Supporting Information

Substituent Effects on Cobalt Diglyoxime Catalysts for Hydrogen Evolution

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Scheme S1: Equations for Free Energy Changes Corresponding to Each Step in Mechanistic Pathways

	Pathway 1	**Free Energy Change for Half or Full Reaction**
	$\mathrm{Co(II)} + \mathrm{e^-} \rightarrow \mathrm{Co(I)^-}$	$-F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}}\right]$
	$\mathrm{Co(I)^-} + \mathrm{HA} \rightarrow \mathrm{Co(III)H} + \mathrm{A^-}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) - \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{III}H}\right)\right]$
A:	$\mathrm{Co(III)H} + \mathrm{HA} \rightarrow \mathrm{Co(III)^+} + \mathrm{A^-} + \mathrm{H_2}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) + \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{III}H}\right)\right]$ $+ F\left[E^{\circ}_{\mathrm{Co^{III}/Co^{II}}} + E^{\circ}_{\mathrm{Co^{II}/Co^{I}}} - 2E^{\circ}_{\mathrm{H^+/H_2}}\right]$
A:	$\mathrm{Co(III)^+} + \mathrm{e^-} \rightarrow \mathrm{Co(II)}$	$-F\left[E^{\circ}_{\mathrm{Co^{III}/Co^{II}}}\right]$
B:	$2\mathrm{Co(III)H} \rightarrow 2\mathrm{Co(II)} + \mathrm{H_2}$	$2\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{III}H}\right)\right] + 2F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}} - E^{\circ}_{\mathrm{H^+/H_2}}\right]$
	Pathway 2	
	$\mathrm{Co(II)} + \mathrm{e^-} \rightarrow \mathrm{Co(I)^-}$	$-F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}}\right]$
	$\mathrm{Co(I)^-} + \mathrm{HA} \rightarrow \mathrm{Co(III)H} + \mathrm{A^-}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) - \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{III}H}\right)\right]$
	$\mathrm{Co(III)H} + \mathrm{e^-} \rightarrow \mathrm{Co(II)H^-}$	$-F\left[E^{\circ}_{\mathrm{Co^{III}H/Co^{II}H}}\right]$
A:	$\mathrm{Co(II)H^-} + \mathrm{HA} \rightarrow \mathrm{Co(II)} + \mathrm{A^-} + \mathrm{H_2}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) + \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{II}H}\right)\right]$ $+ F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}} + E^{\circ}_{\mathrm{Co^{I}/Co^{0}}} - 2E^{\circ}_{\mathrm{H^+/H_2}}\right]$
B:	$2\mathrm{Co(II)H^-} \rightarrow 2\mathrm{Co(I)^-} + \mathrm{H_2}$	$2\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{II}H}\right)\right] + 2F\left[E^{\circ}_{\mathrm{Co^{I}/Co^{0}}} - E^{\circ}_{\mathrm{H^+/H_2}}\right]$
B:	$2\mathrm{Co(I)^-} \rightarrow 2\mathrm{Co(II)} + 2\mathrm{e^-}$	$2F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}}\right]$
	Pathway 3	
	$\mathrm{Co(II)} + \mathrm{e^-} \rightarrow \mathrm{Co(I)^-}$	$-F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}}\right]$
	$\mathrm{Co(I)^-} + \mathrm{e^-} \rightarrow \mathrm{Co(0)^{2-}}$	$-F\left[E^{\circ}_{\mathrm{Co^{I}/Co^{0}}}\right]$
	$\mathrm{Co(0)^{2-}} + \mathrm{HA} \rightarrow \mathrm{Co(II)H^-} + \mathrm{A^-}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) - \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{II}H}\right)\right]$
A:	$\mathrm{Co(II)H^-} + \mathrm{HA} \rightarrow \mathrm{Co(II)} + \mathrm{A^-} + \mathrm{H_2}$	$\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{HA}\right) + \mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{II}H}\right)\right]$ $+ F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}} + E^{\circ}_{\mathrm{Co^{I}/Co^{0}}} - 2E^{\circ}_{\mathrm{H^+/H_2}}\right]$
B:	$2\mathrm{Co(II)H^-} \rightarrow 2\mathrm{Co(I)^-} + \mathrm{H_2}$	$2\ln(10)RT\left[\mathrm{p}K_{\mathrm{a}}\left(\mathrm{Co^{II}H}\right)\right] + 2F\left[E^{\circ}_{\mathrm{Co^{I}/Co^{0}}} - E^{\circ}_{\mathrm{H^+/H_2}}\right]$
B:	$2\mathrm{Co(I)^-} \rightarrow 2\mathrm{Co(II)} + 2\mathrm{e^-}$	$2F\left[E^{\circ}_{\mathrm{Co^{II}/Co^{I}}}\right]$

Isodesmic References, Reactions, and Equations

The isodesmic reactions used in our calculations are:

$$\begin{aligned} &\text{A:} \quad \mathrm{Co^{III}\left(dmgBF_2\right)_2 L_2^+ + e^- \rightarrow Co^{II}\left(dmgBF_2\right)_2 L_2} \\ &\text{B:} \quad \mathrm{Co^{II}\left(dmgBF_2\right)_2 L_2 + e^- \rightarrow Co^{I}\left(dmgBF_2\right)_2 L^- + L} \\ &\text{C:} \quad \mathrm{Co^{III}H\left(dmgBF_2\right)_2 L \rightarrow Co^{I}\left(dmgBF_2\right)_2 L^- + H^+} \end{aligned} \tag{S1}$$

where L is an axial acetonitrile ligand that is lost to bulk solvent upon reduction in the Reference B reaction. The justification for the assumption of acetonitrile ligand loss in Reference B is given in our previous work.[S1] The loss of an axial ligand or acidic proton will cancel in the isodesmic reactions in Table S1. The reduction potentials for Reference A, E°(RefA) = 0.2 V vs SCE, and Reference B, E°(RefB) = –0.55 V vs SCE, were obtained from Ref. S2, and the pK_a for Reference C, pK_a(RefC) = 13.3, was obtained from Ref. S3. The reduction potential for Reference A was determined by cyclic voltammetry from an irreversible couple and thus is not as reliable as the reduction potential for Reference B, which was determined from a reversible couple. The pK_a for Reference C was not obtained by a direct experimental measurement but rather was determined from simulations of cyclic voltammograms. These limitations in the reference values are not problematic for the present study because we are interested in only relative values of these properties for varying substituents. An error in a reference value would shift the line representing the correlation up or down but would not alter the slope.

Table S1: Isodesmic Reactions for Calculating Reduction Potentials and pK_as in Cobaloximes

Process	Isodesmic Reaction	Resulting Equation[a]
$\mathrm{Co^{III}\left(dRgBF_2\right)_2 L_2^+ + e^-} \rightarrow \mathrm{Co^{II}\left(dRgBF_2\right)_2 L_2}$	$\mathrm{Co^{III}\left(dRgBF_2\right)_2 L_2^+ + Co^{II}\left(dmgBF_2\right)_2 L_2} \rightarrow \mathrm{Co^{II}\left(dRgBF_2\right)_2 L_2 + Co^{III}\left(dmgBF_2\right)_2 L_2^+}$	$E^{\circ}\left(\mathrm{Co^{III/II}}\right) = -\frac{\Delta G_r^{\circ}}{F} + E^{\circ}\left(\mathrm{RefA}\right)$
$\mathrm{Co^{II}\left(dRgBF_2\right)_2 L_2 + e^-} \rightarrow \mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + L}$	$\mathrm{Co^{II}\left(dRgBF_2\right)_2 L_2 + Co^{I}\left(dmgBF_2\right)_2 L^-} \rightarrow \mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + Co^{II}\left(dmgBF_2\right)_2 L_2}$	$E^{\circ}\left(\mathrm{Co^{II/I}}\right) = -\frac{\Delta G_r^{\circ}}{F} + E^{\circ}\left(\mathrm{RefB}\right)$
$\mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + e^-} \rightarrow \mathrm{Co^{0}\left(dRgBF_2\right)_2^{2-} + L}$	$\mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + Co^{I}\left(dmgBF_2\right)_2 L^-} \rightarrow \mathrm{Co^{0}\left(dRgBF_2\right)_2^{2-} + Co^{II}\left(dmgBF_2\right)_2 L_2}$	$E^{\circ}\left(\mathrm{Co^{I/0}}\right) = -\frac{\Delta G_r^{\circ}}{F} + E^{\circ}\left(\mathrm{RefB}\right)$
$\mathrm{Co^{III}H\left(dRgBF_2\right)_2 L + e^-} \rightarrow \mathrm{Co^{II}H\left(dRgBF_2\right)_2^- + L}$	$\mathrm{Co^{III}H\left(dRgBF_2\right)_2 L + Co^{I}\left(dmgBF_2\right)_2 L^-} \rightarrow \mathrm{Co^{II}H\left(dRgBF_2\right)_2^- + Co^{II}\left(dmgBF_2\right)_2 L_2}$	$E^{\circ}\left(\mathrm{Co^{III/II}H}\right) = -\frac{\Delta G_r^{\circ}}{F} + E^{\circ}\left(\mathrm{RefB}\right)$
$\mathrm{Co^{III}H\left(dRgBF_2\right)_2 L} \rightarrow \mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + H^+}$	$\mathrm{Co^{III}H\left(dRgBF_2\right)_2 L + Co^{I}\left(dmgBF_2\right)_2 L^-} \rightarrow \mathrm{Co^{I}\left(dRgBF_2\right)_2 L^- + Co^{III}H\left(dmgBF_2\right)_2 L}$	$\mathrm{p}K_a\left(\mathrm{Co^{III}H}\right) = \frac{\Delta G_r^{\circ}}{\ln(10)RT} + \mathrm{p}K_a\left(\mathrm{RefC}\right)$
$\mathrm{Co^{II}H\left(dRgBF_2\right)_2^-} \rightarrow \mathrm{Co^{0}\left(dRgBF_2\right)_2^{2-} + H^+}$	$\mathrm{Co^{II}H\left(dRgBF_2\right)_2^- + Co^{I}\left(dmgBF_2\right)_2 L^-} \rightarrow \mathrm{Co^{0}\left(dRgBF_2\right)_2^{2-} + Co^{III}H\left(dmgBF_2\right)_2 L}$	$\mathrm{p}K_a\left(\mathrm{Co^{II}H}\right) = \frac{\Delta G_r^{\circ}}{\ln(10)RT} + \mathrm{p}K_a\left(\mathrm{RefC}\right)$

[a] ΔG_r° for each equation is the free energy for the corresponding isodesmic reaction. For the calculations presented in this paper, the references were chosen to be the $Co(dmgBF_2)_2$ complexes, as indicated in this table. The experimental reference values are: RefA = –0.55 V vs SCE; RefB = 0.2 V vs SCE; RefC = 13.3.

Benchmarking of Computational Methods

Previously, we benchmarked this computational methodology for the $Co(dmgBF_2)_2$ and $Co(dpgBF_2)_2$ (dpg=diphenylglyoxime) systems.[S1] For completeness, we include the results of this benchmarking here.

Table S2. Comparison of Calculated and Experimental Reduction Potentials of Cobaloximes[a]

		$E^{o}_{Co^{III}/Co^{II}}$	$E^{o}_{Co^{II}/Co^{I}}$	$E^{o}_{Co^{I}/Co^{0}}$	$E^{o}_{Co^{III}H/Co^{II}H}$	$E^{o}_{Co^{II}H/Co^{I}H}$
$Co(dmgBF_2)_2$	Experiment[c]	~0.2	–0.55			
	DFT/B3P86	0.20	–0.55[b]	–0.94	–0.53	–1.25
$Co(dpgBF_2)_2$	Experiment[c]	~0.3	–0.28			
	DFT/B3P86	0.26	–0.27	–0.85	–0.40	–1.07

[a] Values given in V vs SCE in acetonitrile.

[b] $E^{o}_{Co^{II}/Co^{I}}$ for $Co(dmgBF_2)_2$ is used as a reference in the isodesmic reactions.

[c] Ref. S2. In the cyclic voltammetry experiments, $E^{o}_{Co^{III}/Co^{II}}$ is determined from an irreversible couple, and $E^{o}_{Co^{II}/Co^{I}}$ is determined from a reversible couple.

Table S3. Comparison of Calculated and Experimental pK_as of Cobaloximes in Acetonitrile

		$Co^{III}H$	$Co^{II}H$
$Co(dmgBF_2)_2$	Experimental[a]	13.3	23.0
	DFT/B3P86	13.3[b]	20.2
$Co(dpgBF_2)_2$	DFT/B3P86	8.9	16.3

[a] Ref. S3.

[b] The pK_a for $Co^{III}H(dmgBF_2)_2$ was used as a reference in the isodesmic reactions.

In addition, we calculated the pK_a of $Co^{III}H(dmgBF_2)_2$ and $Co^{III}H(dpgBF_2)_2$ in DMSO relative to acetonitrile. Using the differences between the solvation energies of the cobaloximes, which correspond to 0.3 pK_a units for $Co^{III}H(dmgBF_2)_2$ and 0.4 pK_a units for $Co^{III}H(dpgBF_2)_2$, and the difference in the solvation energy of the proton, which corresponds to 9.6 pK_a units,[S4] we determined a decrease in the pK_a of 9.9 and 10.0 for $Co^{III}H(dmgBF_2)_2$ and $Co^{III}H(dpgBF_2)_2$, respectively, in DMSO versus acetonitrile. These values are in qualitative agreement with the 11 pK_a unit change reported in Ref. S5.

Table S4: Calculated Reduction Potentials and pK_as for Cobaloximes with Substituents[a,b]

–R	$E^o(Co^{III/II})$	$E^o(Co^{II/I})$	$E^o(Co^{III/II}H)$	$E^o(Co^{I/0})$	$E^o(Co^{II/I}H)$	$Co^{III}H$ pK_a	$Co^{II}H$ pK_a
–CN	1.15	0.75	0.53	0.032	0.12	–13.2	–4.8
$–CF_3$	0.92	0.50	0.27	–0.24	–0.19	–7.4	1.2
–Cl	0.71	–0.11	–0.16	–0.57	–0.74	2.9	9.9
–H	0.44	–0.21	–0.31	–0.78	–0.90	6.8	14.7
$–C_6H_5$	0.27	–0.27	–0.40	–0.85	–1.07	8.9	16.3
$–CH_3$	0.20	–0.55	–0.53	–0.94	–1.25	13.3	20.2
$–OCH_3$	0.19	–0.81	–0.73	–0.97	–1.31	16.5	20.6
–OH	0.35	–0.78	–0.66	–1.09	–1.08	15.3	22.6
$–NH_2$	–0.047	–1.18	–0.92	–1.25	–1.82	22.8	28.3

[a] Reduction potentials given in V vs SCE in acetonitrile.
[b] $E^o(Co^{III/II})$, $E^o(Co^{II/I})$, and $Co^{III}H$ pK_a for $–CH_3$ substituent are used as references in the isodesmic reactions.

Table S5: Slopes and Intercepts of Linear Fits

Function	Slope	Intercept
$E^o(Co^{III/II})$	0.861 V/σ_p	0.469 V
$E^o(Co^{II/I})$	1.450 V/σ_p	–0.290 V
$E^o(Co^{III/II}H)$	1.092 V/σ_p	–0.318 V
$E^o(Co^{I/0})$	0.951 V/σ_p	–0.736 V
$E^o(Co^{II/I}H)$	1.335 V/σ_p	–0.907 V
$Co^{II}H$ pK_a	–24.6 pK_a/σ_p	14.2 pK_a
$Co^{III}H$ pK_a	–26.9 pK_a/σ_p	7.2 pK_a
$E^o(Co^{III/II})$	–0.032 V/ pK_a	0.700 V
$E^o(Co^{II/I})$	–0.053 V/ pK_a	0.093 V
$E^o(Co^{III/II}H)$	–0.041 V/ pK_a	–0.027 V
$E^o(Co^{I/0})$	–0.035 V/ pK_a	–0.483 V
$E^o(Co^{II/I}H)$	–0.050 V/ pK_a	–0.550 V

Table S6: Optimal Hammett Constants for Proposed Mechanisms[a]

Mechanism	Optimal σ_p
1A	[1.11–0.27*(HA pK_a)]/5.73
2A	[2.77–0.28*(HA pK_a)]/6.06
3A	[10.0–0.85*(HA pK_a)]/17.5
1B	[9.23–1.01*(HA pK_a)]/24.6
2B	[23.2–2.42*(HA pK_a)]/54.4
3B	[79.6–6.99*(HA pK_a)]/147

[a] Optimal Hammett constants determined by minimizing the sum of the squared deviations of each point on the free energy diagram from the HA/H_2 reference with respect to the Hammett constant. The optimal Hammett constant depends on the mechanism and the pK_a of the acid, HA. This procedure weights all points equally and does not consider the free energy barriers. Thus, the results are only qualitative and may not lead to the optimal catalyst in practice.

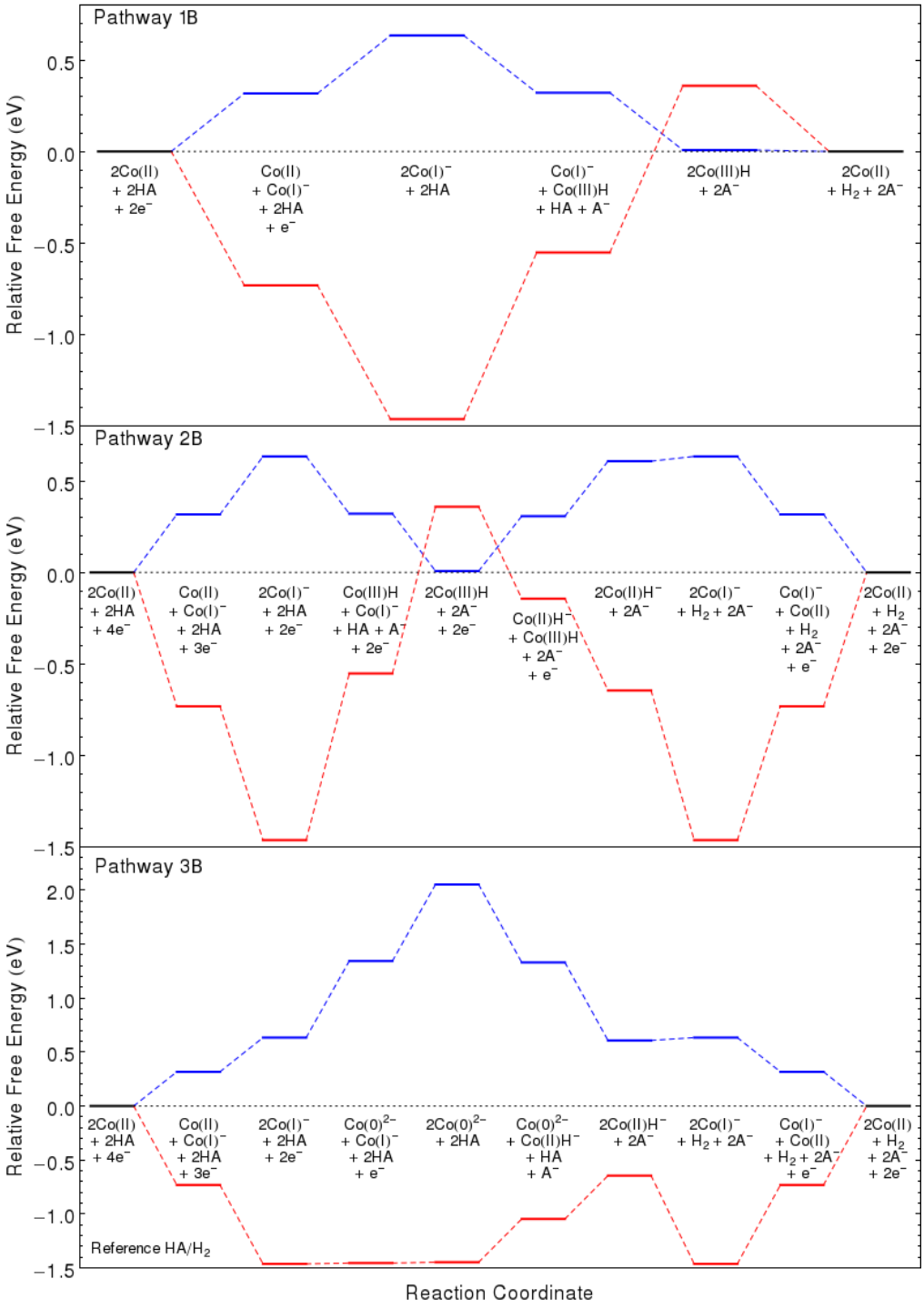

Figure S1. Thermodynamic free energy diagrams for bimetallic pathways (1B, 2B, and 3B) for CH_3 substituents (denoted by blue lines) and CF_3 subsituents (denoted by red lines). Relative free energies for half reactions corresponding to electron transfer are calculated with respect to the HA/H_2 couple in acetonitrile, where HA is tosic acid (pK_a = 8.0). The free energy barriers are not shown.

