Supporting Information for:

Quantifiable Polarity Match Effect on C–H Bond Cleavage Reactivity and its Limits in Reaction Design

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Proof of equivalence between $\omega_{\mathrm{Sub}^{\cdot}}$ and ω_{SubH}

Following the thermocycle from **Figure 1A** for a generic C-H substrate radical, Sub$^{\cdot}$, the potential disparity, $\omega_{Sub^{\cdot}}$, is:

$$\omega_{\mathrm{Sub}^{\cdot}} = \frac{1}{\sqrt{2}}\left(E^{o}_{\mathrm{Sub}^{\cdot}} - \frac{RT}{F}\ln(10) \times pK_{a,\mathrm{Sub}^{\cdot}}\right) \quad \text{(S1)}$$

which can be expressed in terms of the Gibbs free energy for each species in the thermocycle as:

$$\omega_{\mathrm{Sub}^{\cdot}} = \frac{1}{F\sqrt{2}}((G_{\mathrm{Sub}^{\cdot}} - G_{\mathrm{Sub}^{-}} - FE^{o}_{\mathrm{Ref}}) - (G_{\mathrm{Sub}^{\cdot}} + G_{H^{+}} - G_{\mathrm{SubH}^{+}})) \quad \text{(S2)}$$

ultimately leading to:

$$\omega_{\mathrm{Sub}^{\cdot}} = \frac{1}{F\sqrt{2}}(G_{\mathrm{SubH}^{+}} - G_{\mathrm{Sub}^{-}} - FE^{o}_{\mathrm{Ref}} - G_{H^{+}}) \quad \text{(S3)}$$

which, as seen, only depends on the Gibbs free energy of the off-diagonal states from the thermocycle. By analogy, the potential disparity of the native substrate, ω_{SubH}, is:

$$\omega_{\mathrm{SubH}} = \frac{1}{F\sqrt{2}}((G_{\mathrm{SubH}^{+}} - G_{\mathrm{SubH}} - FE^{o}_{\mathrm{Ref}}) - (G_{\mathrm{Sub}^{-}} + G_{H^{+}} - G_{\mathrm{SubH}})) \quad \text{(S4)}$$

ultimately leading to:

$$\omega_{\mathrm{SubH}} = \frac{1}{F\sqrt{2}}(G_{\mathrm{SubH}^{+}} - G_{\mathrm{Sub}^{-}} - FE^{o}_{\mathrm{Ref}} - G_{H^{+}}) \quad \text{(S5)}$$

Equations S3 and S5 demonstrate the equivalence between $\omega_{\mathrm{Sub}^{\cdot}}$ and ω_{SubH}

Thermodynamic data for all organic substrates and solvents from Figure 3

Table S1. Thermodynamic data and relevant H-atom q_{ESP} charges for the set of substrates and solvents from **Figure 3**. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in MeCN. All values are given in kcal mol^{-1}. Charges were obtained using the Atoms-in-Molecules approach on the DFT-obtained electron density, on the 0.001 isosurface.

Substrate	$(RT\ln(10)/F)pK_a$[a]	$E°$[b]	BDFE[c]	ω[d]	μ[e]	q_{ESP}[f]	q_{AIM}[g]
CHD	2.973	0.935	65.2	0.403	-2.234	0.008	0.012
DHA	2.651	1.365	68.1	0.935	-2.132	0.013	0.033
Xanthene	2.658	1.012	66.7	0.681	-1.973	0.018	0.036
Fluorene	2.248	1.104	72.5	1.036	-1.390	0.017	0.048
Ph_2CH_2	2.771	1.557	74.2	0.986	-1.976	0.014	0.027
9-^{t}Bu-fluorene	2.382	1.056	72.2	0.907	-1.473	0.014	0.031
9-Ph-fluorene	1.984	1.102	67.1	1.221	-1.535	0.017	0.046
MeCN	2.694	4.520	87.5	3.135	-3.199	0.043	0.095
THF	4.237	2.085	84.4	0.322	-2.760	0.004	0.006

[a] Acidobasic potential, expressed in V.
[b] Reduction potential, expressed in V using the Cp/Cp^+ pair in MeCN as a reference.
[c] Bond dissociation free energy, in kcal mol^{-1}.
[d] Potential disparity, calculated as shown in **Figure 1** in the main text, expressed in V.
[e] Potential duality, calculated as shown in **Figure 1** in the main text, expressed in V.
[f] Electrostatic potential (ESP)-derived atomic charges, expressed in *e*.
[g] AIM-integrated atomic charges, expressed in *e*.

Linear regressions for H-donors from Figure 4

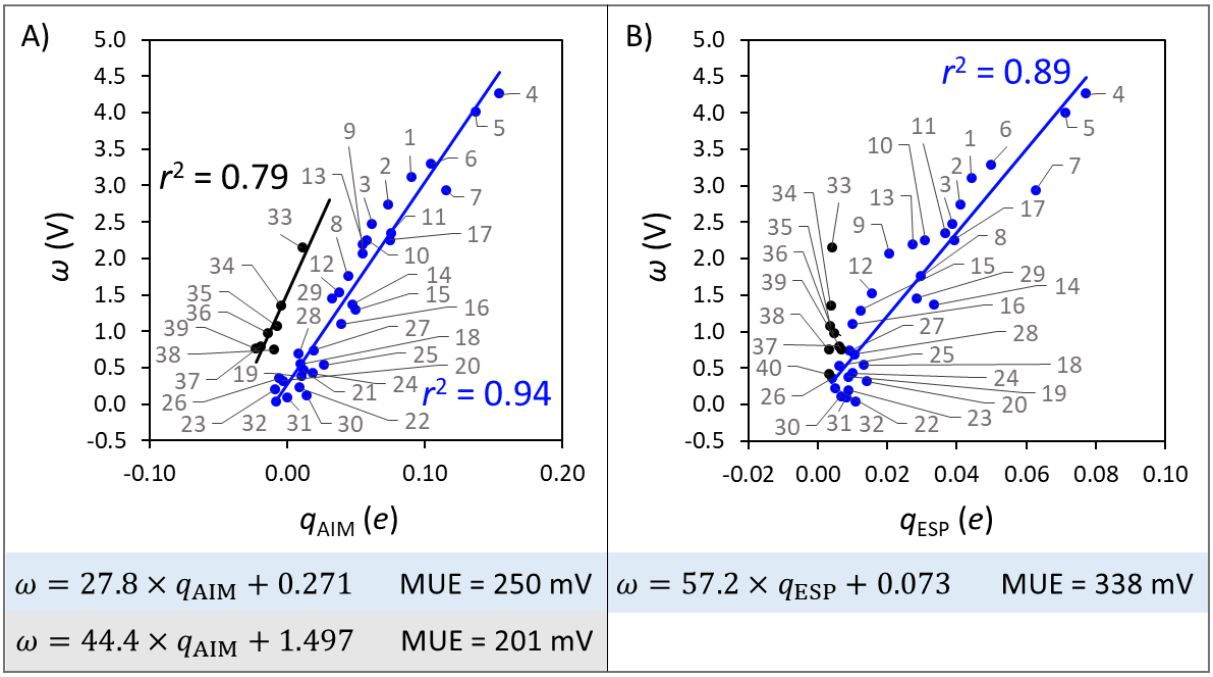

Figure S1. **A**) Correlation between the AIM charge of polar and nonpolar hydrogen atoms (in *blue* and *black*, respectively) and the potential disparity ω of the corresponding C–H bond substrates from **Figure 4**. **B**) Correlation between the AIM charge of polar hydrogen atoms (in *blue*) and the potential disparity ω. No meaningful fit was obtained for the set of nonpolar substrates (in *black*) under this charge scheme. Least-squares linear fits, and their corresponding mean unsigned errors (MUE) are included.

Thermodynamic data for all model organic substrates from Figure 4

Table S2. Energetics and charges for the polar model substrates 1-32 from **Figure 4** (blue set), containing electrophilic H-atoms. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in MeCN. All values are given in kcal mol^{-1}. Charges were obtained using the Atoms-in-Molecules approach on the DFT-obtained electron density, on the 0.001 isosurface.

Substrate	pK_a[a]	E°[b]	BDFE[c]	ω[d]	μ[e]	q_{ESP}[f]	q_{AIM}[g]
1	56.5	4.243	86.6	3.114	5.362	0.0442	0.0900
2	61.0	3.907	81.4	2.740	5.313	0.0410	0.0734
3	62.7	3.612	76.7	2.477	5.175	0.0388	0.0614
4	25.5	4.525	78.7	4.264	4.266	0.0771	0.1540
5	27.9	4.271	73.1	4.009	4.186	0.0712	0.1366
6	30.9	3.389	82.2	3.295	3.688	0.0497	0.1045
7	28.9	2.794	81.0	2.937	3.184	0.0627	0.1150
8	54.2	2.226	87.2	1.757	3.840	0.0297	0.0442
9	58.2	2.836	90.1	2.068	4.439	0.0207	0.0549
10	35.4	2.116	82.7	2.256	2.976	0.0309	0.0580
11	35.8	2.268	85.3	2.351	3.100	0.0367	0.0751
12	54.5	1.922	81.0	1.532	3.638	0.0157	0.0380
13	57.4	2.986	83.8	2.199	4.511	0.0274	0.0547
14	84.4	2.986	88.4	1.370	5.640	0.0335	0.0475
15	83.4	2.836	89.6	1.294	5.492	0.0122	0.0496
16	87.6	2.743	87.9	1.099	5.602	0.0101	0.0390
17	56.6	3.031	90.7	2.255	4.510	0.0392	0.0744
18	92.0	2.159	86.7	0.552	5.373	0.0131	0.0097
19	94.8	2.044	86.1	0.384	5.409	0.0087	0.0101
20	96.0	2.008	84.6	0.321	5.433	0.0142	-0.0032
21	91.3	2.008	83.3	0.467	5.237	0.0185	0.0115
22	96.8	1.911	84.5	0.229	5.398	0.0050	0.0087
23	98.7	1.956	82.8	0.202	5.510	0.0087	-0.0093
24	93.1	2.031	86.6	0.427	5.328	0.0101	0.0184
25	92.4	2.156	99.0	0.539	5.388	0.0063	0.0269
26	97.7	2.130	88.8	0.358	5.591	0.0041	-0.0061
27	72.5	1.581	83.3	0.741	4.149	0.0091	0.0194
28	72.7	1.521	76.7	0.691	4.115	0.0106	0.0081
29	58.2	1.976	81.0	1.458	3.830	0.0285	0.0322
30	76.6	0.876	80.7	0.116	3.822	0.0066	0.0141
31	77.6	0.885	77.3	0.094	3.870	0.0082	0.0000
32	78.8	0.866	75.7	0.042	3.907	0.0109	-0.0082

[a] Unitless. Calculated in MeCN using the free energy of solvation of the proton, G_H = -260.2 kcal mol^{-1}.
[b] Reduction potential, expressed in V using the Cp/Cp$^+$ pair in MeCN as a reference.
[c] Bond dissociation free energy, in kcal mol^{-1}.
[d] Potential disparity, calculated as shown in **Figure 1** in the main text, expressed in V.
[e] Potential duality, calculated as shown in **Figure 1** in the main text, expressed in V.
[f] Electrostatic potential (ESP)-derived atomic charges, expressed in *e*.
[g] AIM-integrated atomic charges, expressed in *e*.

Table S3. Energetics and charges for the nonpolar model substrates 33-40 from **Figure 4** (black set), containing nucleophilic H-atoms. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in MeCN. All values are given in kcal mol^{-1}. Charges were obtained using the Atoms-in-Molecules approach on the DFT-obtained electron density, on the 0.001 isosurface.

Substrate	pK_a[a]	E°[b]	BDFE[c]	ω[d]	μ[e]	q_{ESP}[f]	q_{AIM}[g]
33	90.1	4.334	95.6	2.149	6.832	0.0041	0.0109
34	96.0	3.474	90.1	1.357	6.470	0.0037	-0.0046
35	96.7	3.094	91.6	1.071	6.231	0.0036	-0.0074
36	99.7	3.094	87.5	0.978	6.356	0.0046	-0.0144
37	98.8	2.802	85.1	0.799	6.112	0.0061	-0.0196
38	97.4	2.078	87.3	0.751	5.541	0.0032	-0.0100
39	98.7	2.728	84.1	0.760	6.055	0.0067	-0.0228
40	98.4	2.730	88.8	0.418	6.044	0.0031	-0.0152

[a] Unitless. Calculated in MeCN using the free energy of solvation of the proton, G_H = -260.2 kcal mol^{-1}.
[b] Reduction potential, expressed in V using the Cp/Cp$^+$ pair in MeCN as a reference.
[c] Bond dissociation free energy, in kcal mol^{-1}.
[d] Potential disparity, calculated as shown in **Figure 1** in the main text, expressed in V.
[e] Potential duality, calculated as shown in **Figure 1** in the main text, expressed in V.
[f] Electrostatic potential (ESP)-derived atomic charges, expressed in *e*.
[g] AIM-integrated atomic charges, expressed in *e*.

