423	7.2044072865
C	15.4393853244	3.0630448702	7.4713293653
C	16.3260073658	2.6336396622	6.4815451658
C	15.8224292932	2.2290999503	5.2429725677
C	14.4390871998	2.2690149640	5.0168501830
C	13.0486874289	3.5081108220	8.1982941621
H	15.8133542694	3.3819790563	8.4345792352
H	17.3924072472	2.6131219718	6.6728583539
H	16.4945720694	1.8878118871	4.4674786464
C	13.8152081311	1.8585556601	3.7341282108
C	14.7008681261	1.3917372047	2.6088295252
H	14.1398274989	1.2630482306	1.6837013359
H	15.5005449970	2.1173789413	2.4221382186
H	15.1815956567	0.4350328163	2.8485289623
C	13.5118056198	3.9201057511	9.5716691038
H	12.6742882899	4.0478501387	10.2567281161

H	14.1815662767	3.1622655410	9.9932567429
H	14.0694056614	4.8645360399	9.5418166433
N	12.5173947871	1.9713936538	3.6837906793
N	11.8098079751	3.4548292088	7.7939856114
C	10.0849683667	0.7360906597	0.4420055277
C	10.1067421798	2.0857332699	0.8507636934
C	10.9162783375	2.4842632058	1.9122698700
C	11.7380064661	1.5473696303	2.5625536467
C	11.7337048093	0.2034649755	2.1444332938
C	10.9078249533	-0.2015148388	1.0960294907
C	9.2221944471	0.3221570533	-0.6195571657
H	9.4911723406	2.8100136492	0.3293888923
H	10.9417129321	3.5229991996	2.2200595395
H	12.3711320541	-0.5215608215	2.6386423213
H	10.9007370935	-1.2368946945	0.7746652958
C	8.4838548204	4.7869289580	10.0583639802
C	8.5499738884	3.4591004149	9.5885137817
C	9.6483865246	3.0317000427	8.8458101640
C	10.7117527395	3.9132979023	8.5849868299
C	10.6520409503	5.2375602408	9.0595832373
C	9.5439648929	5.6732859888	9.7856794975
C	7.3448490671	5.2282385182	10.8001213542
H	7.7415715826	2.7734867499	9.8154376004
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H	9.4974705393	6.6923637417	10.1521574702
N	16.3419899379	9.4031168944	5.0587779371
N	15.6760707219	-3.8870334611	8.3920009073
N	6.4026191290	5.5861801587	11.4001122995
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L$_2$Co^{III} – R=H

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N	11.4397958877	0.8083169732	6.2512719133
C	9.3769174301	3.7944515621	4.9066545750
C	8.0005920787	3.7888240251	4.6402648632
C	7.2842236567	2.5976561768	4.8296340053
C	7.9375708534	1.4404012697	5.2817289302
C	9.3103588830	1.5092742342	5.5471026982
C	10.3307309852	4.9127622710	4.7422752426
C	9.8491962505	6.2300647686	4.2172595707
C	10.1925472337	0.4395809848	6.0652042242
C	9.6388293222	-0.9197402509	6.3576544084
C	12.6249942630	5.6137877123	4.9780380637
C	13.6418689767	5.4943873593	4.0154510131
C	14.6322719651	6.4788029800	3.9316794463
C	14.6226159779	7.5710658533	4.8103994296
C	13.6078563492	7.6860100395	5.7697178263

C	12.6058944669	6.7135643478	5.8546472488
C	12.4282126782	-0.0911684349	6.8110489292
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C	14.1043937577	-1.8172672866	6.5353138287
C	14.3057254439	-1.8431903434	7.9219605272
C	13.5642442396	-0.9914702515	8.7519582417
C	12.6263032338	-0.1099147864	8.2022759372
H	7.4966163129	4.6817286011	4.2927572013
H	6.2202366800	2.5705651446	4.6243524625
H	7.3874651251	0.5187060250	5.4243348060
H	10.6721849034	6.8757923939	3.9135463870
H	9.1890454754	6.0779250549	3.3563222806
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H	15.3988931131	6.4064715822	3.1680644094
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H	14.6597417731	-2.4930650165	5.8943164062
H	15.0217647651	-2.5331653003	8.3535990796
H	13.7007821319	-1.0272922182	9.8272423505
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H	12.0329623828	0.5285336233	8.8479849852
H	11.8045988711	6.8191725216	6.5771242765

H	13.6282573698	4.6754579526	3.3061945854
N	13.6604995941	2.7194341949	6.0453652225
C	14.0874528252	3.1129396179	7.2628425797
C	15.4606407116	3.1274184113	7.5440728675
C	16.3552082938	2.7126776963	6.5464580399
C	15.8773345273	2.2932220552	5.2951299193
C	14.4960219790	2.3101729291	5.0673955603
C	12.9721453223	3.4778257883	8.1630820233
H	15.8278346726	3.4499984735	8.5100955037
H	17.4210038474	2.7140398686	6.7440401309
H	16.5654580112	1.9660644884	4.5257825284
C	13.7716335929	1.9346202838	3.8324700124
C	14.5279832505	1.4679824139	2.6278550139
H	13.8785985029	1.3161096734	1.7673834395
H	15.3017089843	2.1963764358	2.3551530024
H	15.0426117991	0.5215039077	2.8402366126
C	13.2582391704	3.9104739851	9.5677785221
H	12.3587444649	3.9289612872	10.1818333647
H	13.9845947841	3.2346299376	10.0326389485
H	13.6978811160	4.9168878999	9.5850947941
N	12.4668252207	2.0735887028	3.9057365083
N	11.7747211266	3.3556036511	7.6291564167
C	9.9731799722	1.1652650011	0.5920547668
C	10.3531539152	2.4906333336	0.8443808106
C	11.1632229409	2.7968181238	1.9438629333