References

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(S5) Wayner, D. D. M.; Parker, V. D., *Acc. Chem. Res.* **1993,** 26, 287-294.

Complete Reference 16:

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Coordinates and Energies of Optimized Structures:

$Co^0(dRgBF_2)_2$ R = C_6H_5

Co	0.005905348585	0.004878502520	-0.000515471329
N	0.013438601440	0.022721127944	1.835736927054
O	1.138119998494	-0.064090763872	2.600298766132
B	2.287113604791	0.686592776445	2.053881574797
O	2.760335607810	0.214857802698	0.732251697276
N	1.825527503678	0.122219882423	-0.250904264095
C	2.264453670538	0.164849160931	-1.511580988272
C	1.176310349391	0.040993386575	-2.457690254359
N	-0.006902990254	-0.009288212135	-1.841027133981
O	-1.110213520225	-0.112809367915	-2.629171368168
B	-2.324124554632	-0.680189161549	-1.999446369987
O	-2.732400015940	-0.018912653516	-0.743086574601
N	-1.808241490288	-0.117476965673	0.253505019765
C	-2.254716028449	-0.110014114668	1.509506635659
C	-1.161964235640	-0.080798622830	2.455962352042
F	1.983093436460	2.061542647626	2.004828325622
F	3.351003453191	0.451816993053	2.933161557416
F	-2.165970432512	-2.063802087886	-1.784552474100
F	-3.359484558043	-0.442300125917	-2.911420664091
C	1.342147324391	-0.130567397665	-3.908754892841
C	0.487184753135	0.503282251171	-4.835551893302

C	2.364215396113	-0.958194910059	-4.420307018622
C	0.665887889925	0.331898639273	-6.207532940127
H	-0.326950899344	1.110328528852	-4.461034344844
C	2.538877287388	-1.126216922752	-5.792973797061
H	3.015316735568	-1.476525517711	-3.725179199675
C	1.693531469768	-0.479077299168	-6.698670621242
H	-0.009575421248	0.830678260023	-6.897655059685
H	3.334205337616	-1.772618391389	-6.155077015311
H	1.826312695138	-0.613264450287	-7.769036459052
C	3.664112036955	0.428621472472	-1.876604595457
C	3.974262297298	1.328021727566	-2.919349862016
C	4.739514869296	-0.183872380907	-1.198228459619
C	5.295067629982	1.585125795526	-3.282751738940
H	3.163916990459	1.830795839974	-3.435392856345
C	6.058912113940	0.076830783805	-1.565696469981
H	4.521922242737	-0.846253636852	-0.370356682908
C	6.348844296069	0.958147432860	-2.611746668380
H	5.500937897083	2.285081573876	-4.088475596121
H	6.866908678115	-0.407486393485	-1.023598386539
H	7.379151523660	1.161603543843	-2.891790589996
C	-3.679989619271	-0.034500313249	1.862235528396
C	-4.127779589924	0.835951858378	2.876883456923
C	-4.642074096842	-0.824860856427	1.198167016446
C	-5.476148983445	0.900268051438	3.227633367624
H	-3.405093709727	1.466158929834	3.383751684018
C	-5.988173973900	-0.756240030918	1.552157406499
H	-4.316361514967	-1.476092483477	0.396504340580
C	-6.416391853642	0.102802171980	2.570143895817
H	-5.792368973978	1.581262784313	4.013633187663
H	-6.708710059682	-1.375711476180	1.024744276471
H	-7.467891878985	0.154983418389	2.840425827496
C	-1.300413054545	-0.250648256668	3.909730046026
C	-0.541828709262	0.522044183306	4.814707034022
C	-2.199475489604	-1.197398851699	4.442613100775
C	-0.695823102711	0.362943895347	6.190606546697
H	0.173982944754	1.231967918632	4.419345215418
C	-2.350004579085	-1.351908931745	5.820467472871
H	-2.775094318313	-1.814793821920	3.761581254148
C	-1.601628006967	-0.571141629069	6.705110011766
H	-0.099558712350	0.970674318841	6.866068991837
H	-3.050442647836	-2.090093906918	6.202541800182
H	-1.715510962157	-0.693462725408	7.779137393615

E = -3437.09464285 Hartrees

$Co^0(dRgBF_2)_2$ R = CF_3

Co	0.000010708206	-0.000257342943	-0.000000967663
N	0.015154643177	-0.061095874384	1.837984382515
O	1.120312010135	-0.140814204199	2.608243832617
B	2.329451041252	0.514854080949	2.040981291085
O	2.746312934166	-0.050869388233	0.729176845703
N	1.821938024125	0.039544458084	-0.249822012128
C	2.255379307632	0.123818702633	-1.508155726726
C	1.169278108779	0.067665404895	-2.450255032082
N	-0.015135494992	0.060572808255	-1.837984968710
O	-1.120291283494	0.140294135578	-2.608247011036

B	-2.329428574480	-0.515381614322	-2.040988966348
O	-2.746292876260	0.050334456020	-0.729181578127
N	-1.821915563926	-0.040074309998	0.249816189299
C	-2.255358016696	-0.124369299118	1.508147219863
C	-1.169261545793	-0.068204476578	2.450252331811
F	2.113502831993	1.891408444791	1.919992215449
F	3.363331824592	0.224214463211	2.921667327303
C	3.691140753011	0.362206628718	-1.847211128408
C	1.303421678536	-0.078152691579	-3.931539077497
F	-2.113475073602	-1.891935565197	-1.920006003676
F	-3.363309760399	-0.224741369397	-2.921674167078
C	-3.691118278294	-0.362787421778	1.847185185915
C	-1.303419799015	0.077610089937	3.931537760836
F	0.350450637924	-0.838459298023	-4.486067753335
F	1.279817521514	1.105193673188	-4.605968496609
F	2.475225255645	-0.671932955756	-4.272108800745
F	3.822456875305	1.052752798910	-3.008370553706
F	4.415452387762	-0.779805151055	-2.013300157207
F	4.348011121096	1.086147792186	-0.932432841955
F	-4.347963327024	-1.086726335701	0.932386314051
F	-4.415453040486	0.779208319143	2.013281081208
F	-3.822438033019	-1.053355974688	3.008330162647
F	-2.475230014672	0.671381984967	4.272097729585
F	-0.350468578852	0.837927244151	4.486084953543
F	-1.279818163847	-1.105736392667	4.605967599607

E = -3861.00452345 Hartrees

$Co^0(dRgBF_2)_2$ R = CH_3

Co	0.000030784234	-0.000567495856	-0.000003709599
N	0.013915351510	0.024391074932	1.831540139025
O	1.125564815582	0.025701879277	2.637012312439
B	2.323569708931	0.657405345408	2.040924411417
O	2.768003639641	0.116170005034	0.736994049388
N	1.810692925627	0.125229660930	-0.247098368227
C	2.245244544904	0.136250739895	-1.505401443733
C	1.166007790282	0.059530075320	-2.441636522123
N	-0.013863020437	-0.025361911601	-1.831553662668
O	-1.125510350281	-0.026673598440	-2.637024044963
B	-2.323532940151	-0.658333001892	-2.040919735287
O	-2.767945200731	-0.117028364252	-0.737008979703
N	-1.810646343128	-0.126176721217	0.247091778796
C	-2.245217197577	-0.136881981753	1.505390247894
C	-1.165977220297	-0.060184198162	2.441624886611
F	2.138824141778	2.058322937788	1.947868837305
F	3.376358049564	0.381963258965	2.937896155334
C	3.700198482413	0.191079109890	-1.829704485942
C	1.275272584910	0.097011215531	-3.928803829112
F	-2.138829080960	-2.059249406522	-1.947817365556
F	-3.376311890405	-0.382884753107	-2.937903088279
C	-3.700192700044	-0.191268289013	1.829680880635
C	-1.275275161515	-0.097370179817	3.928795872332
H	-0.891521525020	-1.040244682820	4.342770612335
H	-0.668251660075	0.699733101895	4.371216637637
H	-2.311898001977	0.023055442411	4.254835447132
H	-3.865309150994	-0.441512429302	2.880918662980

H	-4.204311646717	0.763021933735	1.622114164290
H	-4.193325724634	-0.940662110788	1.202920291427
H	0.891096065983	1.039770612087	-4.342592113485
H	0.668604767852	-0.700268839908	-4.371361458915
H	2.311925862451	-0.022900356659	-4.254890358474
H	3.865227757248	0.441634542450	-2.880878465893
H	4.204575074517	-0.763128753227	-1.622395851034
H	4.193145467516	0.940438138791	-1.202759903984

E = -2668.07061562 Hartrees

$Co^0(dRgBF_2)_2$ R = Cl

Co	0.000063402926	-0.000653560764	0.000022897638
N	0.035995378695	0.065176867187	1.846551489967
O	1.135321167462	0.087035246313	2.640538751675
B	2.310986875989	0.767464597782	2.036805886856
O	2.769801846029	0.180531222254	0.750011024307
N	1.826482115539	0.166844636302	-0.224346359194
C	2.220828335974	0.154554924480	-1.484344605084
C	1.151323646331	0.035605337802	-2.415101277622
N	-0.035871101301	-0.066441206985	-1.846508464841
O	-1.135196505694	-0.088305307698	-2.640493931031
B	-2.310864817124	-0.768727839727	-2.036759223497
O	-2.769677178719	-0.181790311150	-0.749966139595
N	-1.826360289007	-0.168106551573	0.224392622992
C	-2.220713223386	-0.155719165838	1.484388387672
C	-1.151207370679	-0.036771592698	2.415143974764
F	2.044414990290	2.135917505506	1.873995151339
F	3.361154145821	0.563525675044	2.934396374596
F	-2.044300698751	-2.137182211067	-1.873947653044
F	-3.361030981187	-0.564784912582	-2.934350269220
Cl	-1.379279869608	-0.089238575505	4.133429853076
Cl	-3.887937804448	-0.210481233350	1.957800093359
Cl	1.379385678027	0.088159249097	-4.133385816097
Cl	3.888048196821	0.209411977172	-1.957762639016

E = -4349.90207751 Hartrees

$Co^0(dRgBF_2)_2$ R = CN

Co	0.000039540582	-0.000502034426	0.000010111602
N	0.028256447674	0.036757283844	1.836194879318
O	1.116087795739	0.062380781814	2.622803071497
B	2.299471626123	0.756368410528	2.026529744901
O	2.751108952095	0.156828088303	0.731977624771
N	1.816833927656	0.138360697217	-0.232093380497
C	2.242750439195	0.139754829658	-1.494572842228
C	1.157330780322	0.051920668481	-2.437408017051
N	-0.028181490502	-0.037702759786	-1.836177379405
O	-1.116011002912	-0.063348307656	-2.622783155478
B	-2.299390922465	-0.757335238616	-2.026502119111
O	-2.751031387439	-0.157780739208	-0.731958686665
N	-1.816760758167	-0.139301725381	0.232113477793
C	-2.242685145665	-0.140575006979	1.494591788857
C	-1.157263610213	-0.052744531890	2.437425160997
F	1.999852175320	2.105227251756	1.834800348175
F	3.339604190538	0.563632206593	2.915984778581

F	-1.999765143809	-2.106190607004	-1.834756882591
F	-3.339523595578	-0.564615724737	-2.915960344426
C	1.330535793948	0.070865120775	-3.836932636554
C	3.601163280849	0.208075360439	-1.867339799786
C	-3.601103644198	-0.208788270492	1.867355190317
C	-1.330477345383	-0.071589694900	3.836950733365
N	1.505993143392	0.089360747255	-4.982816766997
N	4.708399585734	0.262729364228	-2.206786218268
N	-4.708346329142	-0.263350339517	2.206796084589
N	-1.505944883694	-0.089999820300	4.982834514291

E = -2880.13297297 Hartrees

$Co^0(dRgBF_2)_2$ R = H

Co	0.000077781698	-0.000758275242	0.000028750774
N	0.023169820322	0.062789923550	1.836578353149
O	1.127369351095	0.110148413031	2.643729957825
B	2.310447553312	0.762876658208	2.036219911285
O	2.770793998839	0.203867792333	0.743320983068
N	1.815004658395	0.164492264362	-0.235427949611
C	2.227563987111	0.155285517499	-1.494238622441
C	1.160496019646	0.035461057369	-2.423080071974
N	-0.023021840330	-0.064208161646	-1.836526396736
O	-1.127222358463	-0.111538092013	-2.643673749478
B	-2.310316181823	-0.764245265675	-2.036172043435
O	-2.770646243518	-0.205240530346	-0.743266293283
N	-1.814860369461	-0.165906345526	0.235484324305
C	-2.227433172570	-0.156518132287	1.494290468274
C	-1.160363044994	-0.036697401685	2.423129931159
F	2.085205373518	2.153461614733	1.909916639446
F	3.367899056791	0.535548552328	2.939416446004
F	-2.085111370927	-2.154837734002	-1.909889373127
F	-3.367762188147	-0.536876003564	-2.939364887931
H	1.262867184189	0.032764838151	-3.502607080548
H	3.279285709952	0.223542276439	-1.749302753216
H	-3.279165548095	-0.224628736885	1.749349628184
H	-1.262746776540	-0.033865339131	3.502655458308

E = -2510.16964455 Hartrees

$Co^0(dRgBF_2)_2$ R = NH_2

Co	0.000459582943	0.021484096798	0.001443309670
N	0.019753443781	0.085490059508	1.829252055866
O	1.127751755290	0.107627767351	2.652070485622
B	2.326156677473	0.747172993639	2.053558356459
O	2.778420513432	0.204522860338	0.748235632047
N	1.807116702511	0.193652143166	-0.233092501825
C	2.233507178506	0.162159117989	-1.490537988477
C	1.164004152155	0.064805908204	-2.423470890664
N	-0.018396406713	-0.047458680181	-1.825684846888
O	-1.125778314794	-0.075994909404	-2.648920663442
B	-2.322352983550	-0.717330286461	-2.048816909022
O	-2.776447716752	-0.172578727694	-0.745033019926
N	-1.805141004180	-0.155531414411	0.236010917057
C	-2.231313443892	-0.134451511657	1.494253153739
C	-1.161300924051	-0.037138924047	2.426602830901

F	2.138017446726	2.143903328661	1.962443575246
F	3.378595142466	0.472131481814	2.952585111137
F	-2.129910848335	-2.113329114349	-1.953688715158
F	-3.375524923721	-0.448334746297	-2.948741500357
N	-3.591378620753	-0.244643598770	1.854509812341
H	-3.885711248668	0.556412565901	2.405495896261
H	-4.119867608560	-0.262222033074	0.985387756969
N	-1.327353621495	-0.024694176458	3.828639219383
H	-0.393636388525	0.038819916948	4.228006011475
H	-1.762545880459	-0.885205437342	4.148866353252
N	1.332100562968	0.038864102392	-3.825606483961
H	0.399460584558	-0.046202175589	-4.223770871175
H	1.747611599829	0.905364388946	-4.156339554945
N	3.594283648609	0.258806754362	-1.849841680586
H	4.124934143527	0.255758669866	-0.982027973539
H	3.875432799673	-0.535109420150	-2.417411877461

E = -2732.25823958 Hartrees

$Co^0(dRgBF_2)_2$ R = OCH_3

Co	0.013294531044	-0.070029438352	0.019268683539
N	0.026723590015	0.060307026624	1.856194538850
O	1.125193653712	0.149908196977	2.673196899491
B	2.329486277802	0.733456276816	2.039419354784
O	2.781099734218	0.079758812607	0.788925382522
N	1.834280979124	0.062349181189	-0.204459588740
C	2.257322034767	0.008616404804	-1.460687962482
C	1.188759408570	-0.099518270971	-2.399400301285
N	-0.000701629749	-0.176174840055	-1.817405873098
O	-1.108722020956	-0.194728878183	-2.627147033572
B	-2.280291083063	-0.873066672634	-2.026558831224
O	-2.759252229263	-0.314982319949	-0.740696694067
N	-1.807394494308	-0.227422293794	0.243169755012
C	-2.228233622166	-0.178791126393	1.500236640252
C	-1.163993141456	-0.011920035086	2.436043041578
F	2.147950387856	2.116616380589	1.819690247059
F	3.369680780527	0.529160154116	2.963798941511
F	-2.020132027805	-2.254905024442	-1.895704451327
F	-3.335533376439	-0.669280582003	-2.933796092037
O	1.405186319069	-0.075478613398	-3.744240365956
O	3.562694171718	0.005622637201	-1.850886663628
O	-3.527152004599	-0.289210440804	1.897873514060
O	-1.390763684331	0.075992259733	3.777068635970
C	4.258727582619	1.201657561307	-1.521311908740
H	3.809104016797	2.059280653785	-2.037586410683
H	4.244443272763	1.370801769301	-0.442479558392
H	5.286487088407	1.065984892017	-1.869405436431
C	1.000780108813	-1.266881771087	-4.408237601987
H	1.213909935447	-1.115334639805	-5.470055556685
H	1.578050626133	-2.123974314696	-4.039049047286
H	-0.065712913210	-1.448422660003	-4.258852056299
C	-4.351891126394	0.787454523385	1.473806897121
H	-3.994723818353	1.734410138994	1.899250209167
H	-4.368464709539	0.852416047188	0.383152635512
H	-5.355663940658	0.576570142705	1.853295108258
C	-0.843395938007	-1.000834378598	4.525596987439