Classification of C-H substrates from Figure 4 as polar or nonpolar

As seen in **Figure S2**, visual inspection of the key thermodynamic descriptors from **Tables S2-S3**, suggests that the potential duality μ of the reacting C-H bonds and the atomic charges are important factors in determining their classification as polar or nonpolar. The relevance of BDFE and potential disparity ω, however, are less clear.

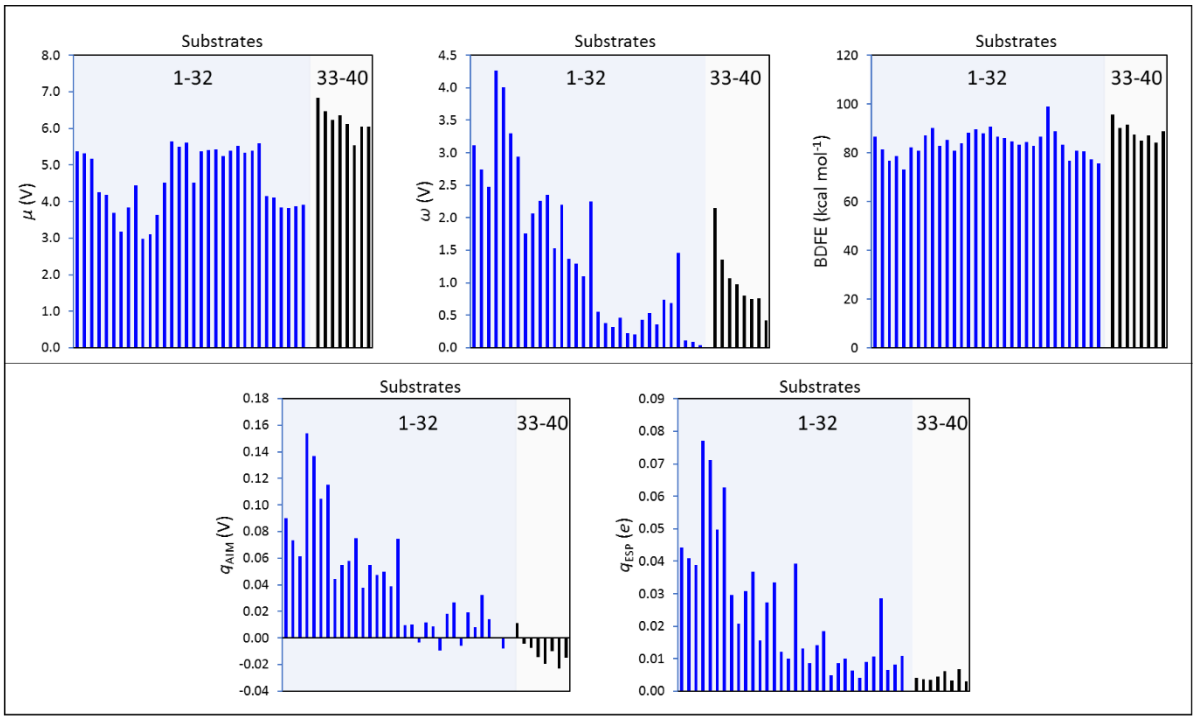

Figure S2. Thermodynamic descriptors (potential duality μ, potential disparity ω, and BDFE) of the 40 C-H substrates from **Figure 4** (*top*), and atomic charges obtained through the q_{AIM} and q_{ESP} schemes (*bottom*). Blue and black colors indicate polar and nonpolar C-H bonds, respectively.

A straightforward to weight the importance of all these descriptors in substrate classification is through the training of an artificial neural network (ANN). Consequently, we trained an ANN consisting of three layers (input, hidden and output) and eight neurons (four inputs; three hidden; one output). The structure of the trained ANN and the relative importance of the evaluated descriptors derived from it are presented in **Figure S3**.

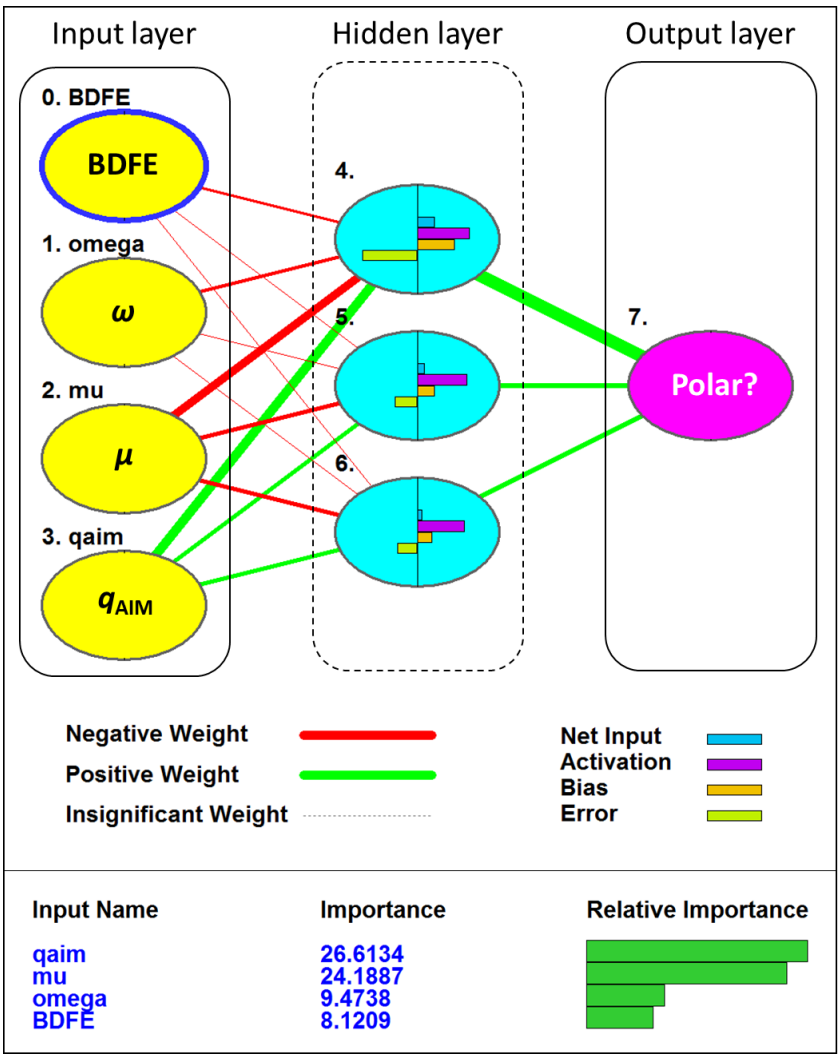

Figure S3. Schematic representation of the artificial neural network trained with the data from **Tables S2-S3** (*top*), and relative importance of the input descriptors in the classification of C-H substrates as polar or nonpolar (*bottom*).

As shown in **Figure S3**, the ANN model confirms the qualitative observation of potential duality and atomic charge as being the dominant determinants in the classification of substrates as polar or nonpolar, whereas the potential duality and the C-H bond BDFE are much less decisive for this classification.

Correlation between C-H bond BDFE and atomic charges

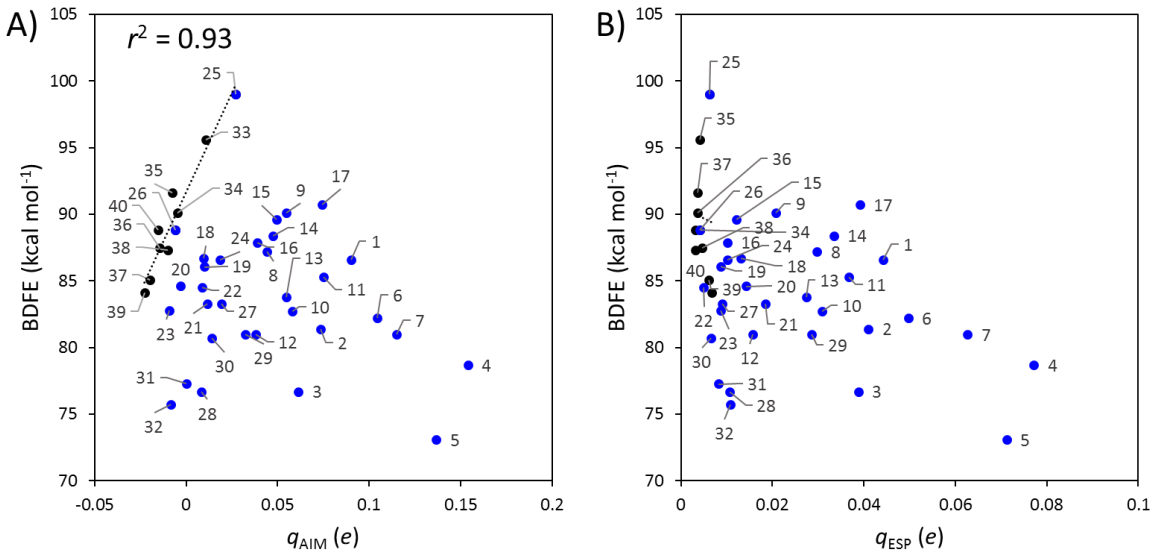

Figure S4. **A**. Correlation between bond dissociation free energy (BDFE) and AIM-integrated atomic charges. **B**. Correlation between bond dissociation free energy (BDFE) and ESP-mapped atomic charges.

Reactivity data for all reactions presented in Figures 5-6

Table S4. Reactivity data for reactions between $L_1Co^{III}O$ and all substrates and solvents from **Figure 3**. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in THF. All values are given in kcal mol^{-1}. Charges were obtained using the Atoms-in-Molecules approach on the 0.001 isosurface of the DFT-obtained electron density.

Substrate	$\Delta G^{\neq}_{\mathrm{DFT}}$ [a]	ΔG_0 [b]	$\Delta G^{\neq}_{\mathrm{intrinsic}}$ [c]	$F\eta$ [d]	$F\sigma$ [e]	Δq_{ESP} [f]	Δq_{AIM} [g]	$\Delta G^{\neq}_{\mathrm{thermo}}$ [h]
CHD	14.0	-15.2	21.6	-29.3	38.3	-0.098	-1.022	-5.3
DHA	10.1	-12.3	14.4	-41.6	35.9	-0.103	-1.042	-7.6
Xanthene	9.3	-13.7	16.2	-35.7	32.3	-0.108	-1.046	-7.7
Fluorene	7.4	-7.8	11.3	-43.9	18.8	-0.107	-1.058	-10.2
Ph_2CH_2	14.2	-6.1	17.3	-42.8	32.4	-0.104	-1.036	-5.7
9-^{t}Bu-fluorene	11.2	-8.2	15.3	-41.0	20.7	-0.104	-1.040	-9.1
9-Ph-fluorene	3.5	-13.3	10.1	-48.2	22.2	-0.107	-1.056	-13.1
MeCN	17.6	7.2	14.0	-92.3	60.6	-0.133	-1.105	-4.4
THF	20.7	4.1	18.7	-27.5	50.4	-0.094	-1.016	7.8

[a] Gibbs free energy difference between the transition state in its lowest spin state and the separated reactants in solution, expressed in kcal mol^{-1}.
[b] Gibbs free energy difference between separated reactants and separated products in solution, expressed in kcal mol^{-1}.
[c] $\Delta G^{\neq}_{\mathrm{intrinsic}} \approx \Delta G^{\neq}_{\mathrm{DFT}} - {}^1/_2\,\Delta G_0$
[d] Factor of asynchronicity, calculated as shown in **Figure 1** in the main text, expressed in kcal mol^{-1}.
[e] Factor of frustration, calculated as shown in **Figure 1** in the main text, expressed in kcal mol^{-1}.
[f] Electrostatic potential (ESP)-derived atomic charges, expressed in *e*.
[g] AIM-integrated atomic charges, expressed in *e*.
[h] Thermodynamic projection of the HAA barrier, $\Delta G^{\neq}_{\mathrm{thermo}} = {}^1/_2\,\Delta G_0 + {}^F/_4\,(|\sigma| - |\eta|)$

Table S5. HAA barriers for reactions between $L_1Co^{III}O$ and all substrates and solvents from **Figure 3**, in all accessible spin states. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in THF. All values are given in kcal mol^{-1}. Missing values correspond to states that could not be located.

Substrate	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=0, closed shell)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=0, open shell)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=1)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=2)
CHD	17.5	16.3	14.0	15.3
DHA	10.1	-	9.0	11.3
Xanthene	9.3	-	10.3	11.7
Fluorene	7.4	-	10.6	12.5
Ph_2CH_2	14.2	-	15.6	16.2
9-^{t}Bu-fluorene	11.2	-	-	13.7
9-Ph-fluorene	3.5	-	7.0	8.2
MeCN	-	-	-	17.6
THF	-	23.4	23.8	20.7

Thermodynamic descriptors and relevant atomic charges for relevant atoms for oxidants in Figure 7

Table S6. Comparison between thermodynamic descriptors for oxidants $L_0Co^{III}O$ to $L_4Co^{III}O$, obtained using de B3LYP* density functional. The def2-SVP//def2-TZVP basis sets were used for geometry optimization and final potential energy calculation, respectively. The D3 dispersion correction and implicit CPCM solvation in MeCN was used in all cases.