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C   11.6017447634    1.7616637340    2.7865229646

C   11.2252318343    0.4307839530    2.5399233795

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H    9.3557382853    0.9322180544   -0.2679307667

H   10.0371838426    3.2819603651    0.1736295155

H   11.4860130432    3.8174637700    2.1182969869

H   11.5844796639   -0.3691600984    3.1784585174

H   10.1368189971   -0.8899064129    1.2324740375

C    8.2788263642    4.4928349767    9.7615436968

C    8.5060680319    3.1441564412    9.4536280726

C    9.6491016929    2.7624868745    8.7429225931

C   10.5804177010    3.7385528411    8.3501416317

C   10.3626625526    5.0910227594    8.6693489742

C    9.2106139494    5.4630980054    9.3702125903

H    7.3940995524    4.7821030881   10.3169080661

H    7.8025395745    2.3886281202    9.7853059881

H    9.8386188100    1.7148766576    8.5423087201

H   11.0961199615    5.8394065059    8.3917181908

H    9.0501726972    6.5047870269    9.6249020292
```

$[CoCl_4]^{2-}$

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Co    0.0000000000    0.0000000000    0.0000000000

Cl   -1.3894744022    1.3894744022    1.3894744022

Cl   -1.3894744022   -1.3894744022   -1.3894744022

Cl    1.3894744022    1.3894744022   -1.3894744022
```

Cl   1.3894744022   -1.3894744022   1.3894744022

$[CoCl_4]^{3-}$

Co   0.0000000000   0.0000000000   0.0000000000

Cl   -1.2909798591   1.2909719181   1.3572606066

Cl   -1.2909798591   -1.2909719181   -1.3572606066

Cl   1.2909798591   1.2909719181   -1.3572606066

Cl   1.2909798591   -1.2909719181   1.3572606066

Cp_2Fe^0

C   -1.7315576221   -1.0690216476   0.5900541787

C   -1.7304477181   0.2302359624   1.1994698816

H   -1.7147017115   0.4337448969   2.2593794294

C   -1.7302999264   1.2113536241   0.1521253001

H   -1.7148113806   2.2822723943   0.2861086016

C   -1.7319315058   -0.8909327716   -0.8338888666

H   -1.7175903757   -1.6787945261   -1.5715369735

C   -1.7311321019   0.5183804478   -1.1045650134

H   -1.7155293772   0.9766698022   -2.0816938533

C   1.7321297044   -1.2108485224   -0.1521544971

C   1.7319033533   -0.5178931441   1.1045541745

H   1.7167797745   -0.9763369223   2.0816335985

C   1.7307236113   0.8914170541   0.8338983072

H   1.7140454667   1.6792254353   1.5715607830

C   1.7308614703   -0.2296990500   -1.1994663299

H	1.7148024532	-0.4332342475	-2.2593526954
C	1.7301225138	1.0695405947	-0.5900412147
H	1.7133651075	2.0146884290	-1.1110586666
Fe	0.0000068649	-0.0007327857	-0.0000015683
H	-1.7168844832	-2.0142131721	1.1110767659
H	1.7176344197	-2.2817836863	-0.2861033197

Cp_2Fe^+

C	-1.7315576221	-1.0690216476	0.5900541787
C	-1.7304477181	0.2302359624	1.1994698816
H	-1.7147017115	0.4337448969	2.2593794294
C	-1.7302999264	1.2113536241	0.1521253001
H	-1.7148113806	2.2822723943	0.2861086016
C	-1.7319315058	-0.8909327716	-0.8338888666
H	-1.7175903757	-1.6787945261	-1.5715369735
C	-1.7311321019	0.5183804478	-1.1045650134
H	-1.7155293772	0.9766698022	-2.0816938533
C	1.7321297044	-1.2108485224	-0.1521544971
C	1.7319033533	-0.5178931441	1.1045541745
H	1.7167797745	-0.9763369223	2.0816335985
C	1.7307236113	0.8914170541	0.8338983072
H	1.7140454667	1.6792254353	1.5715607830
C	1.7308614703	-0.2296990500	-1.1994663299
H	1.7148024532	-0.4332342475	-2.2593526954
C	1.7301225138	1.0695405947	-0.5900412147

H	1.7133651075	2.0146884290	-1.1110586666
Fe	0.0000068649	-0.0007327857	-0.0000015683
H	-1.7168844832	-2.0142131721	1.1110767659
H	1.7176344197	-2.2817836863	-0.2861033197