H	-1.094738885981	-0.809095652302	5.572536882460
H	-1.292675105763	-1.952544119750	4.213118076158
H	0.241298412640	-1.043174197034	4.400810273177

E = -2969.52589617 Hartrees

$Co^{0}(dRgBF_2)_2$ R = OH

Co	0.004127947815	0.044500162468	0.000383868298
N	0.023036227902	0.069678361395	1.817973844175
O	1.125419431125	0.076775001243	2.655028294845
B	2.333959021056	0.723411145754	2.062800040398
O	2.785077212709	0.190558541214	0.742601311492
N	1.801239919592	0.191070053420	-0.231175938630
C	2.232677636360	0.203046664484	-1.485513503464
C	1.163609187214	0.116518839928	-2.418272064821
N	-0.014771254342	0.019177854387	-1.817177096940
O	-1.117179752668	0.012110769994	-2.654230159347
B	-2.325484114548	-0.635023464391	-2.062057761671
O	-2.776830437482	-0.102374303980	-0.741799809758
N	-1.792954492991	-0.102357097744	0.231940669397
C	-2.224372011530	-0.114618764736	1.486279285724
C	-1.155325588253	-0.027991104720	2.419052222631
F	2.143555182226	2.114984108054	1.980449242129
F	3.380816902768	0.433287952023	2.954197020228
F	-2.134609690106	-2.026473635858	-1.979772213498
F	-3.372464280149	-0.345168181140	-2.953428322383
O	1.272419279988	0.145930734318	-3.775001358175
H	0.345630441802	0.048327975256	-4.055900172569
O	3.559195397117	0.271507732362	-1.783997011719
H	3.964218736569	0.334332632557	-0.901240505675
O	-3.550856262867	-0.183688996575	1.784772513864
H	-3.955859226922	-0.246702501733	0.902018490731
O	-1.264120953484	-0.057633830931	3.775779091699
H	-0.337335458901	0.039984352953	4.056682023040

E = -2811.74886414 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = C_6H_5

Co	0.206993735425	-0.493467896028	0.139433299350
N	0.151991588542	0.043701452298	1.915538287026
O	1.246941628648	0.156792269387	2.693345175099
B	2.326941832096	0.974342768404	2.080020572987
O	2.835018645831	0.413311545783	0.795360188961
N	1.918279744849	0.168959491964	-0.157920639938
C	2.300678287531	0.286543270832	-1.414659027698
C	1.247281317162	-0.068745425416	-2.341119472028
N	0.127211771884	-0.390064731674	-1.716486623262
O	-0.917307036361	-0.742481881493	-2.488411283910
B	-2.076955334009	-1.381555386535	-1.821157279627
O	-2.544315984183	-0.659054319956	-0.618217865420
N	-1.633877341119	-0.483807598608	0.359318598449
C	-2.096421454603	-0.216620499334	1.567186558229
C	-1.026668167031	0.044839880591	2.504968086268
F	1.860696113705	2.278070168088	1.879877155043
F	3.395010691988	0.929561888818	2.957302320450
F	-1.768050706872	-2.720740837458	-1.485272822164

F	-3.115500337402	-1.336322821080	-2.732006237030
N	0.576311848246	-2.378445473740	0.323954532237
C	0.450467412021	-3.508398185541	0.145753786142
C	0.197646996454	-4.897206789140	-0.157616920133
H	1.067261066708	-5.350759707485	-0.637176514182
H	-0.038664170657	-5.454018554872	0.751287722650
H	-0.654864175108	-4.934597425998	-0.840953909489
C	-1.208774747544	0.242496614718	3.957051082680
C	-0.552753259216	1.289460887220	4.628654058729
C	-2.044985524658	-0.614827138802	4.691791119914
C	-0.740023603635	1.473294454873	5.997974671823
H	0.108914220022	1.942506392313	4.071907382723
C	-2.226112300511	-0.428949266932	6.062615262469
H	-2.552328734410	-1.427418541157	4.182451995277
C	-1.575993774747	0.617237108049	6.720272893601
H	-0.225626783181	2.285222808056	6.502324437783
H	-2.874477752671	-1.102149951896	6.615006872476
H	-1.716162246425	0.762572112523	7.787182219795
C	-3.535278267200	-0.106420394178	1.884625304207
C	-4.020049699495	1.003667397371	2.596712635571
C	-4.444088986411	-1.103387075337	1.488663418195
C	-5.374604970343	1.109554423570	2.913617372448
H	-3.329408884330	1.783852792554	2.898179175296
C	-5.796132867790	-0.996502814587	1.811184199744
H	-4.083499273368	-1.947301910553	0.912862796647
C	-6.267128596282	0.108329128361	2.525822268224
H	-5.731077098669	1.975982303776	3.461955731695
H	-6.484546822708	-1.774422107381	1.495879536444
H	-7.321439473128	0.190834978598	2.771906156899
C	1.407371535625	-0.133637794843	-3.808382668147
C	0.451204996381	0.426265955260	-4.673922660501
C	2.527153717666	-0.774056957491	-4.368287046868
C	0.620340125119	0.356314206571	-6.056461182112
H	-0.428917579268	0.897905913404	-4.254928035879
C	2.689767691947	-0.847184815094	-5.751506374907
H	3.269958583870	-1.214990091317	-3.712093103448
C	1.738527217093	-0.279116010154	-6.601837180720
H	-0.129469570456	0.793190753322	-6.708623230663
H	3.560130086778	-1.348547951228	-6.163563108964
H	1.864648378628	-0.335527733991	-7.678778373131
C	3.626373177408	0.801383953299	-1.817910576804
C	3.721243597548	1.814493843364	-2.787521063750
C	4.809088089016	0.306254960497	-1.242487016802
C	4.964011139373	2.310937468542	-3.179416348994
H	2.814360926952	2.214788958596	-3.227513117460
C	6.050715053252	0.800734765980	-1.641674465998
H	4.743971102892	-0.448155707707	-0.468276099942
C	6.134290512521	1.802526873677	-2.611643029144
H	5.016416865997	3.097806036562	-3.925421239028
H	6.954038304531	0.409733520743	-1.183863101290
H	7.102031520291	2.190004449193	-2.915395255892

E = -3570.29666759 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = CF_3

Co	0.183866329218	-0.485951474139	0.118796586819

N	0.156114166061	-0.049293533519	1.926424795911
O	1.240235323629	0.032971067816	2.696351721672
B	2.396738427340	0.775143421193	2.093250432519
O	2.856734651527	0.130953908398	0.818081281981
N	1.940038116515	0.065032884265	-0.146648833178
C	2.327523227595	0.224099012507	-1.396945284493
C	1.262340982415	-0.039701766951	-2.330544413930
N	0.116079848361	-0.287069024578	-1.721239543096
O	-0.958860562985	-0.436726217157	-2.492703790261
B	-2.119166999786	-1.166787653011	-1.903244087115
O	-2.569930141239	-0.549433321337	-0.620540109704
N	-1.655432147615	-0.403659677709	0.335886094498
C	-2.095914153246	-0.264716859590	1.574199173375
C	-1.028031671735	0.006202440360	2.502609939299
F	2.020995475912	2.082912966542	1.838600200057
F	3.433943688789	0.647965955909	2.979358040513
C	3.699975596822	0.727113861847	-1.780587541525
C	1.375949957983	-0.121434136352	-3.831766900209
F	-1.775777010025	-2.505402480194	-1.688640424994
F	-3.155485752902	-1.023205159435	-2.785583783773
C	-3.549983895020	-0.470051425403	1.916168360084
C	-1.221478522830	0.413610855458	3.944690260443
N	0.428632375752	-2.383101106562	0.230716602132
C	0.339692398283	-3.520388370382	0.098085522988
C	0.167041935173	-4.936002198276	-0.123038973616
H	1.076939310493	-5.368029049431	-0.543458071404
H	-0.069447428259	-5.441114767945	0.815163417090
H	-0.657472591965	-5.073343377446	-0.826571427345
F	0.697339841338	-1.162274692055	-4.332408540282
F	0.926699103220	0.984511612240	-4.451056280677
F	2.652942775208	-0.301635288728	-4.217535952668
F	3.608738694807	1.577827752999	-2.824796280457
F	4.525564117376	-0.274598978524	-2.154661128105
F	4.313531104532	1.398437672382	-0.812556828124
F	-0.233433440756	1.163170025488	4.422212187080
F	-1.346810375050	-0.651420064969	4.765623918761
F	-2.344375213630	1.150643122132	4.075395587449
F	-3.702998555039	-0.792782381596	3.214984393772
F	-4.302458693076	0.621002500699	1.686789890014
F	-4.094077693191	-1.481019024947	1.227561628497

E = -3994.17720150 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = CH_3

Co	0.226369550982	-0.575398510055	0.155050018578
N	0.166856384828	-0.015097404283	1.926013377547
O	1.244613435981	0.180032688047	2.719088083845
B	2.362838788695	0.923260347560	2.071104690467
O	2.871267184718	0.286606440898	0.821773953032
N	1.933347946091	0.099156768731	-0.134143643960
C	2.310292235192	0.227172351491	-1.386178816207
C	1.249055905640	-0.076218000196	-2.307947218606
N	0.143255539809	-0.436452432048	-1.692704330654
O	-0.927880759103	-0.678882101642	-2.481505100288
B	-2.060670504845	-1.399657127918	-1.852804731842
O	-2.547551358851	-0.790453967034	-0.591401963242

N	-1.617091043881	-0.553697802144	0.360573604004
C	-2.073092494046	-0.294881993201	1.567193867783
C	-1.017181428856	0.009470327362	2.494738284869
F	1.955408657858	2.233934942516	1.795576780877
F	3.416186522306	0.887050503478	2.972428818308
C	3.684033958348	0.654616889989	-1.776976642715
C	1.338082766824	0.037649264236	-3.791506327065
F	-1.705375849423	-2.752216010152	-1.628001080429
F	-3.113260612952	-1.322041802128	-2.750427937626
C	-3.528912205265	-0.283052388982	1.887305833665
C	-1.216310550710	0.332875770893	3.936398591024
H	-1.298453529854	-0.574525902390	4.546829885266
H	-0.355970280547	0.896193496191	4.297535583268
H	-2.124790608496	0.920877217992	4.086521792029
H	-3.696910592955	-0.408325036460	2.958347544602
H	-3.999732020492	0.656314259375	1.574655466536
H	-4.033926669800	-1.084304645779	1.344130140504
H	0.922871616424	0.988380178581	-4.146023867605
H	0.751479310300	-0.756091186889	-4.258003943965
H	2.373590508640	-0.029025660074	-4.129557360017
H	3.663438979950	1.274188756324	-2.676396458399
H	4.334174169269	-0.206037309840	-1.975242201072
H	4.128839747598	1.219264762610	-0.957466692915
N	0.570826607104	-2.470223895773	0.340848481347
C	0.409980428623	-3.592810615177	0.137135949494
C	0.105123419759	-4.960786720816	-0.212742516150
H	0.970498006138	-5.445277578975	-0.669784728312
H	-0.193722949409	-5.529457167322	0.670313856573
H	-0.721040211161	-4.939636706944	-0.928842042802

E = -2801.30044440 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = Cl

Co	0.203588753499	-0.534806993744	0.137300992475
N	0.172667626651	-0.001302022186	1.929983328313
O	1.241357302847	0.167397530214	2.715431610958
B	2.366521974734	0.926725624717	2.075083044962
O	2.867271883194	0.272896344034	0.819671239764
N	1.937751089864	0.112953848397	-0.127872850370
C	2.297630185505	0.193991653799	-1.379664048577
C	1.234540146910	-0.082061953346	-2.303640265409
N	0.108025838084	-0.404464976006	-1.723711059191
O	-0.956109417541	-0.624418722578	-2.503740102458
B	-2.089006068833	-1.362649961950	-1.876616502478
O	-2.575117213267	-0.734954683940	-0.614759949372
N	-1.654012921241	-0.522566867399	0.331673239823
C	-2.070854952513	-0.301472365619	1.551012617602
C	-1.011302549661	-0.023710464885	2.478497151130
F	1.944302987188	2.217296111036	1.784947566477
F	3.411036067784	0.878402110511	2.968369780960
F	-1.706199980330	-2.692562724165	-1.626467496073
F	-3.133031714414	-1.293016981908	-2.767471452983
N	0.552199117820	-2.437608136395	0.325775824314
C	0.407588148206	-3.563216207032	0.135934328312
C	0.144493971973	-4.948037264760	-0.175520272490
H	1.022006388244	-5.411717506882	-0.630078931380

H	-0.124398762329	-5.500253268452	0.726906275869
H	-0.689036419827	-4.976417115955	-0.882024534307
Cl	1.418723090615	0.044785687041	-4.006298033588
Cl	3.893030096405	0.577253490764	-1.882866358427
Cl	-3.729080626446	-0.297430328698	1.996878569660
Cl	-1.283536173121	0.234826515388	4.153254216484

E = -4483.10179264 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = CN

Co	0.131606455915	-0.505037835486	0.074964218391
N	0.126524114988	-0.060009231483	1.876219979298
O	1.192254424254	0.022235070293	2.662789703884
B	2.366841012348	0.760562045119	2.066437795231
O	2.817459875185	0.134986635210	0.767120302863
N	1.882317039964	0.058118661465	-0.171281755182
C	2.262887359394	0.189337708036	-1.427849683877
C	1.185037564318	0.001240894696	-2.361858383274
N	0.042317753192	-0.301268295795	-1.767663278886
O	-1.019410776862	-0.450088263135	-2.547339461548
B	-2.180594197321	-1.188930497826	-1.947551094607
O	-2.635497548998	-0.557930488163	-0.662782042622
N	-1.711276916552	-0.416724790291	0.277032485865
C	-2.138464843005	-0.220346242666	1.513896542932
C	-1.061575915205	-0.034059984300	2.449325185938
F	1.998937536360	2.069850467114	1.829164931367
F	3.400857777844	0.605082567090	2.943221428585
F	-1.808758945604	-2.509672646688	-1.704654041388
F	-3.214852776613	-1.068442331147	-2.827398580319
N	0.429185250112	-2.390510978547	0.223852156011
C	0.438418186764	-3.536993775032	0.167364930613
C	0.409887356585	-4.976091925862	0.059665443181
H	1.364590897072	-5.343653270673	-0.320768430929
H	0.218273069328	-5.423073103813	1.036777630904
H	-0.387260114066	-5.261230183972	-0.630328148201
C	3.594625789873	0.477399515808	-1.813710741853
C	1.324138539943	0.134814408064	-3.763337092382
C	-3.506783559552	-0.189249691128	1.871578997748
C	-1.252271457463	0.148689468623	3.840641405191
N	4.672009013821	0.701960815528	-2.165352031491
N	1.470423440380	0.241540055098	-4.904781995993
N	-4.615830365303	-0.167926680725	2.196014138982
N	-1.444141201093	0.285108504588	4.971744365569

E = -3013.28429494 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = H

Co	0.221501960623	-0.579943691775	0.150813417964
N	0.179262439469	-0.023509395342	1.922624483612
O	1.244378682617	0.174489926889	2.722061697816
B	2.373506530240	0.914893434387	2.080248008596
O	2.874123289463	0.278794433688	0.822646425749
N	1.932809119912	0.088852119308	-0.121117191230
N	0.126124558083	-0.436641056108	-1.698987912784
O	-0.936148649834	-0.675707659298	-2.491577647222
B	-2.074570062172	-1.395946159478	-1.864933906835

O	-2.558457323945	-0.785506835328	-0.599430771272
N	-1.626110670836	-0.552497374264	0.344124906722
F	1.973023440873	2.225090055008	1.808774805319
F	3.424122335626	0.862192100604	2.979000126124
F	-1.716608187986	-2.745388178493	-1.636309195152
F	-3.124419970126	-1.315406376137	-2.760583791989
N	0.547006128954	-2.465541405469	0.320478094158
C	0.402367083856	-3.591294473015	0.129563722323
C	0.124307727677	-4.970018459911	-0.197139898716
H	0.996284940933	-5.441000089091	-0.655308343411
H	-0.154009544183	-5.530819118242	0.697331765377
H	-0.708121911331	-4.977721843534	-0.905924051976
C	-2.057050620408	-0.293375309167	1.555887202957
C	-1.009277007189	-0.002551308999	2.471627311630
C	1.241022919789	-0.077113054249	-2.289567958036
C	2.290125015134	0.211946680595	-1.374760121853
H	1.306565430950	0.009489899457	-3.367134126429
H	3.291263710663	0.522446116475	-1.647748956236
H	-3.114700755021	-0.281529021565	1.788595986330
H	-1.141638721831	0.233939223056	3.520334528468

E = -2643.39285540 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = NH_2

Co	0.247257021259	-0.635526937191	0.184990908535
N	0.192644864808	-0.038378078835	1.943797187724
O	1.256864666128	0.230222511811	2.750002723158
B	2.356960718149	0.987651601098	2.074653690560
O	2.890435450162	0.334230625310	0.839903478154
N	1.937673442672	0.093885764996	-0.102486623408
C	2.308529551153	0.197493725776	-1.352344820295
C	1.243084726224	-0.107542821506	-2.271262326731
N	0.155311320706	-0.511315089272	-1.665621482401
O	-0.925689978847	-0.725020616137	-2.466415288364
B	-2.068346898249	-1.436079829337	-1.836059567447
O	-2.556033120828	-0.836465709809	-0.564309224066
N	-1.603256324830	-0.587866507190	0.376518292902
C	-2.048868331314	-0.305304127660	1.574549881492
C	-0.991067871958	0.031253759803	2.492427127666
F	1.909940793452	2.277461438075	1.767247934494
F	3.410121603842	1.007982217534	2.978148267696
F	-1.729954454709	-2.793019514288	-1.623499606251
F	-3.121629373938	-1.336899152607	-2.733059204631
N	0.611622242264	-2.558874918523	0.384326206130
C	0.418314756452	-3.663405834648	0.110046871315
C	0.072503987786	-4.996952086811	-0.326800760250
H	0.916765358340	-5.468519755966	-0.834553697823
H	-0.221407268815	-5.619323694999	0.521219959093
H	-0.766538291529	-4.908640790908	-1.022631710365
N	1.373620067269	0.016053358870	-3.650665111823
H	0.466782062448	-0.105294209337	-4.089020627833
H	1.799212908774	0.894837706175	-3.920951066658
N	3.555065101904	0.654614243427	-1.767314296815
H	4.155513423920	0.770253210334	-0.957102001263
H	3.983365783653	0.056618229282	-2.463349706851
N	-1.216897275133	0.355691316319	3.824771429843

H	-0.346560123984	0.679793308822	4.236200324928
H	-1.951641974465	1.045109974910	3.932469681338
N	-3.398539114546	-0.214292037730	1.908766748118
H	-3.620536699399	-0.710991348538	2.763506137024
H	-3.959792748825	-0.551081931247	1.133125273106