	$L_0Co^{III}O$	$L_1Co^{III}O$	$L_2Co^{III}O$	$L_3Co^{III}O$	$L_4Co^{III}O$
E^o_{OxH} (V)	-1.042	-0.482	0.373	0.128	1.090
$pK_{a,Ox}$	33.0	25.6	14.5	17.5	-0.2
E^o_{Ox} (V)	-2.728	-2.325	-1.348	-1.656	0.324
$pK_{a,OxH}$	61.4	56.7	43.6	47.3	12.8
BDFE (kcal mol^{-1})	77.5	80.3	84.9	82.9	81.4
ω (V)	-1.463	-0.869	0.285	-0.042	2.083
μ (V)	1.833	2.031	2.087	2.067	1.304
q_{ESP} (e)	-0.103	-0.090	-0.021	-0.015	0.060
q_{AIM} (e)	-1.028	-1.010	-0.861	-0.925	-0.822

Reactivity data for all reactions presented in Figure 8

Table S7. Reactivity data for reactions between $L_4Co^{III}O$ and all substrates and solvents from **Figure 3**. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in THF. All values are given in kcal mol^{-1}. Charges were obtained using the Atoms-in-Molecules approach on the 0.001 isosurface of the DFT-obtained electron density.

Substrate	$\Delta G^{\neq}_{\mathrm{DFT}}$ [a]	ΔG_0 [b]	$\Delta G^{\neq}_{\mathrm{intrinsic}}$ [c]	$F\eta$ [d]	$F\sigma$ [e]	Δq_{ESP} [f]	Δq_{AIM} [g]	$\Delta G^{\neq}_{\mathrm{thermo}}$ [h]
CHD	7.9	-16.2	16.0	38.7	-33.6	0.052	-0.834	-9.4
DHA	7.1	-13.3	13.8	26.5	-35.4	0.048	-0.855	-4.4
Xanthene	8.7	-14.7	16.1	32.3	-29.8	0.042	-0.859	-8.0
Fluorene	9.3	-8.9	13.8	24.1	-24.6	0.043	-0.870	-4.3
Ph_2CH_2	10.9	-7.2	14.5	25.3	-40.5	0.046	-0.849	0.2
9-^{t}Bu-fluorene	15.3	-9.2	19.9	27.1	-26.0	0.047	-0.853	-4.9
9-Ph-fluorene	8.9	-14.3	16.0	19.9	-20.2	0.044	-0.869	-7.1
MeCN	18.8	6.1	15.7	-24.3	-87.6	0.017	-0.918	18.9
THF	13.1	3.0	11.6	40.6	-73.0	0.056	-0.828	9.6

[a] Gibbs free energy difference between the transition state in its lowest spin state and the separated reactants in solution, expressed in kcal mol^{-1}.
[b] Gibbs free energy difference between separated reactants and separated products in solution, expressed in kcal mol^{-1}.
[c] $\Delta G^{\neq}_{\mathrm{intrinsic}} \approx \Delta G^{\neq}_{\mathrm{DFT}} - {}^1/_2\,\Delta G_0$
[d] Factor of asynchronicity, calculated as shown in **Figure 1** in the main text, expressed in kcal mol^{-1}.
[e] Factor of frustration, calculated as shown in **Figure 1** in the main text, expressed in kcal mol^{-1}.
[f] Electrostatic potential (ESP)-derived atomic charges, expressed in *e*.
[g] AIM-integrated atomic charges, expressed in *e*.
[h] Thermodynamic projection of the HAA barrier, $\Delta G^{\neq}_{\mathrm{thermo}} = {}^1/_2\,\Delta G_0 + {}^F/_4\,(|\sigma| - |\eta|)$

Table S8. HAA barriers for reactions between $L_4Co^{III}O$ and all substrates and solvents from **Figure 3**, in all accessible spin states. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in THF. All values are given in kcal mol^{-1}. Missing values correspond to states that could not be located.

Substrate	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=0, closed shell)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=0, open shell)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=1)	$\Delta G^{\neq}_{\mathrm{DFT}}$ (*S*=2)
CHD	16.1	10.6	7.9	16.0
DHA	13.4	9.6	7.1	12.4
Xanthene	14.3	11.2	8.7	13.5
Fluorene	15.2	-	9.3	18.2
Ph_2CH_2	18.6	13.4	10.9	19.4
9-^{t}Bu-fluorene	20.7	-	15.3	23.6
9-Ph-fluorene	13.7	-	8.9	17.0
MeCN	-	21.6	18.8	34.7
THF	-	14.7	13.1	18.4

Steric effects in the HAA reaction between $L_4Co^{III}O$ and 9-^{t}Bu-fluorene

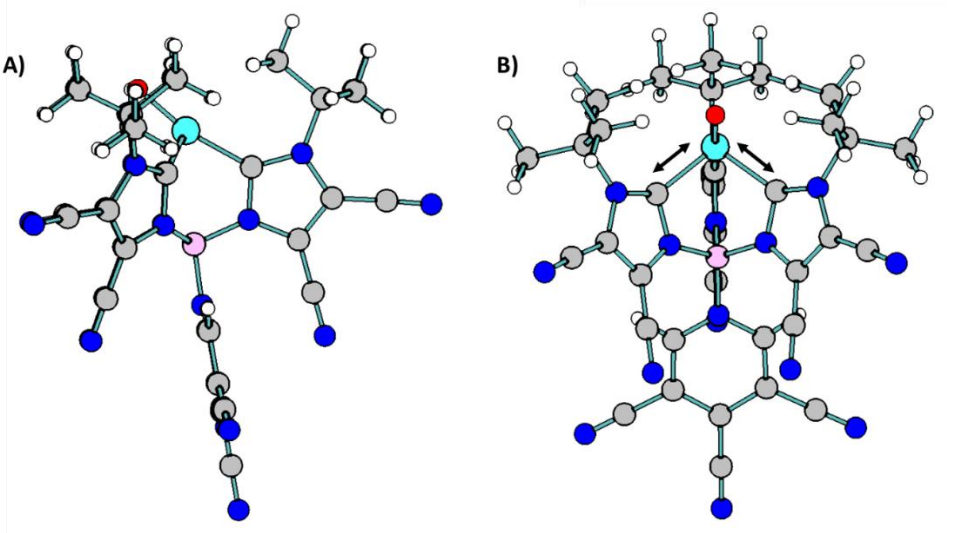

Figure S5. **A**. Lateral view of oxidant $L_4Co^{III}O$ in its ground $S = 2$ state, showcasing an HAA-active oxygen atom that is buried between two ^{t}Bu groups, and inequivalent C-Co bonds. **B**. Frontal view of $L_4Co^{III}O$ in its ground $S = 2$ state, presenting the two equivalent C-Co bonds (black arrows) used to evaluate the effect of sterics at the HAA step in **Figure S6**.

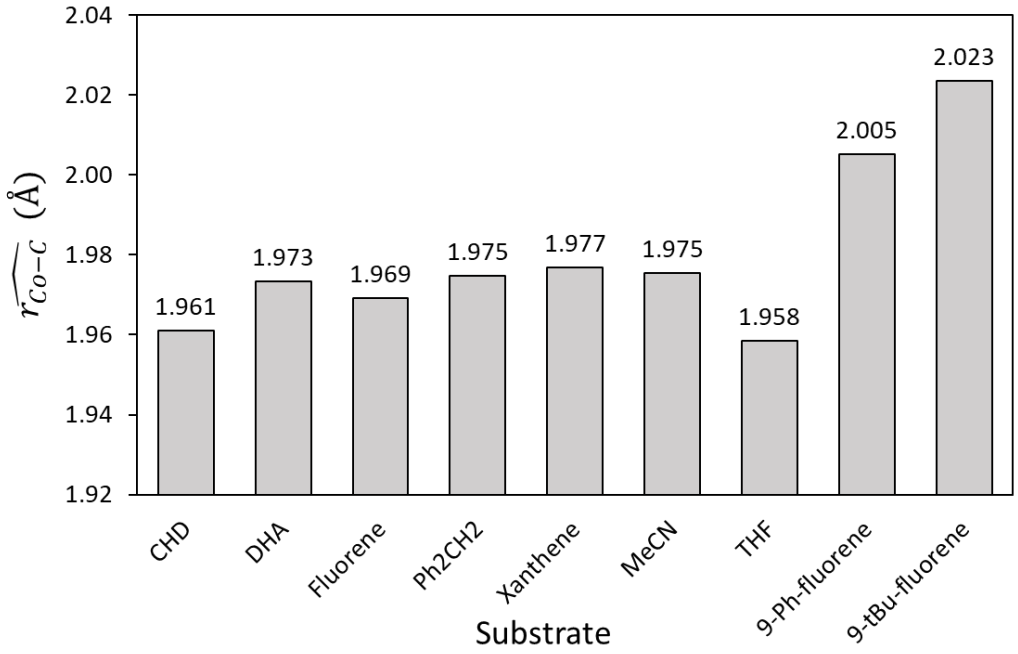

Figure S6. Average C-Co distances ($\widehat{r_{Co-C}}$) for the equivalent C-Co bonds in $L_4CoIIIO$, shown in **Figure S2B**, at the transition state for HAA with all substrates from **Figure 3**. As seen, substrate 9-^{t}Bu-fluorene shows the largest deviations, arising from steric clash between the ^{t}Bu groups in both oxidant and substrate.

Prescription for application of the D3 correction with the B3LYP* functional

All calculations in this work were carried out with Gaussian 16, and the presented prescription applies only to this program. The B3LYP* functional is imposed through the following keywords:[1]

BLYP IOp(3/76=1000001500) IOp(3/77=0720008500) IOp(3/78=0810010000)

The coefficients for the D3 dispersion correction, however, are method-dependent and have not been reported for the B3LYP* functional. For this reason, the values employed in our work with B3LYP* (15% Fock exchange) were obtained by linear interpolation from the values reported for the BLYP (0% Fock exchange) and B3LYP functionals (20% Fock exchange).[2] The coefficients obtained in this way are:

BLYP (0% exchange):
IOp(3/174=1000000) IOp(3/175=1682000) IOp(3/176=1094000)

B3LYP (20% exchange):
IOp(3/174=1000000) IOp(3/175=1703000) IOp(3/176=1.261000)

B3LYP* (15% exchange):
IOp(3/174=1000000) IOp(3/175=1697750) IOp(3/176=1219250)

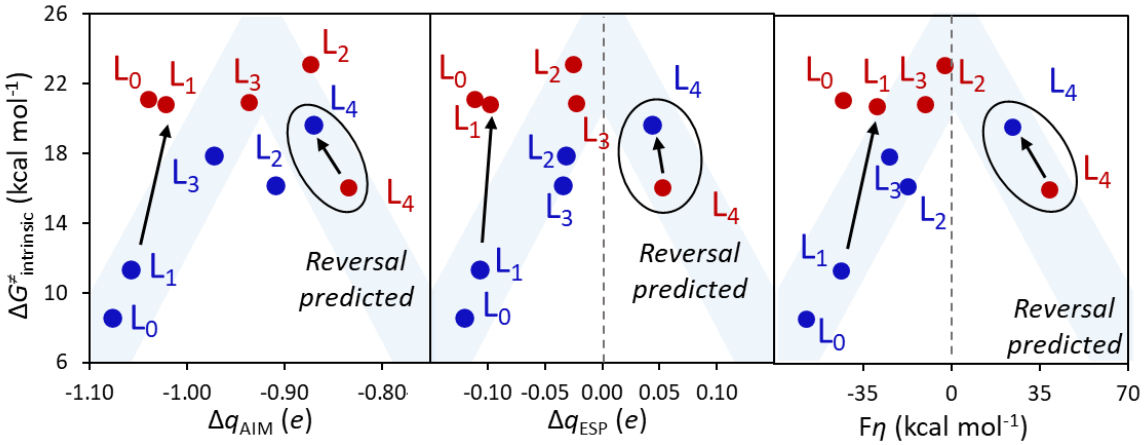

Figure S7. Quantification of PM predicts the substrate selectivity reversal observed through explicit transition state calculations from CHD and fluorene by oxidants L_0-L_4 in **Figure 9**, if spin crossover is not allowed in the HAA reaction from fluorene by L_2-L_4. All energetics is condensed in **Table S9**.