E = -2865.49813969 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = OCH_3

Co	0.235357894086	-0.514767317756	0.131112623252
N	0.194296723763	0.093548811304	1.896178237877
O	1.263064366373	0.391120679724	2.671937126358
B	2.386920530348	1.083631463830	1.975609753482
O	2.891637316190	0.357581512488	0.774816551355
N	1.941108836535	0.187617895748	-0.177369654903
C	2.288560046373	0.301507388866	-1.430591248072
C	1.213319928719	-0.021550037678	-2.341683647241
N	0.122252563767	-0.402892841209	-1.724911013297
O	-0.977673759913	-0.607314662208	-2.486443856695
B	-2.052739464969	-1.416998284596	-1.859253420964
O	-2.552480069308	-0.877216718305	-0.571112981305
N	-1.614932243130	-0.553683194304	0.349808735529
C	-2.042306864220	-0.301173092956	1.563329046636
C	-0.982803315165	0.063800861409	2.469800267191
F	1.994586448500	2.373604334495	1.603950891846
F	3.435090473078	1.098195553485	2.882160322575
F	-1.607262456148	-2.747048908917	-1.686767541596
F	-3.123570057243	-1.371855693438	-2.735689495780
N	0.634450788835	-2.417249899575	0.371368467407
C	0.437035026407	-3.538956808763	0.191173756205
C	0.086646907441	-4.906432104530	-0.116212800475
H	0.936550776465	-5.435348163423	-0.552456115918
H	-0.234531315001	-5.433771665485	0.784419645928
H	-0.736306949458	-4.881681027765	-0.835730314703
O	1.361353032884	0.187803053413	-3.661970967504
O	3.487685309867	0.645160721007	-1.922121291598
O	-3.319086941488	-0.388088247581	1.985713998026
O	-1.262772033888	0.396621454243	3.743458379322
C	4.164680714059	1.739498581684	-1.292199302554
H	4.705137422086	1.403437674800	-0.408725840854
H	4.849551285116	2.129670714202	-2.046439763658
H	3.451114512229	2.511103806802	-0.995281993003
C	-4.232990134581	0.523380467469	1.372761814334
H	-3.902875217627	1.554924935225	1.533368646919
H	-4.322490589262	0.319232662930	0.305003497771
H	-5.189715848392	0.366426693994	1.871360034072
C	-0.589641638907	-0.357160967904	4.752605029025
H	-0.829537508781	-1.421202155930	4.651007067160
H	0.488750018092	-0.209342794973	4.691562129416
H	-0.974859202014	0.011652132314	5.703331206103
C	1.038618146646	-0.907267779550	-4.520053489853
H	1.606653980529	-1.796549454743	-4.227653048767
H	-0.028903199847	-1.124686507433	-4.488823644711
H	1.340534220951	-0.596067340411	-5.520218234336

E = -3102.74833202 Hartrees

$Co^{I}(dRgBF_2)_2L$ R = OH

Co	0.269827398014	-0.679040556753	0.187776391691
N	0.210269247674	-0.051949142524	1.931075224749
O	1.264042779258	0.224220224960	2.753055289273
B	2.362924848918	0.994900271550	2.075104829756
O	2.905849199471	0.326885105675	0.841374037984
N	1.948663396776	0.055078026492	-0.092757974111
C	2.306608516321	0.231678745403	-1.335471295143
C	1.249790303496	-0.081691138084	-2.258947547913
N	0.169519141367	-0.501210898912	-1.654817764853
O	-0.901693265398	-0.704342637143	-2.474320157199
B	-2.057784918232	-1.419308479446	-1.852199033210
O	-2.535107352895	-0.816603620012	-0.569361723522
N	-1.573243467397	-0.614499523615	0.376320641984
C	-2.026426977941	-0.293375547630	1.559443884553
C	-0.970327644555	0.022877970491	2.482824760333
F	1.897705136971	2.266047833108	1.744078962842
F	3.409884756114	1.032189721576	2.976358279381
F	-1.722051480891	-2.769715879258	-1.644497759386
F	-3.106052866421	-1.297291491527	-2.743558586605
N	0.609225348991	-2.609079056629	0.370519780735
C	0.397654998789	-3.714820455417	0.118943624366
C	0.035542873506	-5.055762594232	-0.279312030273
H	0.874522528701	-5.551284770254	-0.772352901798
H	-0.265975781306	-5.648339658051	0.586938847382
H	-0.802314851142	-4.980799699244	-0.977749695112
O	1.329618102330	0.101720468086	-3.586338128546
H	0.450038412538	-0.148277756994	-3.916786256114
O	3.512175099578	0.689443594193	-1.696776779610
H	3.957265051739	0.869701714962	-0.849257352730
O	-3.333875709738	-0.203733800795	1.850157395807
H	-3.781356155548	-0.429550572202	1.017055085649
O	-1.165840016311	0.387762518490	3.756512914633
H	-0.270572002779	0.594668213737	4.079900895006

E = -2944.97663496 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = C_6H_5

Co	-0.009941546185	-0.007608909488	0.010489627873
N	-0.043551924476	0.315863336585	1.870246389570
O	1.062843931725	0.522477784724	2.583331364452
B	2.109551666930	1.370548786416	1.928371870066
O	2.660489390574	0.796409387325	0.655244572152
N	1.799969057257	0.444920464107	-0.296659772707
C	2.218567352741	0.334711209814	-1.523905295593
C	1.161016913368	-0.138995999358	-2.448949119357
N	0.025710835913	-0.347943283396	-1.848783088351
O	-1.031841620483	-0.715662515201	-2.567385322764
B	-2.168296651344	-1.390993866444	-1.856272177968
O	-2.692320769587	-0.631532386896	-0.675628481021
N	-1.823890807822	-0.434258626297	0.315220516826
C	-2.257738013672	-0.267102174823	1.529365653342
C	-1.165502854073	0.066834390142	2.477991984512
F	1.564074261074	2.634662852876	1.665764361239
F	3.161276724015	1.416164878399	2.798949495524

F	-1.756492514485	-2.660123731167	-1.426637667904
F	-3.191246416913	-1.441861344250	-2.760137854540
N	-0.634029492888	2.120707219324	-0.445096914213
C	-0.432958242586	3.239641413497	-0.268858626654
C	-0.143159554752	4.631734073808	-0.016135871119
H	0.121670854547	5.138433645736	-0.945617312192
H	-1.011472358332	5.124555988497	0.424355070080
H	0.696824325084	4.679031920948	0.679949320426
N	0.637061550971	-2.129233539244	0.432107086185
C	0.482276903651	-3.247630357113	0.211798269517
C	0.247159281163	-4.639231291075	-0.094452242720
H	1.150708803467	-5.096379399231	-0.501138192552
H	-0.051806416215	-5.178447261238	0.805969472655
H	-0.555003449431	-4.689246038041	-0.833656757651
C	-1.321015461568	0.036151743320	3.944552240169
C	-2.030284993508	-1.014639198115	4.550929976031
C	-0.759837080407	1.040548596599	4.751722703109
C	-2.171392136083	-1.061802494382	5.937029001050
H	-2.467493007955	-1.794629597306	3.936820734210
C	-0.918248455304	0.995995159741	6.135714079760
H	-0.192446564275	1.841253720761	4.293489245561
C	-1.620642311569	-0.054402314671	6.731933102540
H	-2.713513960018	-1.882457013190	6.394208312728
H	-0.482887916342	1.777248482685	6.749224163174
H	-1.734789625187	-0.089240256177	7.810223433193
C	-3.681405856294	-0.318965402817	1.911695496001
C	-4.216525168616	0.673418570894	2.750512245595
C	-4.519602820421	-1.343563683904	1.439996240018
C	-5.563963435533	0.643414993876	3.106693072495
H	-3.578006324317	1.468845840988	3.119635926845
C	-5.862165704904	-1.376813188541	1.812880957855
H	-4.120098213540	-2.099173740155	0.774681249690
C	-6.388299327138	-0.384339526854	2.643625555469
H	-5.967580542683	1.419608342793	3.747805914245
H	-6.499782986282	-2.173312729742	1.445059601408
H	-7.435595383840	-0.409957355303	2.925505458637
C	1.379646840600	-0.393126992962	-3.887665517522
C	2.482733176798	-1.158106386133	-4.303561633140
C	0.483049688898	0.098363659340	-4.850746785006
C	2.683052513364	-1.426628235033	-5.656743402812
H	3.179066190706	-1.543892505867	-3.566805600722
C	0.697950372888	-0.160028126261	-6.204095072591
H	-0.384505826303	0.664663456366	-4.534974702867
C	1.794875310101	-0.923424231753	-6.610099555715
H	3.533110417405	-2.025358353902	-5.965642461776
H	0.000285682608	0.224993485213	-6.939874391427
H	1.954026478281	-1.129508029178	-7.663304836159
C	3.587384034657	0.687196962375	-1.952926664045
C	3.778447344619	1.530246029280	-3.060992893828
C	4.708037034391	0.210258713533	-1.253179823195
C	5.065209752538	1.889094609419	-3.459471721846
H	2.919799419889	1.906396579827	-3.606584339290
C	5.993119465461	0.559935606929	-1.666461221074
H	4.568143255683	-0.417001278142	-0.381357793934
C	6.175355632149	1.400144945800	-2.767156021997
H	5.199800540482	2.546822837851	-4.311399289751

H	6.851449061905	0.185010241885	-1.119631391750
H	7.176502669431	1.676530431980	-3.080703946450

E = -3703.39049219 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = CF_3

Co	-0.002789748740	-0.000626066006	0.000797401757
N	-0.016884168489	0.245573358282	1.881244046187
O	1.064708153812	0.454424185349	2.595882437654
B	2.202616835624	1.216896540076	1.944501005338
O	2.702930426072	0.545543339192	0.679186580248
N	1.838534258718	0.348844246781	-0.289632090291
C	2.235402605998	0.292524718140	-1.525504523343
C	1.165227223899	-0.103356570656	-2.458942843946
N	0.011295881197	-0.246815319268	-1.879651301408
O	-1.070297527206	-0.455662246690	-2.594292892367
B	-2.208226147836	-1.218118238729	-1.942925132526
O	-2.708520745802	-0.546776874735	-0.677596288222
N	-1.844119557528	-0.350084242130	0.291220570217
C	-2.240990906306	-0.293753267993	1.527090826293
C	-1.170817255396	0.102117741007	2.460533099210
F	1.756430084513	2.486994903216	1.622935308886
F	3.230025336265	1.169362120671	2.820664133452
C	3.649671815740	0.660870825429	-1.951030000389
C	1.374187926982	-0.378246396836	-3.941679964310
F	-1.762083279595	-2.488241078494	-1.621390505988
F	-3.235635523790	-1.170536537919	-2.819084464703
C	-3.655268666008	-0.662063203293	1.952608824550
C	-1.379793378570	0.376998179187	3.943269833281
N	-0.497439371622	2.121549207906	-0.322329410361
C	-0.371385622323	3.254260656317	-0.171300386072
C	-0.178737057543	4.667560054904	0.046995248285
H	0.055025012290	5.165094288854	-0.895701546679
H	-1.081979535645	5.108698413367	0.471739940218
H	0.652235771563	4.797079236619	0.743787149257
N	0.491851279937	-2.122781567152	0.323931100011
C	0.365805768867	-3.255492576191	0.172895754554
C	0.173187986401	-4.668764028873	-0.045601869124
H	1.076518596459	-5.109879378762	-0.470183180471
H	-0.060805408727	-5.166391622177	0.896987959083
H	-0.657622563971	-4.798187871271	-0.742605390898
F	0.516548460053	-1.278255461027	-4.407793329538
F	1.250963774357	0.735635075893	-4.671871732545
F	2.603284500971	-0.879157877513	-4.139244658714
F	3.615534608877	1.253383980892	-3.155003563227
F	4.436856647792	-0.417292623571	-2.034445112239
F	4.215152764928	1.524925908139	-1.117074400373
F	-4.220758240526	-1.526107219617	1.118646537312
F	-4.442425890473	0.416121668794	2.036006860966
F	-3.621148944274	-1.254564129708	3.156590017525
F	-2.608910384385	0.877865497111	4.140821333826
F	-1.256544624906	-0.736885315531	4.673455492237
F	-0.522185421656	1.277030948013	4.409395387388

E = -4127.22628270 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = CH_3

Co	-0.002455484894	-0.000640499594	0.000271750933
N	-0.031336124243	0.335975729671	1.857297846318
O	1.047709576659	0.619761555858	2.588259621922
B	2.143904127814	1.383211818806	1.896295743857
O	2.688300589154	0.711219519432	0.664768430256
N	1.808511401924	0.439368726026	-0.300178432389
C	2.223638032694	0.297457585350	-1.518939817583
C	1.154804083671	-0.107400647001	-2.449598166996
N	0.026387198240	-0.337179152377	-1.856738665239
O	-1.052649462137	-0.621038710285	-2.587684003754
B	-2.148822847148	-1.384490072803	-1.895707278048
O	-2.693262532938	-0.712415106274	-0.664221650742
N	-1.813476983384	-0.440575428807	0.300719292354
C	-2.228625259796	-0.298533614518	1.519456232069
C	-1.159790714764	0.106302877606	2.450124208262
F	1.659132380822	2.648401321084	1.542176713890
F	3.180559409949	1.434875462704	2.783167829498
C	3.637611821746	0.491044994190	-1.935827315498
C	1.349270102809	-0.211130227161	-3.919976335944
F	-1.664036437288	-2.649633412487	-1.541472774639
F	-3.185469396554	-1.436222348468	-2.782586992671
C	-3.642632715839	-0.491992682718	1.936299613351
C	-1.354309455450	0.210096047920	3.920493035901
H	-1.371055909607	-0.783843129085	4.380264763303
H	-0.530917777984	0.770818935307	4.360226264856
H	-2.301658525427	0.699712219366	4.155983971917
H	-3.700431796561	-1.021761612686	2.889461848088
H	-4.144727056821	0.473302439094	2.061872525567
H	-4.177606860856	-1.051681767537	1.170493435362
H	1.365588628572	0.782812771253	-4.379757182040
H	0.526062274110	-0.772169635407	-4.359653548217
H	2.296790613539	-0.700380351252	-4.155527106535
H	3.695332477726	1.021109972226	-2.888831398408
H	4.139682262490	-0.474216366253	-2.061753736853
H	4.172646613815	1.050500531130	-1.169895446541
N	-0.642787932735	2.129664557748	-0.445929802930
C	-0.466368374914	3.249169676047	-0.247800957239
C	-0.207460320335	4.641839660078	0.034713894143
H	0.084324396080	5.165329225669	-0.877271145497
H	-1.098684975157	5.116673465734	0.448376440901
H	0.606060569877	4.691792777778	0.761441168201
N	0.637193049510	-2.130910957946	0.447230950913
C	0.461434390499	-3.250400227516	0.248441219366
C	0.199665284342	-4.643473597114	-0.029406273702
H	1.087541160104	-5.120173858046	-0.448089226533
H	-0.086225116026	-5.164409267368	0.885903428487
H	-0.618714385282	-4.694489197384	-0.750577971725

E = -2934.40107640 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = Cl

Co	-0.002944939636	-0.000694012376	0.001009315168
N	-0.011256557173	0.321590508143	1.875053428370
O	1.061451959904	0.566086890333	2.605250248557
B	2.169910207937	1.342672069094	1.924855616328

O	2.705214309851	0.659156106324	0.683139186903
N	1.828792407613	0.426660675179	-0.276807638968
C	2.216058233435	0.280164574765	-1.497777218320
C	1.141805879722	-0.087815133045	-2.434538091425
N	0.005345224371	-0.322926714168	-1.873049075446
O	-1.067365084973	-0.567405861004	-2.603249680983
B	-2.175876549942	-1.343943961523	-1.922885090724
O	-2.711134545088	-0.660454503210	-0.681133279793
N	-1.834704871384	-0.427989544273	0.278812937335
C	-2.221979330548	-0.281457921848	1.499775162100
C	-1.147726389539	0.086511952951	2.436538469313
F	1.679343491187	2.593135999771	1.565331459881
F	3.199184738494	1.372438623374	2.806603893815
F	-1.685433273981	-2.594481361284	-1.563444060504
F	-3.205158433545	-1.373568472034	-2.804626997447
N	-0.598076085114	2.099182769417	-0.408921277328
C	-0.457573104116	3.228618887386	-0.244274138221
C	-0.244853853265	4.636569319070	-0.008263191052
H	-0.028400015471	5.148077031534	-0.947568203269
H	-1.132569106345	5.080516989016	0.445255822479
H	0.603549534226	4.742946128452	0.671109170324
N	0.592167774690	-2.100511348896	0.410937373262
C	0.451784286687	-3.229966181892	0.246326148008
C	0.239512940632	-4.637923345547	0.009956874306
H	1.127581604442	-5.081630322103	-0.443107241414
H	0.022617921507	-5.149602421020	0.949066032979
H	-0.608463334347	-4.744379835770	-0.669934802845
Cl	1.391901144021	-0.139763277270	-4.117560482955
Cl	3.834226568036	0.440766317949	-2.000962849072
Cl	-3.840161637634	-0.441985045142	2.002943501839
Cl	-1.397842474652	0.138519069648	4.119556148797

E = -4616.17845036 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = CN

Co	-0.002835703340	-0.000596440635	0.000804601845
N	-0.003242698739	0.277598871105	1.873962958721
O	1.058424395760	0.501250570502	2.604696831982
B	2.201290506966	1.271101769451	1.945033704288
O	2.709059571469	0.592630834753	0.673221254555
N	1.831864463408	0.379027254351	-0.273467222822
C	2.228399342956	0.258012343824	-1.508771342661
C	1.148263435571	-0.072262681295	-2.447631319917
N	-0.002413953807	-0.278819737598	-1.872347989402
O	-1.064077305903	-0.502477586434	-2.603080078243
B	-2.206928792199	-1.272326079732	-1.943405036242
O	-2.714714826351	-0.593843180187	-0.671604367673
N	-1.837525572107	-0.380247706538	0.275086505379
C	-2.234049541607	-0.259273065363	1.510398697319
C	-1.153909072029	0.071000843037	2.449254094270
F	1.733871564607	2.524333332189	1.604458509285
F	3.225083572814	1.239601834480	2.818755866405
F	-1.739458212134	-2.525521957141	-1.602774817784
F	-3.230722861891	-1.240887822645	-2.817131743052
N	-0.536199339945	2.106851850616	-0.357305649844
C	-0.451335863303	3.246963706968	-0.235668605136

C	-0.314841472320	4.672426167513	-0.058481452261
H	-0.114662286400	5.152215580734	-1.018003917418
H	-1.230961309773	5.086678039877	0.365868146433
H	0.518013011268	4.858996005692	0.622940588606
N	0.530484059726	-2.108095644471	0.358899194434
C	0.445478646985	-3.248210642315	0.237381754800
C	0.308972876266	-4.673730014276	0.060651606026
H	1.225176336701	-5.088155442093	-0.363346963003
H	0.108562023222	-5.153186150778	1.020292935498
H	-0.523744117082	-4.860508544613	-0.620880797516
C	3.577774078131	0.411945324693	-1.916598352806
C	1.344829551843	-0.140787617181	-3.850335075765
C	-3.583416261798	-0.413244524408	1.918236947427
C	-1.350457471706	0.139476838697	3.851962554609
N	1.532958925073	-0.192815652565	-4.987589663888
N	4.666875809635	0.534359441149	-2.277600587494
N	-4.672506806179	-0.535689016439	2.279262630720
N	-1.538560513791	0.191468567073	4.989223220327