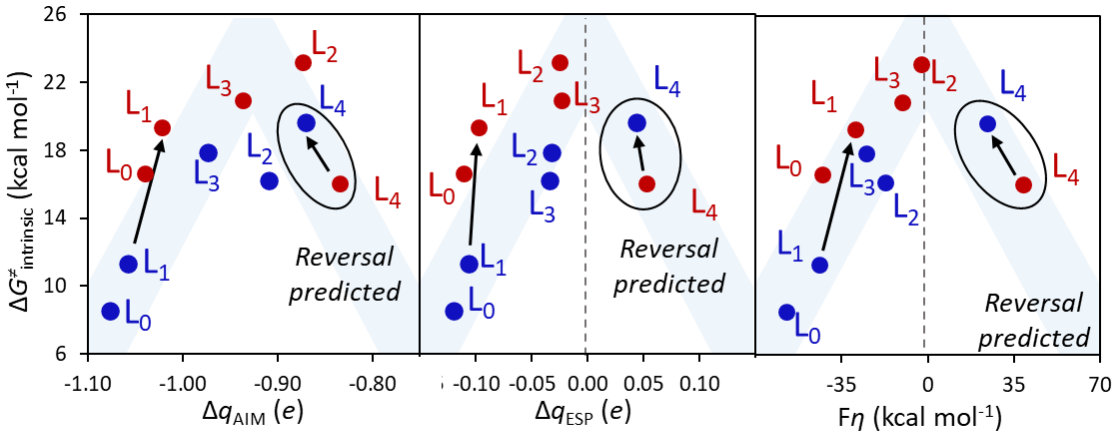

Figure S8. Subtraction of the singlet → triplet spin crossover penalty from the HAA reactions between L0-L1 and CHD partly corrects their outlying behavior shown in **Figure 9**. Energetics is condensed in **Table S9**.

Table S9. HAA barriers for reactions between all oxidants $L_0Co^{III}O$ – $L_4Co^{III}O$ and substrates CHD and fluorene, in the singlet, triplet and quintet spin states. All energies were calculated at the B3LYP*(D3)/def2-SVP//def2-TZVP level of theory at 298 K, with CPCM solvation in THF. All values are given in kcal mol^{-1}. The ground spin state is shown as bold text in each case.

Oxidant	Substrate	$\Delta G^{\neq}_{DFT}$ $(S = 0)$	$\Delta G^{\neq}_{DFT}$ $(S = 1)$	$\Delta G^{\neq}_{DFT}$ $(S = 2)$
$L_0Co^{III}O$	CHD	16.1	**14.0**	15.4
	Fluorene	**6.1**	6.9	16.1
$L_1Co^{III}O$	CHD	16.3	**14.0**	15.3
	Fluorene	**7.4**	10.6	12.5
$L_2Co^{III}O$	CHD	15.5	**12.1**	12.9
	Fluorene	11.1	**9.8**	15.5
$L_3Co^{III}O$	CHD	13.3	**12.1**	13.5
	Fluorene	12.7	**10.3**	19.5
$L_4Co^{III}O$	CHD	10.6	**7.9**	16.0
	Fluorene	15.2	**9.3**	18.2

Half-reaction thermocycle for the $L_1Co^{III}O$ oxidant

For the oxidant $L_1Co^{III}O$, the one-electron reduced species was not reported in ref. 3 and, thus, the experimental half-reaction thermocycle reported is not complete (**Figure S4**). Thus, we applied DFT calculations to fill this gap. All species were optimized at the B3LYP*(D3)/def2-SVP level with implicit CPCM solvation in MeCN. Final electronic potential energies were calculated with the B3LYP*(D3)/def2-TZVP(CPCM) method, as described in the *Methods* section in the main text.

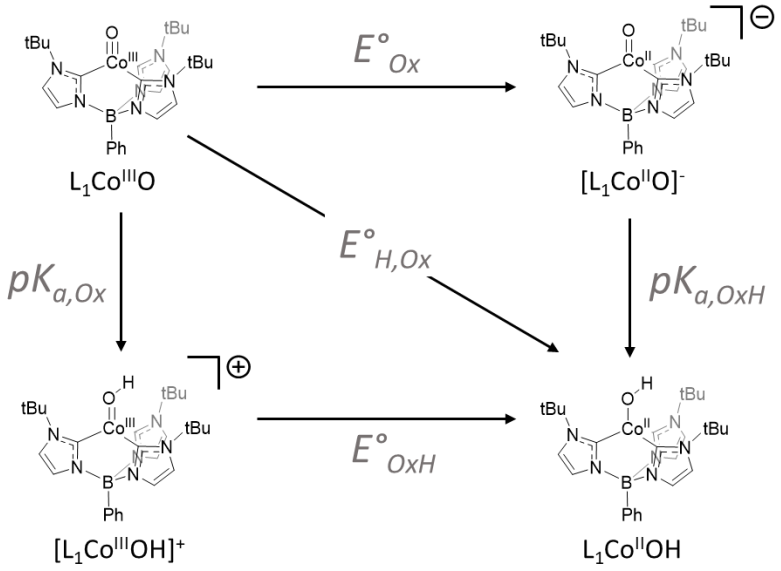

Figure S9. Half-reaction HAA thermocycle for the oxidant $L_1Co^{III}O$. Species $L_1Co^{III}O$, $[L_1Co^{III}OH]^+$ and $L_1Co^{II}OH$ were experimentally characterized in reference 3. Species $[L_1Co^{II}OH]^-$ was not observed experimentally. All three possible spin states were calculated for all species. All values were computed at the B3LYP*(D3)/def2-SVP//def2-TZVP level at 298K with implicit CPCM solvation in MeCN and are condensed in **Table S10**.

All species from **Figure S9** can exist in three spin states each. Systems $L_1Co^{III}O$ and $[L_1Co^{III}OH]^+$ may be singlets, triplets or quintets, while $[L_1Co^{II}OH]^-$ and $L_1Co^{II}OH$ can be doublets, quartets or sextets. For all species, all three potentially accessible states were calculated. The Gibbs energy of the lowest-lying state for each species was employed in all cases to calculate

the thermodynamic descriptors from **Figure S4**. The results for these calculations and their comparison to experimental measurements are provided in **Table S10**.

Table S10. Comparison between experimental thermodynamic descriptors for oxidant $L_1Co^{III}O$, and values calculated using the B3LYP*(D3)/def2SVP//def2TZVP protocol with CPCM solvation in MeCN.

	Experimental[a,b]	Calculated[c]
E^o_{AH} (mV)	-230	-482
$pK_{a,A}$	25.6	25.6
E^o_A (mV)	N/A	-2325
$pK_{a,AH}$	N/A	56.7
BDFE (kcal mol^{-1})	84.6	80.3

[a] Experimental acidity constants were measured in MeCN.
[b] Experimental reduction potentials were measured in MeCN. Reduction potentials are referenced to the Cp^+/Cp pair in MeCN (4.98 V). N. D. stands for *not determined*.
[c] The Gibbs free energy of solvation of the proton, G_{H+}, employed for these calculations, was -260.2 kcal mol^{-1}.[4]

Performance of B3LYP* on the prediction of HAA barriers for the $L_1Co^{III}O$ oxidant

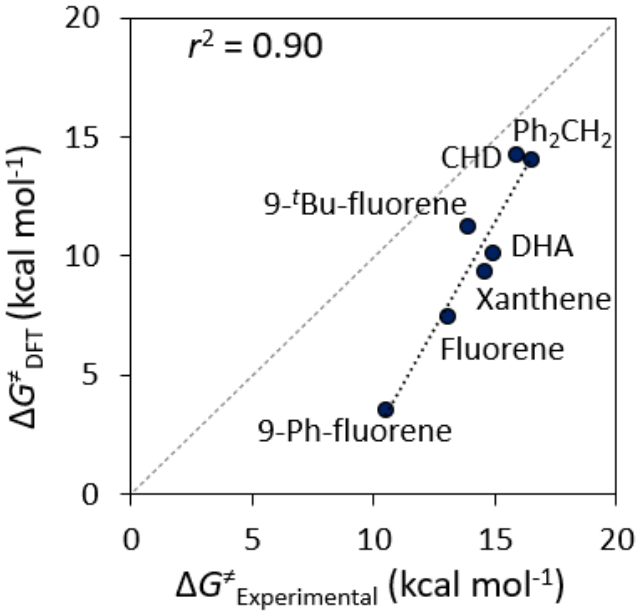

Figure S10. Correlation between HAA barriers calculated with the B3LYP*(D3)/def2SVP//def2TZVP protocol with CPCM solvation in THF, and those obtained experimentally and reported in reference 3.

Prediction of energetics and ground spin states by different density functionals

Table S8. Comparison between ground-state spin multiplicities determined experimentally for the species from **Figure S9**, and those obtained using different density functionals. The def2-SVP//def2-TZVP basis sets were used for geometry optimization and final potential energy calculation, respectively. The D3 dispersion correction and implicit CPCM solvation in MeCN was used in all cases.

	Experiment[a,b]	B3LYP*	B3LYP	BP86
$L_1Co^{III}O$	0	0	2	0
$[L_1Co^{III}OH]^+$	0	0	0	0
$[L_1Co^{II}O]^-$	N/A	3/2	3/2	1/2
$L_1Co^{II}OH$	3/2	3/2	3/2	1/2
BDFE	84.6	80.3	87.4	65.6

[a] From Ref. 3.

[b] Experimental values were measured in MeCN. Reduction potentials are referenced to the Cp^+/Cp pair in MeCN. N. D. stands for *not determined*.

Cartesian coordinates for all species presented in this work

1. Thermodynamic cycle for the $L_1Co^{III}O$ oxidant in all accessible spin states.

$L_1Co^{III}O$ (*S* = 0)

```
74
o_u0.gjf.log     Energy: -1796417.0333958
C          -0.33044         1.47453        -0.42442
N          -0.73758         2.71032        -0.85930
C           0.34382         3.36661        -1.44236
C           1.41994         2.53686        -1.34473
N           1.00269         1.39614        -0.68981
B           1.77334         0.06688        -0.35685
N           1.41991        -0.26288         1.12845
C           0.12098        -0.33149         1.49069
N           0.10868        -0.61137         2.82945
C           1.42232        -0.71483         3.29045
C           2.23780        -0.49641         2.21795
N           1.00499        -0.99832        -1.21983
C          -0.32390        -1.19694        -1.00067
N          -0.72271        -2.15494        -1.89824
C           0.35735        -2.49742        -2.70820
C           1.42563        -1.76361        -2.28815
Co         -1.29627        -0.05876         0.19559
O          -2.94211        -0.02526        -0.06933
C          -2.12212         3.29613        -0.79123
C          -2.06629         4.79099        -1.14512
C          -3.01141         2.55904        -1.80481
C          -2.66113         3.15162         0.64084
C          -1.12423        -0.71514         3.67203
C          -0.74496        -1.10501         5.10670
C          -1.81781         0.65754         3.67479
C          -2.04634        -1.79229         3.07752
C          -2.08717        -2.77680        -2.02842
C          -2.53930        -3.26760        -0.64381
C          -3.05725        -1.73224        -2.60202
C          -2.01432        -3.98396        -2.97735
H          -3.07845         5.20929        -1.03033
H          -1.39231         5.34912        -0.47388
H          -2.59032         2.65105        -2.82096
H          -4.02039         3.00552        -1.80635
H          -3.09397         1.49785        -1.52277
H          -1.97143         3.61795         1.36462
H          -2.80006         2.09272         0.89415
H          -3.63883         3.65555         0.71590
H          -0.10593        -0.34587         5.58660
H          -0.23191        -2.08029         5.14309
H          -1.66686        -1.18745         5.70347
H          -1.15271         1.42770         4.10034
H          -2.73979         0.61638         4.27790
H          -1.51580        -2.75510         2.99090
H          -2.92468        -1.93168         3.72902
H          -2.40593        -1.49257         2.08135
H          -3.51978        -3.76416        -0.73166
H          -1.81561        -3.99255        -0.23379
```

H	-4.03742	-2.20378	-2.78795
H	-3.18937	-0.90966	-1.88037
H	-1.29108	-4.74104	-2.63102
H	-1.76249	-3.69116	-4.00972
H	-3.00810	-4.45749	-3.00626
H	-1.75917	4.96505	-2.18914
H	-2.67480	-1.34122	-3.56081
H	-2.08753	0.95642	2.65045
C	3.37982	0.10098	-0.49947
C	4.12064	1.26269	-0.19254
C	5.52103	1.26696	-0.16346
C	6.23283	0.09065	-0.42469
C	5.52618	-1.08826	-0.68814
C	4.12573	-1.07800	-0.71415
H	3.59867	2.18997	0.06136
H	6.05719	2.19212	0.07462
H	7.32788	0.08874	-0.40536
H	6.06646	-2.02473	-0.86478
H	3.60802	-2.02752	-0.87877
H	0.27643	4.35867	-1.87473
H	2.43666	2.67673	-1.70083
H	1.67705	-0.93410	4.32223
H	3.32316	-0.49104	2.14744
H	0.29473	-3.22543	-3.50929
H	2.43880	-1.72894	-2.67852
H	-2.64128	-2.42342	0.04976

$L_1Co^{III}O$ (*S* = 1)

74
o_u2.gjf.log Energy: -1796413.7952023

C	-0.32780	1.64865	-0.22835
N	-0.67481	2.88650	-0.67561
C	0.39761	3.45651	-1.35738
C	1.42125	2.55654	-1.30337
N	0.97860	1.46332	-0.57906
B	1.71329	0.08617	-0.31966
N	1.37663	-0.32465	1.15228
C	0.09001	-0.43423	1.54607
N	0.09929	-0.81156	2.85206
C	1.42329	-0.93961	3.27985
C	2.21561	-0.63260	2.21170
N	0.96032	-0.94584	-1.25490
C	-0.35135	-1.26532	-1.05058
N	-0.71464	-2.08075	-2.07791
C	0.35413	-2.22911	-2.95866
C	1.39121	-1.50777	-2.44417
Co	-1.27529	-0.05191	0.23814
O	-2.91110	0.03438	-0.01559
C	-2.03110	3.50953	-0.54079
C	-1.91889	5.02682	-0.75070
C	-2.94807	2.88741	-1.60692
C	-2.57128	3.22875	0.86987
C	-1.13438	-1.08141	3.65334
C	-0.75045	-1.43410	5.09517
C	-2.00954	0.18291	3.64432
C	-1.87617	-2.26267	3.00516