E = -3146.31513140 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = H

Co	-0.002925213504	-0.000673442883	0.000954825437
N	-0.019071849389	0.327289365579	1.863307793190
O	1.045486464709	0.609838550273	2.599260388103
B	2.157105803972	1.371754659531	1.913591304213
O	2.695752555542	0.703745312700	0.668227694613
N	1.815713218788	0.432481985303	-0.283972773533
C	2.205301092649	0.292473035459	-1.507733219916
C	1.151825635761	-0.099983162826	-2.427146851021
N	0.013211749300	-0.328610846613	-1.861412510846
O	-1.051344786487	-0.611159603875	-2.597368088590
B	-2.162993249459	-1.373041502234	-1.911709765928
O	-2.701615132810	-0.705031418748	-0.666332349943
N	-1.821573126488	-0.433781999855	0.285869994221
C	-2.211167933035	-0.293760472444	1.509627890746
C	-1.157691746815	0.098686611775	2.429042573357
F	1.677047993061	2.634838997555	1.564051165326
F	3.189957499036	1.402171381217	2.797958447801
F	-1.682997964776	-2.636153351814	-1.562192139288
F	-3.195848123926	-1.403400657822	-2.796074852868
N	-0.609646389333	2.110174191125	-0.417816437395
C	-0.452219582268	3.235335060295	-0.238746598731
C	-0.217077467973	4.636645200467	0.017374632456
H	0.024740576544	5.155438697037	-0.911698851851
H	-1.103165690872	5.093157447575	0.461491961089
H	0.622198043129	4.716696761328	0.711451997920
N	0.603841528037	-2.111464840072	0.419627734560
C	0.446458121923	-3.236645191429	0.240645069580
C	0.211552933926	-4.638011416232	-0.015385954494
H	1.097596345699	-5.094312630452	-0.459812238850
H	-0.029816515541	-5.156858581235	0.913772063048
H	-0.627928588352	-4.718268300780	-0.709190431172
H	1.284185074350	-0.182902418287	-3.500146769491
H	3.238554353022	0.442897208124	-1.800095812475
H	-3.244426083215	-0.444164717788	1.801982737666

H	-1.290052735207	0.181625480047	3.502040543067

E = -2776.47787158 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = NH_2

Co	-0.002828816859	-0.000704276032	0.000844928863
N	-0.032501059960	0.383769054554	1.840069639721
O	1.046532555401	0.660701327758	2.598189356868
B	2.142551949134	1.424645612886	1.900318659739
O	2.694445343310	0.755780220890	0.666572779357
N	1.788609594497	0.486616460594	-0.293949327602
C	2.211018869545	0.297417490575	-1.501446045698
C	1.140051836086	-0.106007463261	-2.433962727490
N	0.026841243337	-0.385131939605	-1.838386141009
O	-1.052188296872	-0.662112512554	-2.596487509885
B	-2.148130090843	-1.426102814629	-1.898561280935
O	-2.700093042022	-0.757172902596	-0.664884389253
N	-1.794278065771	-0.487968424745	0.295639619497
C	-2.216700120717	-0.298707335802	1.503122938357
C	-1.145732505061	0.104713253115	2.435640123578
F	1.653990831631	2.688912832542	1.545680378702
F	3.181026974933	1.481470828828	2.788952939804
F	-1.659403694474	-2.690266017892	-1.543758615320
F	-3.186594594032	-1.483149879149	-2.787197310473
N	-0.706475829820	2.151138472952	-0.501109388562
C	-0.497992848735	3.261226937399	-0.279260812573
C	-0.200020920814	4.640692525430	0.030774524380
H	0.100657584116	5.175222213871	-0.871917352641
H	-1.076057096056	5.130389263277	0.459377522191
H	0.618232406754	4.652960093201	0.753591728192
N	0.700688136280	-2.152464766352	0.502678411774
C	0.492123105082	-3.262535675584	0.280819647265
C	0.194352491237	-4.642015927130	-0.029341737428
H	1.070619354351	-5.131739169327	-0.457444386087
H	-0.106827453309	-5.176506078346	0.873206472679
H	-0.623507826718	-4.654301144422	-0.752605372046
N	1.352177437472	-0.206995093393	-3.781335161398
H	0.496725700715	-0.371479863078	-4.298493379010
H	1.948411362329	0.499964206896	-4.187295065929
N	3.499836666658	0.487021857910	-1.918310321981
H	3.838991395847	-0.166354187434	-2.609851548599
H	4.139584001566	0.641149250107	-1.148149723423
N	-3.505533049258	-0.488240236549	1.919971596557
H	-3.844669944540	0.165170283015	2.611489002597
H	-4.145272107818	-0.642355471525	1.149801718498
N	-1.357877635675	0.205774625960	3.783005174346
H	-1.954136759975	-0.501147886580	4.188992032372
H	-0.502432080952	0.370267254223	4.300171402001

E = -2998.61668247 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = OCH_3

Co	-0.002795602679	-0.000594305073	0.000745753297
N	-0.025386431659	0.349238746341	1.866790993133
O	1.080092134099	0.567975457036	2.603313200112
B	2.164553602546	1.339177502686	1.915482874287

O	2.709705090018	0.658835785888	0.696402495391
N	1.819222787393	0.449015972870	-0.291045996137
C	2.224711556363	0.296839742725	-1.507624646623
C	1.148632383211	-0.114391516872	-2.445948503990
N	0.019790560214	-0.350412499184	-1.865303091559
O	-1.085687319601	-0.569153410065	-2.601825703312
B	-2.170155854824	-1.340347297475	-1.913997807265
O	-2.715301625837	-0.660003357698	-0.694914745273
N	-1.824819517431	-0.450187943701	0.292534484591
C	-2.230311405738	-0.297996888973	1.509110572799
C	-1.154232232529	0.113231711914	2.447434763115
F	1.677319646758	2.605641714020	1.559212725725
F	3.203060142575	1.397726559808	2.805686339113
F	-1.682940044537	-2.606819836542	-1.557733377471
F	-3.208663339137	-1.398880338870	-2.804200973963
N	-0.648742360197	2.135616795926	-0.456099640940
C	-0.466367910060	3.253396670464	-0.253824715676
C	-0.199131525098	4.643762243641	0.033617094633
H	0.084392090094	5.171243064435	-0.878729072531
H	-1.084664448865	5.119595351540	0.458343506290
H	0.621515683932	4.689320440406	0.752542097056
N	0.643141439804	-2.136781026112	0.457588901172
C	0.460775601228	-3.254567726104	0.255345413527
C	0.193574918095	-4.644943652948	-0.032078597025
H	1.079143728140	-5.120782938473	-0.456723275699
H	-0.090013904593	-5.172399190627	0.880261904068
H	-0.627017074016	-4.690529914601	-0.751064784893
O	1.469049683179	-0.130203941543	-3.727681166658
O	3.437640617633	0.397220103375	-2.021934442699
O	-1.474654337524	0.129057168468	3.729166361170
O	-3.443244608536	-0.398358262696	2.023415707955
C	0.725956969268	-0.941315558799	-4.655671032425
H	0.618775036392	-1.954749301776	-4.267297419539
H	-0.257175634910	-0.517017008603	-4.842582779218
H	1.332020224599	-0.946112211712	-5.559409431236
C	4.429227999086	1.230442179294	-1.394779988824
H	4.012401963452	2.215519239701	-1.181691284190
H	4.789379306291	0.780055541837	-0.473430889640
H	5.224771819343	1.309860706462	-2.132963742181
C	-4.434832137139	-1.231590626470	1.396274824995
H	-4.018006407614	-2.216671167333	1.183201666943
H	-5.230376022075	-1.310997527621	2.134459816290
H	-4.794983816733	-0.781218880202	0.474918565214
C	-0.731562334119	0.940174685035	4.657152005858
H	0.251563303110	0.515867700625	4.844081149912
H	-0.624364067686	1.953601126516	4.268764078867
H	-1.337635323686	0.944992119056	5.560883813453

E = -3235.85914586 Hartrees

$Co^{II}(dRgBF_2)_2L_2$ R = OH

Co	-0.002120155091	0.004441439633	0.000588978378
N	-0.017252067780	0.340702028956	1.844465454451
O	1.056898604185	0.606582098398	2.611729628211
B	2.164243368648	1.380296383847	1.921015066819
O	2.709394275417	0.713775016589	0.671193533775

N	1.794630197621	0.457273270427	-0.283054397454
C	2.204869576491	0.313556619117	-1.496639766933
C	1.133209986151	-0.083273033419	-2.430676066465
N	0.012767678338	-0.330824031650	-1.843520541222
O	-1.061405094538	-0.596748968684	-2.610614876186
B	-2.168692020799	-1.370510797974	-1.919859992666
O	-2.713911247298	-0.703825371333	-0.670153024787
N	-1.799184061412	-0.447380581624	0.284129987391
C	-2.209649688137	-0.302554756087	1.497510284075
C	-1.138007601825	0.094321622926	2.431539853664
F	1.676310701320	2.639504804142	1.574856802931
F	3.199828218480	1.414293672795	2.804822770932
F	-1.680641629166	-2.629606357560	-1.573496901123
F	-3.204225768442	-1.404687214254	-2.803712128995
N	-0.646274467511	2.154026020219	-0.435109327477
C	-0.471520500835	3.273070895620	-0.232483724865
C	-0.217480068386	4.666212240166	0.051769040758
H	0.048480659437	5.196235598329	-0.864326082094
H	-1.103607711855	5.130221016474	0.488057093377
H	0.611098873084	4.722623388453	0.760627884898
N	0.641323378399	-2.143741679318	0.435939642899
C	0.467030163680	-3.262924688253	0.233720744816
C	0.213471751191	-4.656264895432	-0.049949235239
H	1.099674732645	-5.120106889396	-0.486255751513
H	-0.052114382012	-5.186048132979	0.866394866442
H	-0.615251663908	-4.713242857056	-0.758600395779
O	1.338110093211	-0.133434653747	-3.737062774659
H	0.492947469145	-0.395983164345	-4.140310033870
O	3.455129915834	0.463481233347	-1.903442714024
H	3.975319592610	0.705356951333	-1.118156963236
O	-1.343163564973	0.145829916462	3.737820725659
H	-0.497864191450	0.408176969538	4.140951811749
O	-3.460142456577	-0.451292670248	1.904050520871
H	-3.980302983894	-0.693209223415	1.118760446490

E = -3078.07551162 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = C_6H_5

Co	-0.014049327362	0.078285322801	-0.010401093085
N	0.001311680776	0.025148669930	1.835623336594
O	1.112598546248	-0.011945429396	2.588916746555
B	2.270787103853	0.753236179227	2.045431895605
O	2.739999625806	0.239939799706	0.722592166829
N	1.825348523597	0.135749715589	-0.252026666129
C	2.250768388505	0.141871036918	-1.499612034548
C	1.158968265980	0.013594791011	-2.451916984330
N	-0.016333044596	-0.023006105429	-1.858738271246
O	-1.114380116478	-0.095107156240	-2.627449727959
B	-2.294641557175	-0.762826313707	-2.003925080141
O	-2.741978936759	-0.091012176905	-0.750532793312
N	-1.833783040165	-0.145026975128	0.238180042295
C	-2.261133436509	-0.154109557117	1.483566689719
C	-1.163719776049	-0.100987963525	2.434554174512
F	1.936081946154	2.101665755576	1.945949251367
F	3.315729435539	0.530697435898	2.919092680168
F	-1.987007533979	-2.097411883423	-1.725790429575

F	-3.327060769970	-0.627170265625	-2.906724816145
H	-0.146103398137	1.522061899010	-0.046815782094
C	1.337839141200	-0.125924530553	-3.910295464414
C	0.547932530231	0.602880261037	-4.816438604918
C	2.304043012646	-1.012937170793	-4.417169706808
C	0.734539196891	0.457114099558	-6.190791568643
H	-0.219461646025	1.265358206934	-4.436314478736
C	2.481430355432	-1.161000631749	-5.791929754499
H	2.909937625516	-1.590556697919	-3.727735296517
C	1.700531467623	-0.423012201863	-6.684190777493
H	0.115251161949	1.025988924376	-6.876981634970
H	3.227829621572	-1.855221011961	-6.164768113725
H	1.838277301144	-0.538386137003	-7.754871686216
C	3.666117392368	0.335722667997	-1.872173953559
C	4.013387745398	1.273135770218	-2.860694032725
C	4.689819586864	-0.395067171351	-1.244632596950
C	5.347104035304	1.468222548798	-3.217657768749
H	3.233643239308	1.853015551081	-3.342174198353
C	6.021498254629	-0.202378107936	-1.610473618534
H	4.435104270225	-1.096560863838	-0.459916477661
C	6.355841287957	0.727734448548	-2.597529696255
H	5.596916149081	2.201042104787	-3.978359248086
H	6.799805660247	-0.773580875070	-1.114549849366
H	7.394187659375	0.879660455564	-2.875689459253
C	-3.689570596500	-0.149654898029	1.853925986859
C	-4.167595369418	0.752144501562	2.819823402083
C	-4.593506284014	-1.042311021214	1.251695385645
C	-5.515478236128	0.758314462406	3.178792961675
H	-3.479511523852	1.450144454107	3.284394036044
C	-5.938016638004	-1.037328257108	1.619865300028
H	-4.235889868145	-1.723987668087	0.489429010482
C	-6.404400825197	-0.138657901720	2.583294122097
H	-5.869239773746	1.464884614853	3.922954849885
H	-6.623847450557	-1.732603491985	1.146422048421
H	-7.453316341615	-0.134653528133	2.863425437085
C	-1.311333672542	-0.233294506155	3.897109233260
C	-0.659711159862	0.658673786272	4.766764400902
C	-2.105239653894	-1.256003526963	4.442409067190
C	-0.813940606894	0.534643375374	6.146599032785
H	-0.025636330602	1.433474693933	4.352356357670
C	-2.250187887605	-1.380438594198	5.824222611333
H	-2.604214212900	-1.954693262196	3.779381895731
C	-1.608441666072	-0.483645061559	6.680703336603
H	-0.304713417829	1.230493430199	6.805686004435
H	-2.863462687673	-2.178971365030	6.229718203227
H	-1.721386425162	-0.580262654363	7.756158997911

E = -3437.70483851 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = CF_3

Co	-0.010029572325	0.063732478141	-0.005704066694
N	0.009733998517	-0.054206291533	1.843770322270
O	1.103720900711	-0.118280416005	2.591823296498
B	2.326439893487	0.565771016830	2.042576572718
O	2.728010360881	-0.020256135774	0.714988679866
N	1.827138191801	0.051839905031	-0.256225535981

C	2.241741415861	0.132063532120	-1.503220375504
C	1.148680834154	0.070914767760	-2.448925223481
N	-0.026220816924	0.068175994092	-1.857351656872
O	-1.122646506586	0.142603808665	-2.603273892561
B	-2.314805255462	-0.573586486069	-2.031975773482
O	-2.741908198604	0.049446675953	-0.731237461142
N	-1.842820075890	-0.036240894230	0.242472136506
C	-2.256367399392	-0.124289325893	1.488364980118
C	-1.165484301814	-0.064822058070	2.436658217975
F	2.072087953292	1.914656883848	1.892931978813
F	3.342038793401	0.270102470694	2.905544842636
C	3.691723223818	0.362401742120	-1.861296263112
C	1.296958661973	-0.061423772160	-3.947775866777
F	-1.980030941172	-1.899727093887	-1.808422459919
F	-3.340489088345	-0.378417172220	-2.908784846004
C	-3.707926803221	-0.350200719786	1.845244650274
C	-1.314446076137	0.067954961315	3.934831450056
H	-0.027184353121	1.505652660012	0.051458267071
F	0.325243060046	-0.784814336143	-4.499882542096
F	1.315446956621	1.132233643345	-4.567954242409
F	2.449100265292	-0.690623348235	-4.249513018187
F	3.785024044864	1.070749740033	-3.003568419604
F	4.345909531139	1.062911255800	-0.937802421153
F	4.363735102075	-0.788912121226	-2.046900768963
F	-4.372296415290	0.802706799124	2.044277023309
F	-3.801970736529	-1.071094011268	2.979480867839
F	-2.472448227486	0.685322340026	4.238857383507
F	-1.320568570216	-1.125401367020	4.557034741808
F	-0.349103365131	0.801392773127	4.484918981556
F	-4.367687394283	-1.036805728517	0.915389791121

E = - 3861.57540646 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = CH_3

Co	-0.017198128856	0.137328815115	-0.007912604957
N	0.009724891773	0.064137341783	1.838839192432
O	1.106382918303	0.092460448244	2.619271426884
B	2.305591839724	0.767860032633	2.033620626054
O	2.743515744805	0.186651275819	0.726147091363
N	1.815347115439	0.167816007541	-0.248981857420
C	2.234288566063	0.136871029188	-1.492156062368
C	1.145751777519	0.055376787834	-2.438744833673
N	-0.026646369954	0.016884618442	-1.851640698103
O	-1.127879599969	0.018331512336	-2.628772020703
B	-2.301851466862	-0.682416963104	-2.026135241002
O	-2.761945107584	-0.077436551209	-0.739211100398
N	-1.834612788121	-0.087717831652	0.239029773198
C	-2.245939136307	-0.139930553704	1.483768916680
C	-1.155845216305	-0.058236878235	2.428623876970
F	2.055635926406	2.130115100877	1.885757317039
F	3.341013448479	0.516646982408	2.915896824224
C	3.678120945529	0.177461695029	-1.853874906424
C	1.305529866921	0.043053554240	-3.919057179445
F	-1.980162317984	-2.027169389644	-1.816489760196
F	-3.343717734210	-0.517510781564	-2.918038835797
C	-3.684109805078	-0.244364863594	1.854814737841

C	-1.301705301787	-0.110423424880	3.909569485798
H	-1.159117565615	-1.128543552070	4.290145976874
H	-0.534831020444	0.513868729004	4.370836028593
H	-2.289705692781	0.233371405412	4.220562971666
H	-3.817133023758	-0.860081622814	2.747015280160
H	-4.116254665895	0.742571822079	2.058622746259
H	-4.238694635360	-0.680887579965	1.024125957551
H	1.346448028486	1.061048851284	-4.324565740080
H	0.445678833726	-0.453092334366	-4.369886511390
H	2.221728745030	-0.473506356116	-4.212459352927
H	3.825807452951	0.637117619707	-2.832962652909
H	4.113401044693	-0.828416357186	-1.881894620875
H	4.223517599335	0.743990796493	-1.097891953833
H	-0.145434168304	1.589983614636	-0.046983297085