C	-2.08464	-2.64826	-2.29409
C	-2.64960	-3.12352	-0.94660
C	-2.96656	-1.53877	-2.89084
C	-1.99654	-3.84052	-3.25833
H	-2.90504	5.48175	-0.56751
H	-1.19703	5.48044	-0.05083
H	-2.54080	3.06322	-2.61752
H	-3.95103	3.34392	-1.55308
H	-3.03932	1.80515	-1.42336
H	-1.86462	3.58518	1.63820
H	-2.74781	2.15246	1.00375
H	-3.52962	3.75739	1.00336
H	-0.20741	-0.60957	5.58592
H	-0.13528	-2.34749	5.14505
H	-1.67093	-1.62031	5.67038
H	-1.45247	1.04500	4.04739
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H	-2.80055	-2.48241	3.56407
H	-2.14920	-2.02720	1.96451
H	-3.61555	-3.62729	-1.11642
H	-1.96228	-3.83816	-0.46343
H	-3.98182	-1.92613	-3.08153
H	-3.03285	-0.70268	-2.17671
H	-1.29703	-4.60907	-2.88855
H	-1.68937	-3.53839	-4.27278
H	-2.99431	-4.29882	-3.34431
H	-1.62724	5.28728	-1.78118
H	-2.54581	-1.18216	-3.84681
H	-2.34100	0.42440	2.62229
C	3.32043	0.11488	-0.47015
C	4.07270	1.25346	-0.11075
C	5.47317	1.24189	-0.08729
C	6.17145	0.07245	-0.40959
C	5.45228	-1.08431	-0.73186
C	4.05200	-1.05871	-0.75153
H	3.55843	2.17324	0.18455
H	6.02035	2.14860	0.19299
H	7.26649	0.05847	-0.39460
H	5.98296	-2.01499	-0.96061
H	3.52088	-1.99050	-0.96929
H	0.36201	4.44166	-1.81176
H	2.42136	2.61906	-1.72454
H	1.69740	-1.23038	4.28902
H	3.29922	-0.60835	2.12371
H	0.30638	-2.83123	-3.86057
H	2.39353	-1.35872	-2.83742
H	-2.81893	-2.26595	-0.28012

$L_1Co^{III}O$ (*S* = 2)

74
o_u4.gjf.log Energy: -1796410.6945776

C	-0.41903	0.86763	1.42942
N	-0.81986	1.73937	2.39061
C	0.21652	2.61116	2.70091

C	1.27397	2.25230	1.91184
N	0.88084	1.16247	1.15457
B	1.64637	0.45219	-0.04116
N	1.42875	-1.10489	0.09015
C	0.20760	-1.70326	0.14810
N	0.43437	-3.03656	0.25727
C	1.80551	-3.28595	0.26876
C	2.42174	-2.07406	0.16371
N	0.87256	0.95380	-1.33427
C	-0.42507	0.60862	-1.55359
N	-0.83269	1.30294	-2.64723
C	0.19737	2.11679	-3.10166
C	1.25747	1.90363	-2.26437
Co	-1.36354	-0.36430	0.03465
O	-2.91401	-1.03305	0.11083
C	-2.20591	1.76037	2.95769
C	-2.26526	2.73945	4.13667
C	-3.17450	2.20951	1.84972
C	-2.55866	0.34208	3.43668
C	-0.65791	-4.05613	0.35334
C	-0.04907	-5.45962	0.46060
C	-1.49425	-3.74882	1.60722
C	-1.52585	-3.95613	-0.91286
C	-2.20930	1.18842	-3.22644
C	-2.48311	-0.29532	-3.52489
C	-3.22161	1.72196	-2.19749
C	-2.29415	2.00808	-4.51956
H	-3.27756	2.71218	4.56938
H	-1.55032	2.46406	4.92981
H	-2.87914	3.19282	1.44660
H	-4.19726	2.28914	2.25405
H	-3.18641	1.47472	1.02985
H	-1.82642	-0.00961	4.18285
H	-2.57693	-0.36161	2.58989
H	-3.55794	0.34810	3.90285
H	0.57648	-5.56900	1.36215
H	0.55502	-5.71467	-0.42606
H	-0.86677	-6.19415	0.53046
H	-0.86008	-3.76631	2.51003
H	-2.28640	-4.50771	1.72252
H	-0.91156	-4.10764	-1.81684
H	-2.30908	-4.73250	-0.88939
H	-2.01384	-2.97030	-0.96025
H	-3.48495	-0.40593	-3.97194
H	-1.73709	-0.69450	-4.23257
H	-4.23094	1.73763	-2.64125
H	-3.24984	1.06892	-1.31113
H	-1.56133	1.66541	-5.26885
H	-2.14036	3.08424	-4.33520
H	-3.29968	1.88511	-4.95143
H	-2.06731	3.77744	3.82218
H	-2.96008	2.74675	-1.88482
H	-1.96915	-2.76028	1.51081
C	3.24192	0.71870	-0.07018
C	3.99132	0.83086	1.12043
C	5.38963	0.91139	1.11519
C	6.09141	0.86446	-0.09491
C	5.37894	0.71327	-1.29008
C	3.98068	0.63394	-1.26968

H	3.47864	0.82718	2.08727
H	5.93309	1.00117	2.06213
H	7.18473	0.92859	-0.10506
H	5.91391	0.64646	-2.24374
H	3.45950	0.47253	-2.21832
H	0.13998	3.40159	3.44140
H	2.26133	2.70046	1.83796
H	2.23692	-4.27893	0.34866
H	3.48133	-1.83434	0.13641
H	0.11549	2.77137	-3.96410
H	2.24123	2.36566	-2.26785
H	-2.44962	-0.88774	-2.59718

[$L_1Co^{III}OH]^+$ (*S* = 0)

75
p_u0.gjf.log Energy: -1796722.1420978

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C	0.03601	-3.22992	-1.79598
C	1.18963	-2.70187	-1.30085
N	0.89561	-1.43961	-0.82700
B	1.72585	-0.49643	0.11835
N	1.52051	0.95385	-0.43726
C	0.29441	1.49795	-0.55677
N	0.45495	2.81687	-0.87463
C	1.82281	3.06773	-0.98967
C	2.47921	1.90682	-0.71387
N	0.88576	-0.54555	1.45575
C	-0.41554	-0.15427	1.41101
N	-0.94113	-0.40594	2.64146
C	0.03049	-0.99185	3.44679
C	1.16552	-1.08637	2.69418
Co	-1.18997	0.38356	-0.30123
O	-2.13332	0.89459	-1.74904
C	-2.41178	-2.54931	-1.98056
C	-2.63561	-4.06802	-2.08501
C	-3.33776	-2.00102	-0.88635
C	-2.69869	-1.89148	-3.33856
C	-0.57769	3.90444	-1.05123
C	0.05838	5.25409	-0.67000
C	-1.02100	3.93336	-2.52168
C	-1.77309	3.65247	-0.12140
C	-2.33760	-0.16303	3.11698
C	-3.13582	0.59862	2.05733
C	-2.99675	-1.52613	3.38861
C	-2.27298	0.68456	4.39971
H	-3.70698	-4.24780	-2.26248
H	-2.09046	-4.51722	-2.92989
H	-3.05156	-2.39267	0.10315
H	-4.37385	-2.31161	-1.09292
H	-3.33345	-0.90201	-0.87507
H	-1.98847	-2.25018	-4.10180
H	-2.62976	-0.79894	-3.25655
H	-3.71896	-2.15067	-3.66588
H	0.84205	5.56999	-1.37601
H	0.48167	5.22663	0.34751

H	-0.72491	6.02710	-0.69595
H	-0.15518	4.07316	-3.18988
H	-1.71991	4.77090	-2.68107
H	-1.43587	3.43180	0.90506
H	-2.40183	4.55587	-0.08773
H	-2.39737	2.83390	-0.50075
H	-4.15579	0.77502	2.43293
H	-2.69113	1.58225	1.83985
H	-4.03186	-1.37892	3.73631
H	-3.02056	-2.13490	2.47000
H	-1.75562	1.63902	4.20754
H	-1.74931	0.16084	5.21481
H	-3.29478	0.90463	4.74769
H	-2.35130	-4.58678	-1.15488
H	-2.45436	-2.09056	4.16387
H	-1.53718	2.99935	-2.78366
C	3.29749	-0.80106	0.22199
C	4.02380	-1.24107	-0.90557
C	5.41643	-1.38311	-0.87968
C	6.13184	-1.06966	0.28182
C	5.44245	-0.59224	1.40217
C	4.04928	-0.45380	1.36392
H	3.50079	-1.45446	-1.84315
H	5.94481	-1.73102	-1.77364
H	7.22090	-1.18066	0.30778
H	5.99172	-0.31599	2.30846
H	3.54934	-0.03382	2.24162
H	-0.13703	-4.19188	-2.26520
H	2.18254	-3.13767	-1.23672
H	2.21989	4.04271	-1.24980
H	3.54323	1.68693	-0.68161
H	-0.15543	-1.28880	4.47565
H	2.13417	-1.50533	2.95249
H	-3.24784	0.01767	1.12729
H	-1.64226	0.90853	-2.58637

[$L_1Co^{III}OH]^+$ (*S* = 1)

75
p_u2.gjf.log Energy: -1796712.8427903

C	-0.60916	-1.36657	-0.86965
N	-1.18716	-2.47196	-1.40180
C	-0.23602	-3.47925	-1.49727
C	0.93234	-2.97174	-1.00116
N	0.69413	-1.66208	-0.63302
B	1.60038	-0.66081	0.19958
N	1.58206	0.76024	-0.49194
C	0.46941	1.52437	-0.58987
N	0.84809	2.74861	-1.03729
C	2.22474	2.73414	-1.26279
C	2.67585	1.49601	-0.91650
N	0.75155	-0.47463	1.51935
C	-0.49023	0.05631	1.41381
N	-1.08801	-0.06674	2.62771
C	-0.21746	-0.71585	3.49554
C	0.92165	-0.98445	2.79001
Co	-1.17120	0.50354	-0.36977

O	-1.95221	0.99930	-1.90097
C	-2.60338	-2.58174	-1.88905
C	-3.01924	-4.06017	-1.89900
C	-3.52920	-1.80364	-0.94222
C	-2.66144	-1.99292	-3.30787
C	-0.00179	3.96979	-1.25262
C	0.79008	5.20213	-0.77816
C	-0.31873	4.08692	-2.75200
C	-1.29260	3.86832	-0.43138
C	-2.46572	0.36007	3.02769
C	-3.12242	1.14753	1.89204
C	-3.28657	-0.90397	3.33350
C	-2.35202	1.26333	4.26752
H	-4.08186	-4.12622	-2.17918
H	-2.45298	-4.64898	-2.63792
H	-3.37129	-2.10648	0.10554
H	-4.57758	-2.01039	-1.20910
H	-3.38142	-0.71868	-1.04167
H	-1.98214	-2.53853	-3.98401
H	-2.37712	-0.92964	-3.28272
H	-3.68673	-2.07539	-3.70497
H	1.67366	5.40436	-1.40325
H	1.11601	5.08149	0.26798
H	0.14039	6.08915	-0.83908
H	0.60523	4.11931	-3.35217
H	-0.88899	5.01022	-2.94378
H	-1.06940	3.68801	0.63293
H	-1.84063	4.82001	-0.51259
H	-1.94761	3.07103	-0.80814
H	-4.12284	1.47808	2.21150
H	-2.54299	2.04788	1.63340
H	-4.31247	-0.62212	3.61971
H	-3.33796	-1.55613	2.44611
H	-1.72262	2.14221	4.05082
H	-1.92272	0.72901	5.12961
H	-3.35451	1.61480	4.55901
H	-2.89606	-4.52008	-0.90445
H	-2.84776	-1.48061	4.16339
H	-0.93029	3.23679	-3.09377
C	3.13152	-1.10790	0.39267
C	3.84986	-1.72372	-0.65489
C	5.22010	-1.99408	-0.55441
C	5.92242	-1.63845	0.60285
C	5.24497	-0.98983	1.64144
C	3.87490	-0.72306	1.52812
H	3.34246	-1.97510	-1.59149
H	5.74211	-2.47603	-1.38783
H	6.99349	-1.84983	0.68735
H	5.78676	-0.67947	2.54119
H	3.38959	-0.17199	2.33911
H	-0.45057	-4.46668	-1.89359
H	1.89419	-3.45892	-0.86921
H	2.76985	3.59601	-1.63561
H	3.68355	1.08906	-0.92737
H	-0.46765	-0.92748	4.53188
H	1.82305	-1.50511	3.10161
H	-3.27824	0.52324	0.99514
H	-1.35815	1.33525	-2.59251