E = -2668.71074049 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = Cl

Co	-0.015814995191	0.125560911019	-0.007449744269
N	0.030094029259	0.055275697294	1.852038818391
O	1.116924186903	0.070442091714	2.623019385922
B	2.315376174406	0.768468990236	2.041404098996
O	2.750849305961	0.167019687069	0.732833332489
N	1.831598035869	0.159735028444	-0.231837524690
C	2.218571735234	0.136917556133	-1.477836778312
C	1.131023093279	0.070571370517	-2.421955704341
N	-0.046508819428	0.014111326877	-1.863765023609
O	-1.136434017100	0.019471271081	-2.632330904286
B	-2.307841870455	-0.705636653206	-2.031765924396
O	-2.767361087870	-0.076942400908	-0.745753768977
N	-1.848953896318	-0.090790402204	0.221136420251
C	-2.231756213080	-0.123191726552	1.467668223212
C	-1.143593235288	-0.056665466279	2.411122157406
F	2.029890469656	2.111046596916	1.863427226670
F	3.343823173223	0.532746147698	2.917881459772
F	-1.949160994676	-2.025808990555	-1.789089711145
F	-3.342076137721	-0.559973174518	-2.917940382739
H	-0.142244834804	1.576163300516	-0.043369855951
Cl	1.366747139916	0.110224833715	-4.115817526539
Cl	3.861883291529	0.173046489907	-1.952521291466
Cl	-3.872932718287	-0.190909813383	1.945108260744
Cl	-1.374757535015	-0.128476111533	4.104893546868

E = -4350.50466280 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = CN

Co	-0.011329118708	0.075698814552	-0.006043521496
N	0.027354492973	0.029617923290	1.843805851407
O	1.103657829166	0.047706166832	2.611062292029
B	2.309989535810	0.758714150669	2.036457340736
O	2.738536286969	0.144988429942	0.720033025489
N	1.824544045916	0.134512711017	-0.234753918571
C	2.231300700655	0.138737357674	-1.488923225320
C	1.140210293874	0.080128168953	-2.434924822997
N	-0.040443354227	0.009871941064	-1.854439799829
O	-1.120382482362	0.013779985420	-2.618440535804

B	-2.301129669490	-0.723828073380	-2.027287851010
O	-2.751367496799	-0.083765822033	-0.732049962786
N	-1.838916859448	-0.095208882598	0.225554519498
C	-2.243697332841	-0.115276311656	1.479327034364
C	-1.152622826623	-0.056511620876	2.425397557647
F	1.993252774916	2.083990040733	1.830688221829
F	3.330499791612	0.535799600441	2.906831330315
F	-1.919643744161	-2.026530055346	-1.764618793058
F	-3.326742226557	-0.581202936938	-2.906191602283
H	-0.120771685020	1.510458928729	-0.027808387633
C	1.318316996595	0.104253579339	-3.838299341474
C	3.593199700675	0.193538551908	-1.867336951033
C	-3.605222105390	-0.179649201498	1.858446345263
C	-1.329565369462	-0.089869858206	3.828501712044
N	1.496904598741	0.123995838814	-4.979489057117
N	-4.707124686519	-0.233356250688	2.201269651762
N	-1.506787017942	-0.121646819927	4.969674871381
N	4.695905687647	0.234911683766	-2.209427573354

E = -2880.67895966 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = H

Co	-0.014942823969	0.119344360382	-0.006909939250
N	0.022644962413	0.060523111687	1.843010107652
O	1.110799104846	0.091316305293	2.624802584126
B	2.312782192800	0.770627894920	2.039375232817
O	2.750646479685	0.187336133015	0.728261057771
N	1.821407874556	0.164313399600	-0.237159837290
C	2.216499757977	0.137562919750	-1.483966679336
C	1.139572617584	0.063666915996	-2.418832448464
N	-0.038147875951	0.015724646318	-1.853177335348
O	-1.129811157698	0.015446686917	-2.632918791433
B	-2.310024633618	-0.686613597163	-2.033163546874
O	-2.766907784277	-0.082296020356	-0.739580481715
N	-1.837560915429	-0.089194331289	0.227818800521
C	-2.227410927812	-0.130217210073	1.475146829685
C	-1.150447401513	-0.055603877686	2.409972681724
F	2.050887003004	2.127352550295	1.881750734408
F	3.345723406638	0.524985168651	2.919709085056
F	-1.984259384293	-2.027162865907	-1.820684714773
F	-3.348534799518	-0.516907934051	-2.921805322585
H	-0.138599052834	1.565094431218	-0.040532990692
H	1.248835449623	0.057418849851	-3.496078429398
H	3.266885251516	0.170721424625	-1.744548928147
H	-3.275521633884	-0.203194803889	1.736976566862
H	-1.256214059846	-0.088357458104	3.487040254681

E = -2510.79954769 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = NH_2

Co	-0.022396546057	0.210808058400	-0.008487252635
N	0.018311854408	0.127278395218	1.836757650127
O	1.112006163765	0.155909919879	2.637736157990
B	2.321376356207	0.822956884579	2.049767001982
O	2.759853314879	0.250110654721	0.732760947148
N	1.811124769442	0.229989154151	-0.235893804636

C	2.222790820757	0.136668667460	-1.473409778204
C	1.133703123751	0.058526059385	-2.421699844728
N	-0.037492989281	0.009931608622	-1.843954493976
O	-1.132816928471	0.003262136951	-2.644848462087
B	-2.315707201375	-0.692330412208	-2.039952674959
O	-2.778267679643	-0.098316063132	-0.742363510502
N	-1.827987132309	-0.097516892878	0.226398566986
C	-2.231272221110	-0.137181442034	1.468927874429
C	-1.140100157026	-0.056318838264	2.414557253916
F	2.091446249548	2.187393845577	1.918600470147
F	3.354989094911	0.545485771432	2.930164325568
F	-2.009707947989	-2.040898580334	-1.847730937969
F	-3.357630402118	-0.505279209443	-2.930660763440
H	-0.205387423302	1.672012656278	-0.091009781545
N	-3.551980610827	-0.287845910525	1.857818668672
H	-3.828235296148	0.353403042743	2.590996733026
H	-4.161107863624	-0.225591142520	1.049074833721
N	-1.327423058173	-0.105323045441	3.786961155350
H	-0.429488431022	-0.112278708699	4.258869567994
H	-1.915736242067	-0.873563885897	4.084205321007
N	1.332917786721	-0.004754508492	-3.790877776678
H	0.441769335967	0.041101302492	-4.273402492924
H	1.985010631170	0.690317273265	-4.132492272248
N	3.553961913026	0.172608430408	-1.857403570238
H	4.151927756527	0.144281120683	-1.038533321522
H	3.797106959461	-0.546082342376	-2.527510789772

E = -2732.91083038 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = OCH_3

Co	-0.008225172626	0.135325454435	-0.002049702303
N	0.026334339555	0.084461575622	1.859081537427
O	1.106840540930	0.216042465408	2.657062408233
B	2.323476840116	0.819637546338	2.032333768871
O	2.746460534608	0.138233412145	0.768798647281
N	1.832486367551	0.166070452405	-0.225299302911
C	2.247304416912	0.092756688080	-1.461691828942
C	1.159465776687	-0.017895527307	-2.419237821949
N	-0.015798266889	-0.058749744478	-1.851558650241
O	-1.122175876095	-0.031987442495	-2.628704181849
B	-2.268050982065	-0.785912000551	-2.036694746476
O	-2.758714680950	-0.204632239502	-0.750184643346
N	-1.829782983205	-0.125220632772	0.227713564360
C	-2.230595291178	-0.161877177740	1.472466548271
C	-1.146190758552	-0.043162911745	2.426004140025
F	2.120519739917	2.174145652929	1.791369057178
F	3.349051704296	0.592447340597	2.933452722075
F	-1.890965071331	-2.115975475191	-1.838670980991
F	-3.313101262731	-0.653790452425	-2.930561755053
H	-0.159121315973	1.593518686558	-0.074845012418
O	1.443379971736	-0.003563266989	-3.725160028669
O	3.510222927208	0.055952343804	-1.899668925343
O	-3.488447823343	-0.327641335946	1.905623114701
O	-1.412886855571	-0.005285913699	3.740011848682
C	4.439723158940	0.976053044283	-1.313606153075
H	3.992261602055	1.970316826314	-1.239003661320

H	4.741740077418	0.644794192096	-0.321632970065
H	5.288441869062	1.000512365562	-1.996993877139
C	0.694827793697	-0.875382356302	-4.581137109123
H	1.287294871984	-0.959277162789	-5.492336000036
H	0.580909890403	-1.857751889983	-4.116633314466
H	-0.291253079583	-0.464525569623	-4.789512350536
C	-4.462014870421	0.603231385001	1.421358349966
H	-4.153098056079	1.625853997758	1.658886075097
H	-4.599551149315	0.495549093067	0.345878870302
H	-5.381808987820	0.366989906445	1.955575045470
C	-0.704058991767	-0.930855727825	4.568932149429
H	-1.133909581609	-0.819745946074	5.564043982573
H	-0.866318910043	-1.953273992648	4.213132814836
H	0.361850654071	-0.705299652762	4.579649101474

E = -2970.15901444 Hartrees

$Co^{II}H(dRgBF_2)_2$ R = OH

Co	-0.016290718711	0.244338977126	-0.005430173065
N	0.023008955910	0.097860458418	1.827045608478
O	1.110201259796	0.102070270043	2.640130981267
B	2.334719127323	0.774490288283	2.066871281329
O	2.767042624218	0.216560941857	0.731103618078
N	1.808805858114	0.220152914395	-0.230582620567
C	2.224151382268	0.165443080768	-1.466799311637
C	1.135066815137	0.103666418879	-2.415372039280
N	-0.033843632790	0.095711179100	-1.835547913120
O	-1.122635393463	0.095949424203	-2.648957331468
B	-2.313582844578	-0.611103981379	-2.050646222205
O	-2.777208296556	-0.020081427510	-0.742085068480
N	-1.818082681133	-0.028902698378	0.221043033571
C	-2.224837805141	-0.126091170371	1.457247099286
C	-1.135722240345	-0.063922671416	2.405670951086
F	2.108607206385	2.136105565667	1.952402710830
F	3.359659787518	0.470009938532	2.938042979687
F	-1.996252129191	-1.951832433080	-1.857439173919
F	-3.349305605581	-0.419064844468	-2.937401871265
H	-0.140202537278	1.709788692026	-0.025123268575
O	1.301072994389	0.075156582508	-3.740570429880
H	0.398569320920	0.014978567147	-4.099389631783
O	3.515595940129	0.155678404310	-1.811814168003
H	3.995992427652	0.226961403276	-0.968917172429
O	-3.508859599043	-0.251751477356	1.803871431061
H	-3.989315146996	-0.282602247536	0.958296953656
O	-1.290711240555	-0.172733352397	3.728948070662
H	-0.393025978397	-0.073877472646	4.090668696685

E = -2812.38563969 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = C_6H_5

Co	0.082551174957	-0.211156064177	0.080550806696
N	0.055483024113	0.041393968671	1.936306362817
O	1.164304025876	0.076782704824	2.666422847630
B	2.272632649670	0.904956180578	2.070973125476
O	2.784086009601	0.315735994506	0.781431731493
N	1.901797488891	0.162988279207	-0.197103727267

C	2.302138328948	0.214400803832	-1.433946788994
C	1.210318732689	-0.042995119539	-2.391670790940
N	0.068580177804	-0.250715805409	-1.801333544310
O	-1.013735102725	-0.450069783019	-2.543520339295
B	-2.189413346257	-1.118449929765	-1.892126775080
O	-2.649386529335	-0.389226898276	-0.664987655278
N	-1.776262149183	-0.336063661611	0.334716337145
C	-2.208220920372	-0.165278593374	1.550138553015
C	-1.104984144180	-0.012723469461	2.518076710000
F	1.796832247527	2.183589971844	1.838388104633
F	3.313824260721	0.833038003165	2.949289268544
F	-1.851596739991	-2.426950261956	-1.545008080935
F	-3.211098970130	-1.038565001173	-2.791262823263
H	1.352211853829	-5.122196719521	-0.239701750025
H	0.211656672982	-5.180308898723	1.123088650311
H	-0.401232670832	-5.054251990565	-0.545603157763
C	0.396715783603	-4.752802599587	0.136242019298
C	0.416205183715	-3.312112528164	0.214966625103
N	0.399456774816	-2.166387029669	0.251588424584
H	-0.148923807488	1.200628436864	-0.048514699352
C	1.391277940221	-0.099988106125	-3.855743180513
C	2.434109031480	-0.867811727790	-4.401202809164
C	0.523447620156	0.590862330593	-4.717371506047
C	2.602672507514	-0.944724973247	-5.782750682882
H	3.108976799581	-1.405948417666	-3.744398588665
C	0.707919552713	0.523326586432	-6.097647433822
H	-0.297107960261	1.165618828071	-4.305792783787
C	1.744057979515	-0.244886385977	-6.633435777585
H	3.405627652961	-1.547307213105	-6.193165494073
H	0.034275667254	1.062922810782	-6.754213692731
H	1.879226691993	-0.301176851543	-7.708322288292
C	3.685279286204	0.547497515357	-1.828882262142
C	3.913071581158	1.540876378754	-2.796192593113
C	4.781457872835	-0.099388678456	-1.235706570846
C	5.214791763011	1.879271612794	-3.161959293027
H	3.073210441400	2.053188750948	-3.252500836602
C	6.080574163141	0.232027583123	-1.618358385324
H	4.613726437224	-0.843510849156	-0.466715690450
C	6.300342346056	1.221348765330	-2.579356255386
H	5.380079949231	2.655819678814	-3.900692032542
H	6.920877566154	-0.273124332211	-1.154804822005
H	7.312753521917	1.483480122407	-2.867719808780
C	-3.635838697358	-0.056894312248	1.905664766232
C	-4.071470063286	0.992009999563	2.732509177464
C	-4.571560842555	-0.984323238870	1.417983839863
C	-5.420841989430	1.111551340392	3.062161872185
H	-3.356730654206	1.715535271258	3.109341021390
C	-5.916385424813	-0.868176894738	1.764777469642
H	-4.245107040406	-1.781222571871	0.760567041874
C	-6.344310056428	0.179482013055	2.584124937513
H	-5.748791868820	1.930911154145	3.692392523425
H	-6.631586190117	-1.589611716489	1.385150469748
H	-7.393306077944	0.271652011261	2.844790115695
C	-1.287433242999	0.025728037267	3.981331346552
C	-2.120034301734	-0.914456344199	4.610253304473
C	-0.630279381419	0.995199788480	4.757356889073

C	-2.287831371259	-0.888707551153	5.994142102483
H	-2.633067382925	-1.664140753742	4.017199260732
C	-0.815269922440	1.024638365864	6.138451770551
H	0.025069057798	1.712730542754	4.278142325543
C	-1.639849458089	0.083044211090	6.759683650638
H	-2.926941045699	-1.623173525074	6.472051361897
H	-0.307620290706	1.778658391899	6.729798051379
H	-1.775221175871	0.105808363725	7.835807055184

E = -3570.79837549 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = CF_3

Co	0.074844081057	-0.183391105970	0.073806730260
N	0.065970866414	0.006236568498	1.946167061256
O	1.157835959724	0.041743053411	2.669196973528
B	2.333928417509	0.800727961480	2.067387464588
O	2.788368649736	0.118802362448	0.782072138341
N	1.916112600789	0.096134553294	-0.194997395145
C	2.307035795201	0.175239113403	-1.430696826433
C	1.212833124547	-0.017199668239	-2.386556622022
N	0.054030119311	-0.138075742703	-1.809095100993
O	-1.037069170954	-0.173997170372	-2.532917690603
B	-2.230347347954	-0.908299930255	-1.952830906798
O	-2.664625676397	-0.262821751702	-0.649794153045
N	-1.791214560579	-0.230785408303	0.325542672194
C	-2.197672357680	-0.183463290178	1.559929471742
C	-1.101925469398	0.011780009444	2.513459199588
F	1.925253796129	2.072856646640	1.765277881183
F	3.351605544630	0.669573683155	2.941294204792
C	3.746391718643	0.499074605142	-1.814902039460
C	1.389506889652	-0.124352298740	-3.896749612644
F	-1.868879043046	-2.215946070492	-1.702843889939
F	-3.245288158518	-0.729501221595	-2.820464787708
C	-3.659858052686	-0.371888739427	1.946213374040
C	-1.287899862171	0.265779055575	4.005416615504
H	1.341183100741	-5.073592707564	-0.231112196230
H	0.193625829895	-5.132529204202	1.127722279854
H	-0.412719592274	-5.081548574607	-0.547503285525
C	0.369609788304	-4.730169636166	0.128508340681
C	0.341997162975	-3.289075473473	0.168015947963
N	0.299076892957	-2.143327315149	0.183099115801
H	-0.073562218608	1.247789395125	0.008444443688
F	0.462655169222	-0.894219351094	-4.453244304906
F	1.350936016886	1.074316492068	-4.481346217157
F	2.574777208189	-0.692488515331	-4.163957640867
F	3.756653301395	1.217045704081	-2.945181684316
F	4.362333651895	1.220428070684	-0.890963043394
F	4.451617090972	-0.620540781461	-2.016827945229
F	-4.307785398780	-1.141065941792	1.079869764015
F	-4.298406966294	0.796100608724	2.035634860806
F	-3.727549721504	-0.988255606865	3.135281943932
F	-2.429384036768	0.937620110791	4.204014736613
F	-1.349636828336	-0.885980095112	4.684421424716
F	-0.311152494822	0.999888336830	4.515627927330

E = -3994.62607331 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = CH_3

Co	0.084807355306	-0.227888079145	0.081496013380
N	0.062620829782	0.047209243519	1.935676683933
O	1.157016084276	0.152401482369	2.682999584375
B	2.301106184589	0.906031248128	2.044292078593
O	2.796370891588	0.228508915175	0.786408737037
N	1.902938115645	0.134544905983	-0.193698395240
C	2.295852033544	0.173103329545	-1.427382452856
C	1.199756917255	-0.030750698597	-2.379322431302
N	0.063878770140	-0.257825644642	-1.797448971391
O	-1.031558837119	-0.371709093184	-2.543161710549
B	-2.185253571922	-1.109662007888	-1.918847614921
O	-2.666334925518	-0.455374720375	-0.651053323657
N	-1.774068606813	-0.346953978650	0.329286692534
C	-2.193278460131	-0.191419567347	1.546197567688
C	-1.101644262414	0.014960219623	2.502547586668
F	1.877558621071	2.183187270986	1.728655770255
F	3.332530669383	0.842502898880	2.933432570440
C	3.707131147380	0.400676713242	-1.833574675905
C	1.358921437640	0.058213723215	-3.854239898697
F	-1.793447848826	-2.417226977557	-1.638505931886
F	-3.215966389646	-1.020162098529	-2.805199948124
C	-3.631439079206	-0.180517156891	1.920569349444
C	-1.307711310512	0.173363401899	3.965844098542
H	-1.515433972944	-0.792804424246	4.437426125896
H	-0.408455967016	0.587175606773	4.419106394100
H	-2.156378562466	0.830442686615	4.166668842663
H	-3.785051470518	-0.649160245230	2.894026679566
H	-4.005119236765	0.847342157378	1.980481431912
H	-4.214233867774	-0.701695514329	1.162247865224
H	1.314255732228	1.102136955403	-4.182624731696
H	0.548337529806	-0.478473503221	-4.345583430087
H	2.320127990787	-0.350981394907	-4.169365228139
H	3.760898677044	1.111997265762	-2.660400285886
H	4.171862694117	-0.533096394770	-2.166874295750
H	4.274655825930	0.780826613621	-0.985947652881
H	1.385578324667	-5.135488928696	-0.177489341177
H	0.186795483896	-5.195416140934	1.133805809919
H	-0.353967825009	-5.081930812896	-0.559631630135
C	0.411955742115	-4.770793518634	0.153914063364
C	0.418303619862	-3.329473925369	0.227436774624
N	0.391744967838	-2.183685522858	0.262272635957
H	-0.137226451918	1.184693710738	-0.051077405339

E = -2801.80997872 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = Cl

Co	0.068426393072	-0.208446876133	0.063298665785
N	0.069222209768	0.041616039161	1.932015365945
O	1.153313992508	0.114859073443	2.676105729438
B	2.311349422005	0.881184715480	2.052446380986
O	2.793364067200	0.199179120894	0.779444668508
N	1.903953868358	0.137378422880	-0.189788853752
C	2.276197355590	0.154942921486	-1.425420436673
C	1.178161794931	-0.016816133915	-2.379338024574

N	0.030888503452	-0.230392769630	-1.825448723555
O	-1.053875205117	-0.319368062595	-2.567929856055
B	-2.216925098964	-1.070853272087	-1.953931921000
O	-2.689776286631	-0.407979834614	-0.675889289210
N	-1.802537077763	-0.326909240566	0.294776844245
C	-2.193396722767	-0.191817487548	1.518615195309
C	-1.099168440211	-0.019521585060	2.476795328495
F	1.882043646652	2.147429689396	1.736738121595
F	3.334615598028	0.791854761570	2.933576107517
F	-1.810717205079	-2.362539327693	-1.663337982073
F	-3.239711016235	-0.969749859707	-2.833164734660
H	1.428845046556	-5.098943868830	-0.154076353618
H	0.310688714388	-5.147177386328	1.228353458382
H	-0.330491261966	-5.120622995130	-0.434198034788
C	0.463177963878	-4.755814093077	0.221068063041
C	0.426376375910	-3.313960293551	0.241685026065
N	0.374412283469	-2.168536650826	0.239925547920
H	-0.146112463784	1.205701734366	-0.057762255157
Cl	1.402118164442	0.105128883212	-4.057088749587
Cl	3.890197362369	0.333664994372	-1.917878912577
Cl	-3.824739833866	-0.166151072240	1.985122480512
Cl	-1.360486680195	0.065304513267	4.151415123537

E = -4483.57883863 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = CN

Co	0.059951919555	-0.203323249776	0.059051500191
N	0.059829988766	0.040211377365	1.921175421608
O	1.130076309262	0.116311043762	2.664440976717
B	2.311788814330	0.880811036150	2.053698070009
O	2.776865202202	0.196677020537	0.760783597795
N	1.890469027096	0.129910211815	-0.194912859177
C	2.275109982401	0.154340659534	-1.439391825120
C	1.178520852556	-0.006170877282	-2.391244786239
N	0.022034506243	-0.205884998627	-1.822458019172
O	-1.049056195685	-0.290075743635	-2.564069849612
B	-2.237079461421	-1.039302153858	-1.965933793803
O	-2.689896498907	-0.375009147424	-0.667057873665
N	-1.805439016359	-0.296466587486	0.289853604526
C	-2.208822842316	-0.170391848089	1.523802906093
C	-1.115932180454	-0.009442453036	2.479844016579
F	1.884932966689	2.139750516858	1.736676039863
F	3.326168508795	0.763329888198	2.926274962183
F	-1.836747557492	-2.324360576387	-1.677505857273
F	-3.250638352079	-0.904390685817	-2.836002040654
H	1.486772519538	-5.059541029402	-0.113273283416
H	0.361317317421	-5.114993735801	1.264155627722
H	-0.270118349360	-5.137638213421	-0.402692138142
C	0.508940676468	-4.738547301885	0.250288159666
C	0.432722974977	-3.298849474645	0.246274348193
N	0.353411498164	-2.154829324894	0.229221945740
H	-0.139950842845	1.218126929760	-0.052850381503
C	-3.574354135941	-0.175301374823	1.901867952453
C	-1.316794044802	0.073285514217	3.880521547526
C	1.354494165975	0.062290493378	-3.795566907606
C	3.627501295384	0.309362781206	-1.834341227614

N	1.530644049144	0.111640687248	-4.934580085962
N	4.719538056422	0.422280033827	-2.188346702441
N	-1.511967443194	0.126959148141	5.016140543784
N	-4.676595590533	-0.185858855709	2.242119460751

E = -3013.71162514 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = H

Co	0.081806587292	-0.230383650990	0.073820267882
N	0.073242914295	0.036831091454	1.931197201294
O	1.153611037621	0.142147000087	2.682849560218
B	2.310815199342	0.898904862643	2.052583860835
O	2.799290976870	0.229151472139	0.778669762711
N	1.903696054483	0.133953087028	-0.186791858840
C	2.273253995191	0.168789030389	-1.424310445509
C	1.193318606840	-0.022684560448	-2.363737422787
N	0.047505767184	-0.245316282736	-1.807413567011
O	-1.034250200753	-0.356778622357	-2.557262246460
B	-2.200319726549	-1.095361353192	-1.939700356377
O	-2.675087869457	-0.445488344232	-0.658704476196
N	-1.781547581508	-0.342424429101	0.308695046936
C	-2.174673205212	-0.199491213818	1.532312797298
C	-1.097706991032	-0.008440893788	2.475232161663
F	1.886932233988	2.172613606458	1.743699487277
F	3.337632621888	0.815497410586	2.936501276760
F	-1.807044853267	-2.398182407151	-1.660709293592
F	-3.226172040097	-0.990562784435	-2.821183679398
H	1.388646548329	-5.121950781405	-0.177372162805
H	0.244052089508	-5.170600660774	1.182702648515
H	-0.365200974792	-5.100780905059	-0.490287835858
C	0.423648897952	-4.764508136893	0.185805506175
C	0.414401725807	-3.322536876511	0.229976338358
N	0.380829749392	-2.176691056428	0.243840114622
H	-0.137030607712	1.186159026128	-0.050159606887
H	1.298321905974	0.035249725082	-3.440436321688
H	3.307157046783	0.334524538800	-1.702228724832
H	-3.226099545763	-0.201539336583	1.793343671620
H	-1.229373822598	0.096972715105	3.545395246078

E = -2643.88475825 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = NH_2

Co	0.109427660037	-0.229993536090	0.097932214214
N	0.100623105439	0.031093857189	1.946123527032
O	1.187464275435	0.192693387930	2.718732511607
B	2.313269093718	0.959400069135	2.055935757660
O	2.838040402115	0.275824067530	0.809541809984
N	1.923426907614	0.122712176595	-0.162313266855
C	2.310711594123	0.189538427950	-1.394201980146
C	1.216943419095	-0.047555220871	-2.350353162616
N	0.079367309110	-0.260258849028	-1.770793217191
O	-1.011869384510	-0.387309661555	-2.545482478055
B	-2.174264919993	-1.113494581383	-1.916381870048
O	-2.659709955035	-0.472702521914	-0.639719701792
N	-1.740847349944	-0.351775552414	0.334133707318
C	-2.157647634356	-0.213233129464	1.551717030054

C	-1.063927267456	0.023864056420	2.507838930798
F	1.857207055370	2.221633398924	1.716318319360
F	3.346633022956	0.947851200203	2.949162977511
F	-1.799886323129	-2.431828405550	-1.652058324208
F	-3.206554408819	-1.009529620917	-2.804132438976
H	1.218861701425	-5.202334473974	-0.328657145304
H	0.072160680903	-5.255919865697	1.028291736777
H	-0.529218900493	-5.048565077693	-0.636008254870
C	0.278799531080	-4.804098498725	0.056689255498
C	0.359288442807	-3.368228764105	0.181501808202
N	0.390248971391	-2.224039193437	0.253266851153
H	-0.097241426109	1.180104785690	-0.019474438203
N	1.386881953604	0.062264354260	-3.701195996904
H	2.241464178350	-0.325252484163	-4.074299892169
H	0.555881742885	-0.188437833404	-4.223608892818
N	3.603209275905	0.393026625211	-1.790221090402
H	4.203550921983	0.648636676831	-1.014030232935
H	3.719628848711	0.986685982434	-2.599855308019
N	-3.472695449688	-0.175422244953	1.918498517086
H	-4.099968526641	-0.418920294924	1.161260275378
H	-3.700863341171	-0.610651642507	2.800624319034
N	-1.276942565622	0.156190089993	3.851854100539
H	-2.083340623351	0.708371397027	4.109481220867
H	-0.432759017740	0.423051899445	4.346341821440

E = -2866.02270146 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = OCH_3

Co	0.054086532188	-0.175897370772	0.055877051666
N	0.051713941622	0.065507135743	1.923442913278
O	1.162509881381	0.075363252581	2.675259050973
B	2.323962658203	0.810261494645	2.061640534998
O	2.792565923540	0.155892658342	0.788941119055
N	1.889025932658	0.158498331843	-0.202610055560
C	2.275667195297	0.197755655588	-1.434432448286
C	1.171394501146	0.003499451233	-2.399916408511
N	0.028903764193	-0.209692309159	-1.833572990034
O	-1.087561867142	-0.245791955429	-2.577672992029
B	-2.235899883666	-0.988139999535	-1.961442347496
O	-2.712641012123	-0.335144095012	-0.697354346640
N	-1.815727711490	-0.304729605955	0.300967326514
C	-2.218198355492	-0.164972599013	1.521792848091
C	-1.111469087117	0.031839111590	2.483830218461
F	1.952259598146	2.118182405321	1.796178520414
F	3.356677403913	0.680733470054	2.948561103639
F	-1.850342004906	-2.300775406783	-1.691569578028
F	-3.269596175004	-0.887785897335	-2.849580990632
H	1.488264783280	-5.070177260755	-0.103989270454
H	0.338538876750	-5.128468683914	1.249739527791
H	-0.261737005380	-5.131938782692	-0.426648971083
C	0.507112432666	-4.741880320334	0.243173760850
C	0.441461701180	-3.299421893729	0.250080272209
N	0.368004892288	-2.155073210419	0.239179176734
H	-0.165948306019	1.232959176240	-0.071874592391
O	1.477433073821	0.127016606538	-3.676401840978
O	3.487358979215	0.336798703267	-1.934211797301

O	-3.440134495467	-0.116016417638	2.014547644317
O	-1.433681120878	0.103017836019	3.759974801229
C	0.666184190681	-0.491830957474	-4.693446361243
H	0.472512261091	-1.533883884768	-4.437170751176
H	-0.275426183826	0.037349879446	-4.813544008790
H	1.270710947245	-0.430594018827	-5.595857336977
C	4.492017430707	1.070027003634	-1.203464254205
H	4.076740252059	2.009232022397	-0.836950561793
H	4.866569815755	0.483491873622	-0.368604828320
H	5.274028939513	1.261115483232	-1.935137809479
C	-4.540033778323	-0.744157019684	1.328679428494
H	-4.815625150147	-0.181290672466	0.440831982123
H	-4.275723388265	-1.764753473183	1.050279332019
H	-5.346590834181	-0.748426375043	2.058763777065
C	-0.598385084845	0.842546236458	4.674670231837
H	-1.222074192078	0.989257278803	5.553855200727
H	0.299653792861	0.280176012524	4.917329368243
H	-0.324418065049	1.803306130799	4.238074350682

E = -3103.26566477 Hartrees

$Co^{III}H(dRgBF_2)_2L$ R = OH

Co	0.103353306827	-0.254570027991	0.084868156049
N	0.084790852447	0.032866799167	1.925274270227
O	1.163900107079	0.172521925087	2.711067690107
B	2.308489020183	0.941100119255	2.059965062437
O	2.828925469505	0.248567915779	0.804639046156
N	1.910910131919	0.117322453046	-0.165614028659
C	2.307766792169	0.143304179462	-1.392570849713
C	1.215977136128	-0.073880372705	-2.351798470131
N	0.082237576233	-0.308809664693	-1.781306362852
O	-1.003537405330	-0.409253339828	-2.565819548554
B	-2.176358520078	-1.144376998947	-1.943949638252
O	-2.664094938139	-0.488944227857	-0.664252052872
N	-1.744759876931	-0.393587943692	0.310569912693
C	-2.165905883152	-0.228149921816	1.519495867238
C	-1.077546997762	-0.010742486152	2.482493889182
F	1.858557929098	2.196793660350	1.716481801491
F	3.332706192012	0.905818112624	2.953424297817
F	-1.789187882638	-2.446943346727	-1.660771079274
F	-3.199279694576	-1.038042185627	-2.832365770870
H	1.326880652516	-5.205113576973	-0.212004635376
H	0.170954016465	-5.249971464701	1.138552815442
H	-0.422477349121	-5.114980794614	-0.535746204402
C	0.372232257234	-4.823876307580	0.154256202433
C	0.411281002227	-3.383529543940	0.235676969487
N	0.414610747730	-2.237279510881	0.277122657997
H	-0.126032542277	1.149940589435	-0.059125376012
O	1.406216585117	0.016895741672	-3.655284324348
H	0.542181111641	-0.126716764849	-4.078272258381
O	3.552248324607	0.340523364151	-1.786260979541
H	4.079523816412	0.499682116311	-0.984211364424
O	-1.306877170323	0.121636357556	3.775776579688
H	-0.447688848926	0.297057178708	4.197404684483
O	-3.434319294970	-0.203568773696	1.885669712171
H	-3.964148283324	-0.331920669334	1.080182148564

E = -2945.47962644 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = C_6H_5

Co	0.000595310961	0.001113569460	0.000557716827
N	-0.015735515718	0.130013973381	1.892866180493
O	1.109919810592	0.116477303196	2.586128984741
B	2.221506950468	0.971521927234	2.020808322786
O	2.725826190074	0.392160347931	0.717123396361
N	1.864253218981	0.253740963275	-0.274135020676
C	2.275800747527	0.227867995351	-1.508611564283
C	1.177226876058	-0.035710885804	-2.472647781567
N	0.017062056313	-0.146727902417	-1.894263234357
O	-1.078954586903	-0.302915298560	-2.614062353959
B	-2.265199820639	-0.978769415846	-1.962165236061
O	-2.707942594920	-0.207340616132	-0.739072301783
N	-1.861171230539	-0.233456945722	0.276068632808
C	-2.282405549918	-0.146079065859	1.502929777679
C	-1.164127771431	-0.043042891855	2.476645471635
F	1.730286502875	2.248496051215	1.797287851429
F	3.252302967971	0.888502445220	2.890279523761
F	-1.908429754753	-2.260974779589	-1.573256742797
F	-3.276501884049	-0.901728722957	-2.854656247159
N	-0.301675897404	1.845974321494	-0.173070738836
C	-0.415249804905	2.984403953958	-0.209873954838
C	-0.532929857371	4.419689247453	-0.233909815023
H	0.188727686645	4.843423343607	0.468281336993
H	-1.543078605468	4.714138999434	0.056730031545
H	-0.325213286146	4.793107814425	-1.238394465533
N	0.303604255068	-1.843854156743	0.171892219843
C	0.410781794284	-2.982599092278	0.215762634744
C	0.518635054822	-4.418375363865	0.249541566573
H	1.494994388080	-4.727213850976	-0.128246401551
H	0.401035744893	-4.775031433543	1.274527783211
H	-0.266436217633	-4.844501665466	-0.379214919477
C	1.376800738101	-0.210034101860	-3.921078771391
C	2.413967367359	-1.042923938804	-4.381073434204
C	0.527995857273	0.415400051183	-4.851236307133
C	2.591068529640	-1.249142382028	-5.747191460559
H	3.073998779550	-1.532519412208	-3.673458272492
C	0.728717429707	0.223260645755	-6.216794274423
H	-0.289352966030	1.037273736158	-4.508089188272
C	1.754878607948	-0.610877556273	-6.666972143035
H	3.383285343584	-1.903038496891	-6.093372045492
H	0.074495567623	0.713717716739	-6.928411141460
H	1.899701391205	-0.766982967405	-7.730154929342
C	3.670083602963	0.486413562151	-1.903901015087
C	3.934083695028	1.373555434257	-2.964850920227
C	4.743212008439	-0.111132403184	-1.219231252964
C	5.248268292784	1.659593501309	-3.326559259059
H	3.115509992308	1.842949365198	-3.499211377100
C	6.054218336544	0.161678027093	-1.604950344893
H	4.552789902487	-0.774483710436	-0.384990798462
C	6.309575388230	1.048593190731	-2.653653541165
H	5.443702434402	2.354467578923	-4.135256249470
H	6.876271070431	-0.307564834650	-1.076778687259

H	7.331666220860	1.266927371000	-2.942372168139
C	-3.702358315242	-0.079058498152	1.877212877229
C	-4.120152564226	0.849614941824	2.849086802464
C	-4.653072451538	-0.915317668408	1.263975279733
C	-5.467369716822	0.946164994403	3.189854266132
H	-3.396002830463	1.496323669825	3.332502436544
C	-5.994189291948	-0.828506430616	1.629757905034
H	-4.344319231682	-1.623136699594	0.504631397535
C	-6.404689531280	0.103659333777	2.586832736950
H	-5.783767097979	1.672695748364	3.929513007954
H	-6.720301179531	-1.481543304462	1.159523711375
H	-7.451503435582	0.174178155440	2.860443417756
C	-1.326341664860	-0.196937567667	3.929679433612
C	-2.173940117642	-1.203385646278	4.429766684501
C	-0.632109370759	0.634664170231	4.827049684593
C	-2.312810843340	-1.380000553992	5.804561971040
H	-2.717743793641	-1.847286042010	3.747005319435
C	-0.797670250654	0.466722866076	6.199803436570
H	0.033851099873	1.401988759220	4.451780163527
C	-1.631575422196	-0.541769253005	6.690783069341
H	-2.956891127359	-2.165408851521	6.183149673669
H	-0.266838634664	1.116164139171	6.886316953521
H	-1.748626996717	-0.674838808406	7.760487699584

E = -3703.15130547 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = CF_3

Co	-0.002840564516	-0.000617266221	0.000730777166
N	0.003005059314	0.105200563667	1.904572409548
O	1.105844631441	0.141299303885	2.594380587646
B	2.285785600264	0.922938859668	1.999645501017
O	2.723726195413	0.232427150195	0.699407267375
N	1.870719512956	0.209035707539	-0.282982340154
C	2.253566155434	0.204678679291	-1.521618992305
C	1.152597607100	-0.019424803900	-2.472712192379
N	-0.008686637076	-0.106429959918	-1.903106475670
O	-1.111524398538	-0.142547990737	-2.592913830390
B	-2.291444581253	-0.924212170803	-1.998172272164
O	-2.729406794681	-0.233677811631	-0.697944140075
N	-1.876407054941	-0.210271881221	0.284446184728
C	-2.259251697125	-0.205898060880	1.523083440228
C	-1.158281292307	0.018207525570	2.474174188634
F	1.853784658247	2.186125376710	1.691177460522
F	3.297843871777	0.790980703715	2.857033359408
C	3.713945475337	0.445208883543	-1.924924241458
C	1.333055904291	-0.172539821063	-3.988660952400
F	-1.859402556925	-2.187372746839	-1.689671385490
F	-3.303502925513	-0.792299618205	-2.855565395318
C	-3.719629003953	-0.446428848585	1.926394802145
C	-1.338736120063	0.171328399199	3.990122710049
N	-0.281127985942	1.851984649058	-0.147908374390
C	-0.400534381913	2.990954594914	-0.197831785780
C	-0.530262934360	4.422665491007	-0.245023124601
H	-0.414654836254	4.769630182012	-1.274250967046
H	-1.514533473397	4.716290492126	0.126493084912
H	0.245645298571	4.869140278001	0.381893784963