[$L_1Co^{III}OH]^+$ (*S* = 2)

75
p_u4.gjf.log Energy: -1796704.0961240

C	-0.39555	-1.27717	-1.01840
N	-0.77831	-2.39423	-1.68416
C	0.28524	-3.28678	-1.73402
C	1.33362	-2.68850	-1.09579
N	0.91274	-1.43637	-0.68379
B	1.68913	-0.38225	0.20596
N	1.43548	1.05116	-0.42953
C	0.20372	1.56539	-0.66177
N	0.36928	2.80093	-1.19944
C	1.72266	3.06687	-1.31008
C	2.38549	1.96892	-0.82304
N	0.91590	-0.42925	1.59038
C	-0.38781	-0.06077	1.68973
N	-0.79658	-0.34798	2.95098
C	0.24636	-0.94324	3.64247
C	1.31012	-1.00198	2.78285
Co	-1.29188	0.35500	-0.09832
O	-3.08421	0.49232	-0.23269
C	-2.15028	-2.63071	-2.24939
C	-2.13956	-3.90408	-3.10501
C	-3.13418	-2.79323	-1.07976
C	-2.52609	-1.42781	-3.12968
C	-0.76132	3.68706	-1.63627
C	-0.20296	5.02372	-2.13751
C	-1.51023	2.97298	-2.77318
C	-1.68580	3.93036	-0.43234
C	-2.18888	-0.12509	3.47101
C	-2.60814	1.31608	3.14052
C	-3.12007	-1.14353	2.79281
C	-2.20373	-0.32956	4.99106
H	-3.13900	-4.03607	-3.54757
H	-1.41124	-3.83687	-3.92992
H	-2.81747	-3.61641	-0.41794
H	-4.13837	-3.02715	-1.46983
H	-3.20380	-1.86399	-0.49646
H	-1.78516	-1.28473	-3.93337
H	-2.58804	-0.50543	-2.53557
H	-3.51274	-1.60098	-3.58869
H	0.45185	4.89345	-3.01424
H	0.35253	5.55530	-1.34774
H	-1.04521	5.66283	-2.44420
H	-0.83895	2.78412	-3.62689
H	-2.35151	3.59545	-3.11743
H	-1.12380	4.35708	0.41424
H	-2.48307	4.63566	-0.71629
H	-2.16811	2.99910	-0.09857
H	-3.60632	1.51143	3.56435
H	-1.89635	2.03902	3.57174
H	-4.14243	-1.03346	3.18979
H	-3.15924	-0.97923	1.70600
H	-1.49735	0.34678	5.49995
H	-1.97206	-1.36971	5.27187
H	-3.21517	-0.10689	5.36443

H	-1.92322	-4.80343	-2.50592
H	-2.77886	-2.17344	2.98959
H	-1.91440	2.00572	-2.43538
C	3.28309	-0.58810	0.30211
C	4.03109	-1.05271	-0.80107
C	5.43065	-1.09242	-0.78366
C	6.13206	-0.64661	0.34232
C	5.41912	-0.13997	1.43465
C	4.01955	-0.10522	1.40512
H	3.51878	-1.36714	-1.71534
H	5.97477	-1.46416	-1.65835
H	7.22645	-0.67754	0.36139
H	5.95379	0.24012	2.31159
H	3.49882	0.33995	2.25825
H	0.22986	-4.25980	-2.21133
H	2.33378	-3.06725	-0.90504
H	2.12151	3.99185	-1.71498
H	3.45292	1.78559	-0.73121
H	0.17112	-1.27204	4.67423
H	2.30371	-1.41210	2.94138
H	-2.67034	1.47647	2.05454
H	-3.53555	1.06786	-0.87298

[$L_1Co^{II}O]^-$ (*S* =1/2)

74
r_u1.gjf.log Energy: -1796468.1948829

C	-0.40935	-1.34242	-0.90358
N	-0.78929	-2.47858	-1.57953
C	0.30636	-3.32059	-1.76796
C	1.38072	-2.69234	-1.21071
N	0.94197	-1.47744	-0.71199
B	1.69842	-0.40724	0.16656
N	1.41333	1.01734	-0.43577
C	0.14008	1.51592	-0.53202
N	0.28551	2.78001	-1.05706
C	1.63467	3.04451	-1.30451
C	2.33057	1.94082	-0.91112
N	0.93839	-0.46774	1.53377
C	-0.39380	-0.15091	1.50513
N	-0.84565	-0.37278	2.79020
C	0.19015	-0.87139	3.58295
C	1.29488	-0.94179	2.78570
Co	-1.29660	0.29032	-0.15937
O	-2.66553	0.69639	-1.14698
C	-2.17201	-2.74843	-2.07780
C	-2.24621	-4.15917	-2.67950
C	-3.15838	-2.63626	-0.90408
C	-2.50999	-1.69381	-3.14526
C	-0.83726	3.71094	-1.37938
C	-0.28302	5.11772	-1.65136
C	-1.57311	3.17231	-2.61798
C	-1.80588	3.76332	-0.18605
C	-2.22336	-0.05029	3.25489
C	-2.44080	1.46500	3.09228
C	-3.24048	-0.82867	2.40383
C	-2.39035	-0.43939	4.73013

H	-3.27877	-4.34229	-3.01746
H	-1.58677	-4.27241	-3.55648
H	-2.86805	-3.31002	-0.07916
H	-4.17253	-2.91197	-1.24210
H	-3.17134	-1.59383	-0.55017
H	-1.76585	-1.72138	-3.96169
H	-2.52933	-0.69652	-2.65828
H	-3.50467	-1.90472	-3.57817
H	0.35096	5.14992	-2.55330
H	0.29862	5.50282	-0.79592
H	-1.12887	5.80280	-1.82254
H	-0.87080	3.05750	-3.46352
H	-2.36566	3.88011	-2.92217
H	-1.27567	4.04206	0.74111
H	-2.59053	4.51495	-0.38140
H	-2.27690	2.77389	-0.06692
H	-3.46613	1.74235	3.39050
H	-1.72747	2.02749	3.71920
H	-4.26282	-0.64837	2.77768
H	-3.18797	-0.50025	1.35300
H	-1.69420	0.11191	5.38395
H	-2.24314	-1.52130	4.88658
H	-3.41516	-0.19018	5.04891
H	-1.99122	-4.93838	-1.94061
H	-3.03483	-1.91162	2.44326
H	-2.03319	2.19840	-2.34515
C	3.30992	-0.59055	0.24363
C	4.06050	-1.01230	-0.87565
C	5.46119	-1.04061	-0.87101
C	6.16873	-0.62666	0.26389
C	5.45591	-0.16428	1.37621
C	4.05495	-0.14135	1.35490
H	3.54177	-1.30291	-1.79439
H	6.00218	-1.37850	-1.76218
H	7.26400	-0.64843	0.27490
H	5.99286	0.19091	2.26313
H	3.53331	0.26746	2.22530
H	0.25263	-4.28293	-2.26777
H	2.40843	-3.03648	-1.12651
H	1.99770	3.97744	-1.72480
H	3.40151	1.75166	-0.92988
H	0.07428	-1.13695	4.62932
H	2.29090	-1.30701	3.02435
H	-2.28430	1.75331	2.04082

[$L_1Co^{II}O]^-$ (*S* =3/2)

74
r_u3.gjf.log Energy: -1796473.7423302

C	-0.44468	-0.85361	-1.37585
N	-0.87409	-1.75477	-2.31063
C	0.13433	-2.67416	-2.60068
C	1.21377	-2.31105	-1.84858
N	0.86590	-1.17629	-1.12919
B	1.64513	-0.47733	0.05631
N	1.49664	1.08644	-0.09964
C	0.27920	1.70756	-0.16989

N	0.54739	3.03602	-0.32680
C	1.92691	3.25371	-0.35708
C	2.51234	2.02933	-0.21361
N	0.85330	-0.93508	1.34713
C	-0.45614	-0.56545	1.51420
N	-0.88566	-1.22509	2.63183
C	0.12569	-2.04645	3.13070
C	1.20364	-1.86979	2.31163
Co	-1.29539	0.45721	-0.04529
O	-2.96298	0.96435	-0.09575
C	-2.27874	-1.80590	-2.80943
C	-2.36420	-2.74502	-4.02047
C	-3.17266	-2.31868	-1.66674
C	-2.71990	-0.38786	-3.21181
C	-0.53109	4.05484	-0.47702
C	0.08768	5.45143	-0.61121
C	-1.35048	3.70855	-1.73373
C	-1.44283	3.99065	0.76163
C	-2.25503	-1.04908	3.19838
C	-2.46591	0.44940	3.47876
C	-3.29178	-1.52931	2.16712
C	-2.38670	-1.85270	4.49833
H	-3.39347	-2.72992	-4.41325
H	-1.68541	-2.42420	-4.82920
H	-2.84222	-3.31673	-1.32922
H	-4.22099	-2.39310	-2.00425
H	-3.12024	-1.60860	-0.82591
H	-2.00955	0.05009	-3.93445
H	-2.78610	0.25570	-2.31596
H	-3.71531	-0.43562	-3.68718
H	0.73248	5.53157	-1.50283
H	0.68032	5.72318	0.27893
H	-0.72088	6.19255	-0.71561
H	-0.70079	3.67437	-2.62576
H	-2.13031	4.47252	-1.89799
H	-0.85455	4.12738	1.68581
H	-2.20125	4.79135	0.70899
H	-1.95881	3.01421	0.78598
H	-3.46465	0.61370	3.91895
H	-1.70502	0.82633	4.18432
H	-4.29967	-1.51151	2.61808
H	-3.28344	-0.85521	1.29036
H	-1.64871	-1.53547	5.25472
H	-2.27183	-2.93607	4.32428
H	-3.39145	-1.68764	4.91916
H	-2.12853	-3.78944	-3.75563
H	-3.07283	-2.56300	1.84752
H	-1.83806	2.72873	-1.58931
C	3.23810	-0.79507	0.09695
C	3.99012	-0.96260	-1.08547
C	5.38594	-1.08411	-1.07325
C	6.08601	-1.02500	0.13759
C	5.37297	-0.82190	1.32511
C	3.97735	-0.70219	1.29575
H	3.47826	-0.97292	-2.05283
H	5.92971	-1.21573	-2.01560
H	7.17724	-1.12062	0.15396
H	5.90642	-0.74620	2.27944
H	3.45507	-0.50398	2.23691

H	0.02579	-3.48851	-3.31146
H	2.19197	-2.78132	-1.78096
H	2.38403	4.23265	-0.47104
H	3.56743	1.76724	-0.18363
H	0.01791	-2.67843	4.00765
H	2.18030	-2.34644	2.35104
H	-2.39965	1.00810	2.53059

[$L_1Co^{II}O]^-$ (*S* =5/2)

74

r_u5.gjf.log Energy: -1796428.1311079

C	-0.40454	-0.77683	-1.47244
N	-0.80587	-1.65418	-2.44613
C	0.25001	-2.50008	-2.77682
C	1.30736	-2.12630	-1.99479
N	0.90726	-1.05594	-1.21648
B	1.68964	-0.42822	0.02438
N	1.40412	1.16528	-0.04533
C	0.18537	1.76117	-0.08791
N	0.40828	3.10266	-0.14340
C	1.78116	3.35312	-0.13473
C	2.39375	2.13311	-0.07267
N	0.88874	-0.94998	1.30000
C	-0.42100	-0.63344	1.51986
N	-0.83921	-1.41119	2.56789
C	0.20390	-2.23423	2.98386
C	1.26992	-1.94939	2.17606
Co	-1.36130	0.38686	-0.03212
O	-2.92610	1.04023	-0.08656
C	-2.19751	-1.71869	-2.97335
C	-2.25225	-2.66222	-4.18234
C	-3.11972	-2.24266	-1.85726
C	-2.63327	-0.30490	-3.39858
C	-0.68741	4.11486	-0.21330
C	-0.09115	5.52711	-0.26097
C	-1.51044	3.84727	-1.48568
C	-1.57331	3.95989	1.03548
C	-2.21529	-1.34999	3.13580
C	-2.51224	0.10740	3.53340
C	-3.22167	-1.81818	2.06794
C	-2.30878	-2.25582	4.37045
H	-3.27580	-2.66275	-4.58958
H	-1.56754	-2.33442	-4.98241
H	-2.78206	-3.23198	-1.50437
H	-4.15446	-2.33607	-2.22811
H	-3.11866	-1.54324	-1.00737
H	-1.93456	0.10722	-4.14624
H	-2.66757	0.36828	-2.52766
H	-3.64088	-0.34593	-3.84597
H	0.54499	5.67421	-1.14978
H	0.50216	5.75214	0.64109
H	-0.91349	6.25844	-0.31276
H	-0.86817	3.90340	-2.38137
H	-2.31073	4.60093	-1.58174
H	-0.97208	4.07597	1.95358
H	-2.36119	4.73257	1.03428