N	0.275428235639	-1.853212309394	0.149435408911
C	0.395078343104	-2.992151160561	0.199479614582
C	0.524998896308	-4.423840203771	0.246846562752
H	1.509549068443	-4.717317078193	-0.124044648994
H	0.408815471781	-4.770773172706	1.276020577660
H	-0.250457358601	-4.870478858910	-0.380511962575
F	0.366986151309	-0.901961109058	-4.519494056856
F	1.350117516336	1.021765077946	-4.575318483466
F	2.487538326639	-0.798182000057	-4.224786572276
F	3.739406634001	1.124969212619	-3.072353879244
F	4.346442539365	-0.714649130520	-2.084896697925
F	4.352664154358	1.165740400158	-1.019185606054
F	-4.358358117141	-1.166941773911	1.020650253426
F	-4.352118942988	0.713429676594	2.086393426232
F	-3.745081508185	-1.126208091102	3.073814516799
F	-2.493216159360	0.796972515185	4.226250569148
F	-1.355796391835	-1.022974748734	4.576784446356
F	-0.372663840561	0.900752274317	4.520949702803

E = -4126.93354718 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = CH_3

Co	-0.000100694667	-0.000238134318	0.000063178482
N	-0.005219356104	0.114502721726	1.893629069721
O	1.099707522389	0.157226616386	2.614815777733
B	2.267739221303	0.920828045142	2.009696262739
O	2.735144124702	0.250710401321	0.726071379750
N	1.865049708869	0.220467001806	-0.266315840343
C	2.265202553251	0.173797720130	-1.496709347091
C	1.161576878737	0.015299595314	-2.460333306468
N	0.005032671837	-0.114974039152	-1.893495107285
O	-1.099903850008	-0.157568030284	-2.614676353972
B	-2.267899553035	-0.921279832572	-2.009630722709
O	-2.735334871294	-0.251291773499	-0.725930462719
N	-1.865235094487	-0.221009199145	0.266443489653
C	-2.265372064769	-0.174463859030	1.496845904297
C	-1.161753830355	-0.015896792826	2.460466082901
F	1.849820173804	2.204991305858	1.711160633742
F	3.285136912120	0.813986926931	2.885194601326
C	3.692655851479	0.247144812136	-1.895232974075
C	1.353763984236	0.028569101658	-3.931599248989
F	-1.849885664353	-2.205443954494	-1.711197070774
F	-3.285320434369	-0.814426153601	-2.885112409189
C	-3.692819244482	-0.247978303089	1.895364912046
C	-1.353956034084	-0.029178960912	3.931730761939
H	-1.516080885621	-1.052595184120	4.286300268788
H	-0.468997884637	0.365079183987	4.428026271173
H	-2.229702173427	0.558843443932	4.212389914166
H	-3.817319908005	-0.885936955370	2.772295249530
H	-4.067827593640	0.747577502867	2.155465251765
H	-4.292075484731	-0.630608144908	1.071094222126
H	1.515702480538	1.052008276485	-4.286194427337
H	0.468856832651	-0.365841460023	-4.427875637458
H	2.229604633955	-0.559314446499	-4.212257736286
H	3.817250179047	0.885272875801	-2.772028365473
H	4.067473027912	-0.748419228872	-2.155566743075

H	4.291994372998	0.629497948721	-1.070897238984
N	-0.281198029173	1.851263709173	-0.151530279317
C	-0.377594812018	2.991883555906	-0.180929051565
C	-0.473099502045	4.428756866064	-0.197285930227
H	0.304019811565	4.840575856547	0.450798093059
H	-1.454136770294	4.740282651664	0.166405884868
H	-0.334547716910	4.798899500317	-1.214932046220
N	0.280935286784	-1.851749403701	0.151629418493
C	0.377515645811	-2.992348592441	0.181292116410
C	0.473282105680	-4.429212088109	0.197753093080
H	1.458240954342	-4.740301376636	-0.155582997972
H	0.323946359082	-4.799993229524	1.213643479559
H	-0.296891840583	-4.840845476748	-0.458700019820

E = -2934.15215971 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = Cl

Co	-0.002887051014	-0.000646629639	0.000958797340
N	0.018578033527	0.127774915388	1.902317577195
O	1.116537503976	0.160668375088	2.615518679855
B	2.287468052140	0.939010551640	2.008636686963
O	2.742499485118	0.250569011518	0.717956281010
N	1.870874940325	0.228546216212	-0.259316539793
C	2.243992989237	0.166071587285	-1.494621752721
C	1.134861831010	0.013870981071	-2.452423220042
N	-0.024347418021	-0.129070826965	-1.900398377731
O	-1.122307031625	-0.161974929995	-2.613595644894
B	-2.293209676494	-0.940342084756	-2.006695743141
O	-2.748265899434	-0.251880155875	-0.716036917203
N	-1.876645554988	-0.229843174621	0.261237395501
C	-2.249763678433	-0.167366667165	1.496542609466
C	-1.140631472032	-0.015164011163	2.454342737097
F	1.849776719852	2.204618126181	1.693355612250
F	3.303030738917	0.832431544200	2.873512022944
F	-1.855457405030	-2.205915619899	-1.691366416583
F	-3.308775178119	-0.833833531514	-2.871577315849
N	-0.296260057883	1.848520247350	-0.164113182450
C	-0.408694893132	2.987685737250	-0.210385891940
C	-0.530560717638	4.420819482740	-0.253956261743
H	-0.432222760484	4.768997617477	-1.284277341628
H	-1.505465890612	4.720747771508	0.135969757253
H	0.259369203315	4.861387686476	0.359156082445
N	0.290472338318	-1.849817566972	0.166013327940
C	0.402896970019	-2.988984941536	0.212272032870
C	0.524744522375	-4.422121456435	0.255820426563
H	1.499687982849	-4.722050996598	-0.134008744175
H	0.426294000837	-4.770321317639	1.286123328452
H	-0.265125513356	-4.862667410903	-0.357385310799
Cl	1.371177735599	0.066456807035	-4.121061779981
Cl	3.857068004177	0.211316056574	-1.983129389279
Cl	-3.862837752780	-0.212620855024	1.985052599649
Cl	-1.376944460513	-0.067755888295	4.122981345161

E = -4615.90148039 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = CN

Co	-0.002849632314	-0.000634874059	0.000881581678
N	0.019277306733	0.127545293302	1.899535076056
O	1.103247197966	0.180694046514	2.611382292613
B	2.294173031731	0.962158984349	2.012176465561
O	2.737052194071	0.272889221626	0.700712061955
N	1.867976421920	0.229352808150	-0.262145717991
C	2.246210140955	0.171273953789	-1.506107111776
C	1.140830617859	0.010410472218	-2.458914542386
N	-0.024976879544	-0.128814864014	-1.897772115190
O	-1.108946926176	-0.181962975287	-2.609619543073
B	-2.299873771060	-0.963426308585	-2.010414252277
O	-2.742752137286	-0.274157636877	-0.698948910710
N	-1.873675824078	-0.230621812927	0.263908665640
C	-2.251909733136	-0.172542723439	1.507870067498
C	-1.146530264508	-0.011679469495	2.460677516504
F	1.853877303419	2.217937534294	1.695961115188
F	3.302860120850	0.831724878488	2.867918722320
F	-1.859580868018	-2.219206511645	-1.694200174155
F	-3.308560957002	-0.832989551192	-2.866156110643
N	-0.300119367631	1.849587413735	-0.166196942534
C	-0.421400627341	2.988659639619	-0.218524344971
C	-0.556392817172	4.419406355544	-0.271054961776
H	-0.446915694285	4.762572087394	-1.302390091760
H	-1.540149946092	4.711019588736	0.103858708521
H	0.220825288867	4.871435043921	0.350533438089
N	0.294420714025	-1.850856909149	0.167959932614
C	0.415684616114	-2.989930495063	0.220298057677
C	0.550686802437	-4.420676823614	0.272816138240
H	1.534550455726	-4.712261530999	-0.101840206097
H	0.440935200699	-4.763878490895	1.304110100623
H	-0.226354822947	-4.872697188206	-0.348998832052
C	3.601693438980	0.238563765030	-1.909318145212
C	1.329547383194	0.024479501177	-3.862052379242
C	-3.607393115781	-0.239831437358	1.911081025184
C	-1.335247038715	-0.025747532528	3.863815340988
N	1.511259895372	0.040293505914	-5.001223761754
N	4.697530984125	0.289443230737	-2.266445279541
N	-4.703230762594	-0.290709854774	2.268208028991
N	-1.516959739368	-0.041560664434	5.002986707199

E = -3146.00585895 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = H

Co	-0.002841331297	-0.000655198213	0.000918194293
N	0.014104170364	0.128067912405	1.897905094716
O	1.106066526260	0.190725524979	2.617506530499
B	2.281369111482	0.958525536574	2.004984289080
O	2.741380517210	0.280605028794	0.710120639679
N	1.866172061501	0.228721546123	-0.262204939209
C	2.231534689314	0.174292996081	-1.498918324077
C	1.142471610520	0.005593928623	-2.440607555894
N	-0.019788220943	-0.129380192622	-1.896069425536
O	-1.111753216876	-0.192018534763	-2.615670567625
B	-2.287063801002	-0.959814840212	-2.003161446540
O	-2.747066585836	-0.281917679557	-0.708283853944
N	-1.871853951328	-0.230035240664	0.264039569275

C	-2.237216095364	-0.175621559962	1.500754176134
C	-1.148154494147	-0.006917646215	2.442444063057
F	1.849566524093	2.228987608767	1.694213018289
F	3.297546780728	0.851050868556	2.871028543963
F	-1.855284203775	-2.230294870501	-1.692422192292
F	-3.303242267033	-0.852306686701	-2.869200955463
N	-0.292215168893	1.847481967309	-0.161249341069
C	-0.396388706688	2.987529531346	-0.201764337996
C	-0.504290405378	4.422319214369	-0.234977181720
H	-0.391869648481	4.778647584752	-1.260984755809
H	-1.479898100056	4.729337194874	0.147375642881
H	0.283799935803	4.849417626823	0.389886424869
N	0.286541719181	-1.848787998417	0.163082196415
C	0.390583673888	-2.988843455550	0.203710687223
C	0.498296159008	-4.423642452777	0.237093522589
H	1.474160899734	-4.730811613027	-0.144480676007
H	0.385036912675	-4.779881641610	1.263040377387
H	-0.289375116597	-4.850685195408	-0.388336296381
H	1.265341613601	0.002182958461	-3.517896473880
H	3.275900136776	0.239443749921	-1.782991230854
H	-3.281580928338	-0.240783699827	1.784826717662
H	-1.271023990107	-0.003506882729	3.519733036286

E = -2776.21272671 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = NH_2

Co	-0.002855199589	-0.000663805611	0.000854190061
N	0.004932689673	0.187455603271	1.876031582597
O	1.115440267505	0.242357780342	2.618624868244
B	2.263752003196	1.016370025067	1.987054418836
O	2.743265125455	0.335961717182	0.712365989017
N	1.838588970224	0.292514632443	-0.271398781270
C	2.243369065584	0.182469480395	-1.498472590218
C	1.131329134356	0.004571863092	-2.457233505172
N	-0.010643223834	-0.188783799702	-1.874321032707
O	-1.121148870215	-0.243701360222	-2.616915300998
B	-2.269460251945	-1.017704665281	-1.985333056842
O	-2.748974092900	-0.337274245960	-0.710657041916
N	-1.844299846415	-0.293838419896	0.273109230284
C	-2.249080464636	-0.183784773732	1.500182415778
C	-1.137039837286	-0.005895706440	2.458943880051
F	1.820159634606	2.289841973933	1.670982797395
F	3.291418144701	0.947415286589	2.861420463287
F	-1.825863732940	-2.291166490698	-1.669232336506
F	-3.297125972527	-0.948768058068	-2.859701695550
N	-0.347758523161	1.840181268677	-0.204981777772
C	-0.454384965200	2.979284007936	-0.245864043099
C	-0.559000550182	4.415820815240	-0.274128118980
H	-0.426906718812	4.779199436785	-1.294900580968
H	-1.539551079003	4.725584392521	0.091932077328
H	0.219034919962	4.836405217506	0.367089411218
N	0.342038891583	-1.841515269401	0.206701197527
C	0.448670607369	-2.980619265137	0.247534707262
C	0.553496857172	-4.417147112161	0.275494468813
H	1.534088514689	-4.726698591861	-0.090631192190
H	0.421446454286	-4.780758263807	1.296190310879

H	-0.224459502760	-4.837700601964	-0.365840910314
N	1.310767456169	0.005324170742	-3.794572457832
H	0.465023711891	-0.047762639261	-4.348203534690
H	2.066445861822	0.543726963451	-4.188595561347
N	3.534440201604	0.259675214185	-1.882482775222
H	3.827070251950	-0.218331318543	-2.720363361169
H	4.212219116949	0.300547329238	-1.131867776938
N	-3.540152352259	-0.260970379847	1.884190926575
H	-3.832775296575	0.217028074821	2.722078311577
H	-4.217933206666	-0.301835104377	1.133577608859
N	-1.316480360102	-0.006646745742	3.796283463886
H	-2.072152920719	-0.545060311155	4.190303970132
H	-0.470735913021	0.046436675453	4.349914142095

E = -2998.37633800 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = OCH_3

Co	-0.002792214531	-0.000580304444	0.000757591328
N	0.003164153955	0.207448247615	1.893979433039
O	1.129817946842	0.274795745519	2.608791917153
B	2.242544952866	1.074118538352	1.969257184022
O	2.735955781959	0.367398336234	0.726546895976
N	1.855144970640	0.311930395161	-0.276789603063
C	2.247043074640	0.226272218965	-1.507048287103
C	1.138865801965	-0.039924746680	-2.465730733979
N	-0.008748388313	-0.208607685408	-1.892464459224
O	-1.135401459104	-0.275956797980	-2.607277449319
B	-2.248131579488	-1.075278004925	-1.967743435281
O	-2.741539905229	-0.368555762514	-0.725032099579
N	-1.860729682866	-0.313089410526	0.278304734648
C	-2.252627542087	-0.227431535822	1.508563761338
C	-1.144449724301	0.038765095248	2.467245750181
F	1.761817202111	2.327080803315	1.620649231240
F	3.271553731266	1.061780440658	2.846998372015
F	-1.767408550133	-2.328241405450	-1.619137733929
F	-3.277139721435	-1.062933876383	-2.845485029558
N	-0.386020979821	1.826125175615	-0.239565295376
C	-0.561097132135	2.953349273687	-0.337568067909
C	-0.759766088231	4.376364231459	-0.443229742849
H	-0.620774407948	4.694301561550	-1.478315788234
H	-1.770588528127	4.634883095645	-0.122096721121
H	-0.033425217735	4.884676093196	0.194829165504
N	0.380443135618	-1.827280632442	0.241091652061
C	0.555552252534	-2.954497801186	0.339114008491
C	0.754124485850	-4.377535771783	0.444641287451
H	1.764846613346	-4.636114335091	0.123239743346
H	0.615366688415	-4.695524940870	1.479742528119
H	0.027588700795	-4.885755571459	-0.193268771935
O	1.463016842647	-0.027529980851	-3.728634389898
O	3.441824488669	0.296058486389	-2.024348294317
O	-1.468599425371	0.026369749528	3.730149595620
O	-3.447408204362	-0.297217720998	2.025865784431
C	0.606083801690	-0.585680534192	-4.757770220123
H	0.343811229073	-1.611311561772	-4.502334730409
H	-0.290383514206	0.016239958832	-4.874934553746
H	1.220412880363	-0.559297548642	-5.653537512172

C	4.569538219205	0.861825549717	-1.308522604273
H	4.315383934023	1.857167882237	-0.947308153047
H	4.855596796347	0.219931160749	-0.480277236831
H	5.355251230327	0.915059576563	-2.057106676723
C	-4.575124780642	-0.862984407973	1.310043756592
H	-4.320972754304	-1.858327369688	0.948829588970
H	-5.360835350354	-0.916216782565	2.058630515311
H	-4.861185549846	-0.221090445242	0.481798892668
C	-0.611664418639	0.584519510321	4.759283828873
H	0.284802760009	-0.017401601533	4.876446359225
H	-0.349391660137	1.610150406071	4.503847762485
H	-1.225991895807	0.558137003789	5.655052249911

E = -3235.61504042 Hartrees

$Co^{III}(dRgBF_2)_2L_2$ R = OH

Co	-0.002257689529	0.005239257663	0.000576791335
N	0.019506713720	0.147315054494	1.878425950296
O	1.122313498313	0.197636748143	2.626589511001
B	2.284222147457	0.978658757275	2.004899830291
O	2.754874212104	0.303216686792	0.712388554327
N	1.844523940622	0.264104222618	-0.261478091343
C	2.233749538840	0.201258084610	-1.491214174948
C	1.123197875631	0.021670830511	-2.448390499447
N	-0.024021966744	-0.136835507220	-1.877272396406
O	-1.126828604874	-0.187158890152	-2.625435994660
B	-2.288736145596	-0.968182180748	-2.003746041920
O	-2.759388955753	-0.292740192214	-0.711235417497
N	-1.849039076822	-0.253625623201	0.262631452806
C	-2.238265018387	-0.190776965549	1.492367335836
C	-1.127713445848	-0.011189575123	2.449543795080
F	1.840254414756	2.247218370790	1.696186722578
F	3.306937945595	0.886534238042	2.871983349896
F	-1.844766566263	-2.236741127020	-1.695033020089
F	-3.311451983283	-0.876059463594	-2.870829936490
N	-0.316151145912	1.855789194282	-0.166872858114
C	-0.430880287304	2.994710347585	-0.206676221804
C	-0.552403331833	4.429012306262	-0.239159619830
H	-0.433403859669	4.788112353296	-1.263371974051
H	-1.534300846259	4.726548360723	0.134265685449
H	0.225351591029	4.863395476886	0.393362067137
N	0.311638136768	-1.845313389129	0.168026663769
C	0.426375938070	-2.984234144338	0.207816546891
C	0.547881568044	-4.418536951525	0.240319752737
H	1.529688791634	-4.716101299688	-0.133320352187
H	0.429109485556	-4.777602800173	1.264570465603
H	-0.230025532305	-4.852927233652	-0.392009996814
O	1.342443043356	0.056701786065	-3.738764203374
H	0.499653378444	-0.075112888636	-4.207075189890
O	3.472893974355	0.257633419044	-1.910380130105
H	4.061534535662	0.373538026630	-1.144228998396
O	-1.346959195650	-0.046219733801	3.739917376341
H	-0.504169671988	0.085594247463	4.208228785924
O	-3.477409573403	-0.247151037187	1.911532959568
H	-4.066049922533	-0.363057546221	1.145381960502

E = -3077.81225030 Hartrees