H	-2.05403	2.96881	1.03246
H	-3.52243	0.18007	3.97057
H	-1.78055	0.46357	4.27839
H	-4.23318	-1.87773	2.50429
H	-3.25219	-1.10222	1.23159
H	-1.58674	-1.95882	5.14929
H	-2.13990	-3.31531	4.11527
H	-3.32024	-2.17278	4.79878
H	-2.00443	-3.70078	-3.90724
H	-2.94684	-2.81415	1.68175
H	-1.97232	2.84922	-1.42696
C	3.23975	-0.72437	0.04486
C	4.03602	-0.72536	-1.16646
C	5.42162	-0.81072	-1.16313
C	6.15926	-0.86835	0.05607
C	5.41397	-0.74987	1.26749
C	4.02834	-0.66434	1.25762
H	3.53238	-0.62919	-2.13686
H	5.95903	-0.81584	-2.12211
H	7.25268	-0.92862	0.06076
H	5.94543	-0.70624	2.22871
H	3.52002	-0.51788	2.21918
H	0.18448	-3.28052	-3.52931
H	2.31085	-2.54058	-1.93735
H	2.21076	4.34972	-0.17209
H	3.44928	1.87191	-0.04635
H	0.12456	-2.94255	3.80334
H	2.26619	-2.38422	2.16163
H	-2.46626	0.76041	2.64780

[$L_1Co^{II}OH$] (*S* =1/2)

75
h_u1.gjf.log Energy: -1796813.6612540

Co	1.16585	0.46218	-0.32087
N	1.05104	-0.23468	2.61700
C	0.14748	-0.87227	3.47013
C	-0.99171	-1.07951	2.74956
N	-0.78719	-0.55575	1.48365
C	0.48435	-0.07083	1.38363
H	0.38115	-1.11852	4.50306
H	-1.91648	-1.56593	3.04862
C	2.43158	0.14112	3.02263
C	3.12438	0.90205	1.88644
C	3.21734	-1.14376	3.33938
C	2.34996	1.05121	4.26140
H	4.12958	1.21026	2.21643
H	2.56346	1.80810	1.60956
H	3.25420	0.26554	0.99609
H	2.75591	-1.70519	4.16813
H	4.25140	-0.89538	3.62990
H	3.25160	-1.79984	2.45379
H	1.76066	1.95574	4.03585
H	3.36268	1.36125	4.56669
H	1.88411	0.53800	5.11808
B	-1.62712	-0.61160	0.15361
N	1.09646	-2.41610	-1.53945

C	0.10535	-3.38383	-1.70673
C	-1.04549	-2.85800	-1.20037
N	-0.76121	-1.57781	-0.75472
C	0.56333	-1.30330	-0.95055
H	0.28449	-4.35534	-2.15637
H	-2.02801	-3.31357	-1.11312
C	2.52075	-2.58952	-1.96280
C	2.71338	-1.91397	-3.33121
C	2.84544	-4.08894	-2.06378
C	3.44859	-1.94446	-0.92167
H	3.73781	-2.09175	-3.70063
H	2.56218	-0.82936	-3.22497
H	2.00247	-2.32058	-4.07051
H	2.63439	-4.61194	-1.11597
H	3.91706	-4.20637	-2.28931
H	2.28726	-4.58479	-2.87435
H	3.33665	-0.85109	-0.93822
H	4.49640	-2.18361	-1.16717
H	3.23011	-2.32328	0.09020
N	-0.76119	2.81486	-0.92607
C	-2.14193	2.87877	-1.12969
C	-2.64303	1.65005	-0.81957
N	-1.57702	0.84984	-0.44007
C	-0.41360	1.55557	-0.52651
H	-2.65447	3.77614	-1.46290
H	-3.67007	1.29330	-0.83098
C	0.16918	3.96536	-1.13842
C	1.35424	3.85554	-0.16709
C	-0.58294	5.27931	-0.86519
C	0.67426	3.93275	-2.59099
H	1.97921	4.75951	-0.25552
H	1.97393	2.98358	-0.41785
H	1.00523	3.77089	0.87537
H	-1.37133	5.47458	-1.60987
H	0.12906	6.11810	-0.92004
H	-1.03854	5.27753	0.13925
H	1.27913	3.02606	-2.74229
H	1.30276	4.81659	-2.79431
H	-0.17199	3.93986	-3.29902
C	-3.91357	-1.53484	-0.78983
H	-3.40296	-1.73096	-1.73792
C	-5.29298	-1.76808	-0.72231
H	-5.82136	-2.16710	-1.59519
C	-5.99685	-1.48081	0.45319
H	-7.07516	-1.66332	0.51306
C	-5.30780	-0.93694	1.54312
H	-5.84796	-0.67924	2.46083
C	-3.92813	-0.70752	1.45999
H	-3.43251	-0.23776	2.31453
C	-3.18246	-1.02553	0.30544
O	2.13451	1.02879	-1.81971
H	1.60149	0.93113	-2.62330

[$L_1Co^{II}OH$] (*S* =3/2)

75
h_u3.gjf.log Energy: -1796820.1033728

C	0.43989	-0.74389	1.45798
N	0.86833	-1.53577	2.47678
C	-0.14757	-2.40466	2.86599
C	-1.22205	-2.12262	2.07163
N	-0.86271	-1.07991	1.23138
B	-1.65315	-0.48596	-0.01096
N	-1.49852	1.09133	-0.00032
C	-0.29623	1.73014	0.00015
N	-0.56421	3.06084	0.00591
C	-1.94242	3.26947	0.00974
C	-2.52016	2.03271	0.00478
N	-0.85996	-1.05617	-1.25862
C	0.44575	-0.71914	-1.47298
N	0.87207	-1.48960	-2.50915
C	-0.14597	-2.34580	-2.92028
C	-1.22171	-2.07752	-2.12374
Co	1.26504	0.45227	0.00916
O	3.08409	0.94153	-0.11155
C	2.25279	-1.47086	3.03910
C	2.36269	-2.40190	4.25281
C	3.25014	-1.90051	1.94931
C	2.53327	-0.02040	3.46711
C	0.50782	4.10184	0.03409
C	-0.12278	5.49838	-0.01500
C	1.30798	3.93051	1.33691
C	1.42726	3.89436	-1.18230
C	2.26624	-1.44499	-3.04838
C	2.61710	0.01566	-3.37885
C	3.21651	-1.99266	-1.97050
C	2.35810	-2.30130	-4.31779
H	3.37452	-2.31316	4.67858
H	1.63989	-2.13306	5.04110
H	2.98291	-2.89058	1.54324
H	4.26561	-1.96113	2.37598
H	3.26545	-1.16243	1.13174
H	1.79463	0.32006	4.21197
H	2.49132	0.64824	2.59375
H	3.54022	0.05192	3.91042
H	-0.77509	5.68564	0.85402
H	-0.70752	5.64804	-0.93783
H	0.67966	6.25265	0.00091
H	0.65204	4.03420	2.21751
H	2.10298	4.69211	1.39785
H	0.84414	3.91586	-2.11836
H	2.17949	4.70019	-1.22126
H	1.95683	2.93080	-1.10650
H	3.62047	0.05960	-3.83490
H	1.89033	0.43690	-4.09402
H	4.25015	-2.01496	-2.35502
H	3.19360	-1.34575	-1.08117
H	1.65607	-1.95443	-5.09447
H	2.16391	-3.36708	-4.11275
H	3.37854	-2.22384	-4.72495
H	2.21049	-3.45790	3.97461
H	2.92892	-3.01809	-1.68212
H	1.77719	2.93451	1.36237
C	-3.24116	-0.80203	-0.01245
C	-3.98377	-0.84664	1.18692
C	-5.37935	-0.96656	1.19563

C	-6.08661	-1.02882	-0.01058
C	-5.38250	-0.94601	-1.21742
C	-3.98692	-0.82607	-1.21044
H	-3.46789	-0.75736	2.14789
H	-5.91669	-1.00140	2.14973
H	-7.17770	-1.12437	-0.00996
H	-5.92238	-0.96457	-2.17054
H	-3.47362	-0.71998	-2.17104
H	-0.04533	-3.13816	3.65998
H	-2.20133	-2.59336	2.04771
H	-2.40420	4.25225	0.01374
H	-3.57228	1.75990	0.00327
H	-0.04383	-3.06069	-3.73106
H	-2.20335	-2.54367	-2.11405
H	2.62906	0.62909	-2.46518
H	3.41201	1.53483	0.58101

[$L_1Co^{II}OH$] (*S* =5/2)

75

h_u5.gjf.log Energy: -1796739.7126202

C	0.36120	-0.87529	1.38962
N	0.79314	-1.93162	2.16174
C	-0.22357	-2.87279	2.27154
C	-1.29373	-2.38778	1.57702
N	-0.94956	-1.14561	1.06362
B	-1.69596	-0.37892	-0.09594
N	-1.50874	1.18241	0.16037
C	-0.29608	1.77827	0.25193
N	-0.51457	3.11487	0.36096
C	-1.88295	3.36299	0.34096
C	-2.49680	2.14765	0.20779
N	-0.91107	-0.72432	-1.39015
C	0.42838	-0.26976	-1.58845
N	0.95477	-1.08526	-2.63560
C	0.04222	-2.08643	-2.90464
C	-1.07878	-1.86652	-2.14565
Co	1.24745	0.44657	0.08747
O	3.00077	0.93353	0.33465
C	2.14321	-2.01516	2.78581
C	2.17833	-3.16981	3.79659
C	3.19574	-2.25237	1.68815
C	2.42873	-0.68902	3.51267
C	0.57984	4.12380	0.50896
C	-0.01605	5.53632	0.53478
C	1.31341	3.84158	1.83081
C	1.53991	3.98467	-0.68499
C	2.35809	-1.04872	-3.08750
C	2.81495	0.41905	-3.16586
C	3.23739	-1.82113	-2.08302
C	2.46753	-1.68850	-4.48113
H	3.16268	-3.18090	4.29064
H	1.40785	-3.05156	4.57659
H	2.93721	-3.13801	1.08410
H	4.18570	-2.41835	2.14553
H	3.26794	-1.37383	1.03025
H	1.66203	-0.49041	4.28010

```
H          2.43549        0.14585        2.79697
H          3.41543       -0.73469        4.00274
H         -0.69675        5.68067        1.38976
H         -0.55873        5.76555       -0.39713
H          0.80382        6.26469        0.63487
H          0.62290        3.92130        2.68680
H          2.13444        4.56349        1.97168
H          0.99409        4.09237       -1.63697
H          2.31251        4.76951       -0.63283
H          2.04474        3.00676       -0.67197
H          3.84208        0.46510       -3.56449
H          2.15298        0.99780       -3.83117
H          4.29678       -1.79698       -2.38935
H          3.15347       -1.36857       -1.08412
H          1.78361       -1.19959       -5.19515
H          2.24406       -2.76772       -4.46240
H          3.49815       -1.57547       -4.85417
H          2.04279       -4.14888        3.30818
H          2.91536       -2.87445       -2.01583
H          1.73992        2.82686        1.82323
C         -3.27681       -0.69644       -0.16666
C         -4.04448       -0.84045        1.00957
C         -5.43529       -0.99913        0.97274
C         -6.10860       -1.00741       -0.25556
C         -5.37573       -0.84166       -1.43773
C         -3.98509       -0.68179       -1.38631
H         -3.54429       -0.81492        1.98399
H         -5.99721       -1.11106        1.90677
H         -7.19632       -1.13176       -0.29042
H         -5.89085       -0.82967       -2.40479
H         -3.43866       -0.52618       -2.32233
H         -0.13079       -3.79343        2.83996
H         -2.27259       -2.83434        1.41808
H         -2.31469        4.35557        0.42435
H         -3.55449        1.90331        0.14386
H          0.22213       -2.87326       -3.63387
H         -1.99325       -2.45691       -2.10859
H          2.81592        0.89010       -2.17157
H          3.24390        1.48940        1.09203
```

2. Thermodynamic cycle for the $L_0Co^{III}O$ oxidant

[$L_0Co^{III}O$] (*S* =0)

```
80
o_u0.out Energy: -1900520.4231349
B          1.71929        0.08420       -0.21147
Co        -1.42708        0.00194        0.08267
O         -2.99589        0.02935       -0.48297
C         -2.05817        3.50218       -0.97355
C         -2.00794        5.01293       -1.26976
C         -2.90555        2.80467       -2.06375
C         -2.73867        3.31493        0.40409
C         -1.44925       -0.58937        3.73044
C         -1.26328       -0.51053        5.25738
C         -2.47546        0.49268        3.32166
```

C	-2.00664	-1.98298	3.35391
C	-1.96217	-3.14613	-1.82177
C	-2.66320	-3.32119	-0.45312
C	-2.81693	-2.22124	-2.72016
C	-1.86726	-4.53576	-2.47977
H	-3.03512	5.40973	-1.21597
H	-1.40602	5.56634	-0.53058
H	-2.42557	2.90158	-3.05375
H	-3.90303	3.27678	-2.11956
H	-3.03152	1.73784	-1.81274
H	-2.13734	3.77362	1.20827
H	-2.87822	2.24680	0.62355
H	-3.73131	3.79802	0.39636
H	-0.81724	0.44881	5.56857
H	-0.65246	-1.33380	5.65659
H	-2.25286	-0.58526	5.73776
H	-2.08412	1.50590	3.51450
H	-3.40587	0.36205	3.90040
H	-1.30001	-2.78197	3.63793
H	-2.96434	-2.16730	3.87156
H	-2.17927	-2.04633	2.26710
H	-3.63990	-3.81512	-0.59723
H	-2.05725	-3.94589	0.22580
H	-3.80020	-2.68896	-2.90868
H	-2.97466	-1.25479	-2.21165
H	-1.25772	-5.23951	-1.88965
H	-1.47574	-4.49625	-3.50745
H	-2.88367	-4.95826	-2.54175
H	-1.63182	5.23771	-2.27924
H	-2.32369	-2.05719	-3.69467
H	-2.73042	0.41980	2.25232
C	3.27946	0.15642	-0.55077
C	4.32105	0.10550	0.39444
C	5.66650	0.18852	0.00536
C	6.00404	0.32642	-1.34448
C	4.98374	0.38213	-2.30447
C	3.64667	0.29846	-1.90759
H	4.07820	-0.00318	1.45323
H	6.45442	0.14494	0.76559
H	7.05420	0.39098	-1.64966
H	5.23361	0.49135	-3.36564
H	2.86565	0.34424	-2.67385
H	-2.83929	-2.34204	0.01524
C	-0.69639	2.81025	-0.92506
C	-0.62074	-2.45299	-1.58359
C	-0.17694	-0.37631	2.91555
N	0.93385	1.37387	-0.65366
N	0.96879	-1.08145	-0.95990
N	1.23409	-0.11420	1.27207
C	-0.11382	-0.15439	1.53095
C	-0.38786	-1.26470	-0.86461
C	-0.42591	1.48937	-0.51999
N	1.98905	-0.30061	2.33607
N	1.51768	2.46201	-1.10756
N	1.58245	-2.01005	-1.66039
C	1.72382	-0.71946	4.64437
H	1.44065	0.06624	5.35682
H	1.39971	-1.69849	5.02333
H	2.81313	-0.72083	4.51223

C	0.93274	4.62791	-1.81533
H	0.42169	4.82078	-2.76771
H	0.70688	5.43138	-1.10285
H	2.01598	4.57866	-1.98313
C	1.06157	-3.95400	-2.87689
H	0.85135	-4.91266	-2.38618
H	0.56419	-3.91973	-3.85506
H	2.14446	-3.83913	-3.01148
N	1.13493	-0.46421	3.33207
N	0.53443	3.32839	-1.27673
N	0.62442	-2.83582	-2.04241

[$L_0Co^{III}O$] (*S* =1)

80
o_u2.out Energy: -1900514.0970237

B	1.63671	0.08692	-0.19947
Co	-1.43732	0.02426	0.14109
O	-3.00488	0.08020	-0.40525
C	-2.01359	3.66726	-0.97412
C	-1.89974	5.19163	-1.16106
C	-2.81899	3.05168	-2.14339
C	-2.77200	3.39556	0.34656
C	-1.45338	-0.64781	3.79259
C	-1.25208	-0.58920	5.31798
C	-2.48547	0.43611	3.40296
C	-2.00815	-2.03668	3.39448
C	-1.94839	-3.27256	-1.80263
C	-2.71313	-3.33259	-0.45925
C	-2.75806	-2.40440	-2.79536
C	-1.81807	-4.70630	-2.34883
H	-2.90625	5.63399	-1.07648
H	-1.26827	5.65574	-0.38447
H	-2.29647	3.19482	-3.10557
H	-3.81070	3.53316	-2.21638
H	-2.96014	1.97335	-1.96006
H	-2.20032	3.76392	1.21602
H	-2.95651	2.31711	0.46598
H	-3.74529	3.91623	0.32656
H	-0.80155	0.36603	5.63569
H	-0.63508	-1.41703	5.69797
H	-2.23548	-0.67131	5.80973
H	-2.09913	1.44777	3.61285
H	-3.41472	0.29069	3.97970
H	-1.29822	-2.83874	3.66072
H	-2.96301	-2.23294	3.91284
H	-2.18491	-2.08034	2.30673
H	-3.68240	-3.83950	-0.60866
H	-2.14173	-3.89616	0.29846
H	-3.74511	-2.86349	-2.98400
H	-2.90934	-1.40149	-2.36261
H	-1.19080	-5.33995	-1.69925
H	-1.41563	-4.73913	-3.37253
H	-2.82120	-5.16264	-2.38582
H	-1.51071	5.47432	-2.15083
H	-2.23237	-2.31120	-3.76190
H	-2.74386	0.38328	2.33268
C	3.19784	0.17727	-0.54692

```
C          4.23204        0.24991        0.40545
C          5.57603        0.37403        0.02181
C          5.92154        0.43202       -1.33146
C          4.90921        0.36865       -2.29935
C          3.57387        0.24544       -1.90747
H          3.98663        0.20463        1.46799
H          6.35602        0.42595        0.78970
H          6.97034        0.52813       -1.63310
H          5.16369        0.41760       -3.36396
H          2.80153        0.20295       -2.68162
H         -2.90723       -2.31647       -0.08284
C         -0.67814        2.93510       -0.90652
C         -0.62187       -2.56159       -1.55768
C         -0.18984       -0.41591        2.97239
N          0.86680        1.41170       -0.62834
N          0.89866       -1.11691       -0.93849
N          1.18297       -0.11821        1.29590
C         -0.15427       -0.15271        1.59926
C         -0.44195       -1.39920       -0.80318
C         -0.47504        1.63850       -0.42672
N          1.96120       -0.35165        2.33764
N          1.49069        2.43095       -1.19006
N          1.54262       -1.98554       -1.69546
C          1.74175       -0.83499        4.64121
H          1.48241       -0.06551        5.38017
H          1.40907       -1.81965        4.99807
H          2.82826       -0.84859        4.48859
C          0.98637        4.58543       -2.01202
H          0.41699        4.74789       -2.93768
H          0.85186        5.44252       -1.33902
H          2.05087        4.46780       -2.25135
C          1.07964       -3.92079       -2.96474
H          0.94014       -4.90270       -2.49369
H          0.53228       -3.88506       -3.91673
H          2.14772       -3.74854       -3.14852
N          1.13064       -0.53397        3.34921
N          0.55635        3.34780       -1.36596
N          0.62289       -2.85320       -2.07825
```

[$L_0Co^{III}O$] (*S* =2)

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80
o_u4.out Energy: -1900510.1392336
B          1.53463        0.16623       -0.23323
Co        -1.62039        0.19640        0.16104
O         -3.30322        0.12875       -0.00862
C         -1.98376        3.77219       -1.32506
C         -1.86473        5.22659       -1.81072
C         -2.82374        2.96005       -2.34029
C         -2.71451        3.75886        0.03987
C         -1.31423       -0.91227        3.93691
C         -0.98663       -0.63164        5.42016
C         -2.52055       -0.03261        3.54348
C         -1.69553       -2.39977        3.74619
C         -2.08487       -3.10507       -1.83388
C         -2.67996       -3.37188       -0.42871
C         -3.00829       -2.11872       -2.58747
C         -2.03067       -4.42942       -2.61461
```

H	-2.87584	5.66115	-1.87913
H	-1.28632	5.85321	-1.11252
H	-2.32194	2.91192	-3.32228
H	-3.81104	3.43494	-2.47969
H	-2.97797	1.93511	-1.96510
H	-2.12242	4.27804	0.81318
H	-2.89842	2.72241	0.36634
H	-3.68879	4.27021	-0.05181
H	-0.57133	0.38175	5.55487
H	-0.28313	-1.35817	5.85182
H	-1.91359	-0.69734	6.01372
H	-2.27343	1.03875	3.63544
H	-3.36784	-0.25194	4.21512
H	-0.85838	-3.07181	4.00233
H	-2.55114	-2.66167	4.39270
H	-1.97892	-2.58993	2.69719
H	-3.67084	-3.85032	-0.52292
H	-2.02773	-4.04169	0.15849
H	-4.00312	-2.57586	-2.73323
H	-3.13261	-1.19240	-2.00414
H	-1.44430	-5.20291	-2.09422
H	-1.62474	-4.29805	-3.63069
H	-3.05694	-4.81836	-2.72121
H	-1.41263	5.30014	-2.81234
H	-2.59436	-1.87209	-3.58073
H	-2.84837	-0.21004	2.50738
C	3.11729	0.29119	-0.47134
C	3.97020	0.84362	0.50606
C	5.32897	1.07133	0.25594
C	5.87632	0.75896	-0.99397
C	5.04665	0.22815	-1.98886
C	3.68953	0.00452	-1.72797
H	3.56896	1.10505	1.48862
H	5.96253	1.49860	1.04122
H	6.93932	0.93355	-1.19321
H	5.45743	-0.01041	-2.97628
H	3.06332	-0.40342	-2.52552
H	-2.80421	-2.42276	0.11780
C	-0.65696	3.04116	-1.14525
C	-0.73785	-2.41727	-1.63198
C	-0.15723	-0.60033	2.99818
N	0.81939	1.50298	-0.68440
N	0.80392	-1.00755	-1.00838
N	1.08259	-0.11162	1.27039
C	-0.22799	-0.10110	1.69847
C	-0.55870	-1.18461	-0.99981
C	-0.52971	1.74620	-0.64336
N	1.92089	-0.59208	2.16543
N	1.52165	2.51727	-1.16150
N	1.46376	-2.00935	-1.56167
C	1.86102	-1.45765	4.36978
H	1.86343	-0.74403	5.20598
H	1.36752	-2.38963	4.67869
H	2.89296	-1.67269	4.06428
C	1.14938	4.69008	-2.00870
H	0.73548	4.85852	-3.01197
H	0.90299	5.54072	-1.35978
H	2.23913	4.57928	-2.07389
C	1.00452	-4.07319	-2.61206

H	0.71853	-4.96333	-2.03597
H	0.59262	-4.14257	-3.62743
H	2.09849	-4.00386	-2.66192
N	1.17511	-0.88938	3.21350
N	0.62663	3.44747	-1.44467
N	0.52956	-2.86099	-1.94814

[$L_0Co^{III}OH]^+$ (*S* =0)

81
p_u0.out Energy: -1900834.0174341

C	0.50101	1.25289	-0.89182
N	-0.78714	1.47521	-0.49051
B	-1.58094	0.46058	0.41605
N	-1.49015	-0.88917	-0.38732
C	-0.29335	-1.43334	-0.76030
N	-0.54953	0.20253	1.59010
C	0.74943	-0.16824	1.31396
Co	1.26503	-0.42231	-0.53843
O	2.00366	-0.72592	-2.16425
C	2.25403	2.88478	-2.06483
C	2.57113	4.37275	-1.78167
C	3.37657	2.05113	-1.40806
C	2.25539	2.62636	-3.58850
C	0.29494	-3.83764	-1.72856
C	-0.25610	-5.23693	-1.36761
C	0.47455	-3.72336	-3.25910
C	1.67187	-3.69719	-1.03923
C	2.78490	-0.60043	2.93971
C	3.56213	-0.93348	1.65191
C	3.45920	0.62968	3.59244
C	2.85885	-1.82588	3.87879
H	3.63056	4.55785	-2.02126
H	1.98634	5.06893	-2.39793
H	3.33773	2.13105	-0.30727
H	4.35633	2.42925	-1.74272
H	3.30367	0.99406	-1.69620
H	1.46130	3.19555	-4.10087
H	2.10386	1.55469	-3.79300
H	3.22412	2.92928	-4.02153
H	-1.11187	-5.53950	-1.98657
H	-0.54491	-5.29952	-0.30469
H	0.53592	-5.98250	-1.54328
H	-0.49092	-3.79933	-3.78785
H	1.12771	-4.53449	-3.62424
H	1.56529	-3.66198	0.05897
H	2.29940	-4.56698	-1.29404
H	2.19405	-2.79516	-1.38445
H	4.60605	-1.18294	1.90236
H	3.13114	-1.80411	1.13147
H	4.51811	0.40366	3.80269
H	3.41937	1.50008	2.91640
H	2.34974	-2.69539	3.42989
H	2.40983	-1.63415	4.86461
H	3.91405	-2.09704	4.04974
H	2.41972	4.62467	-0.71826
H	2.99082	0.91755	4.54622

H	0.94115	-2.75932	-3.51402
C	-3.07153	0.92748	0.72367
C	-3.93214	1.10663	-0.38262
C	-5.25381	1.53052	-0.22385
C	-5.75608	1.78958	1.05881
C	-4.92320	1.61971	2.16901
C	-3.59749	1.19415	2.00171
H	-3.56038	0.91176	-1.39429
H	-5.89543	1.66069	-1.10199
H	-6.79129	2.12266	1.18922
H	-5.30481	1.81975	3.17614
H	-2.96494	1.06838	2.88205
H	3.59178	-0.07184	0.96406
H	1.43922	-0.56578	-2.93749
C	-0.61216	-2.70933	-1.24603
C	1.34511	-0.27662	2.57381
C	0.90666	2.45703	-1.48700
C	0.32665	0.00780	4.93413
H	-0.55341	0.57445	5.26393
H	0.25499	-1.02859	5.29641
H	1.23537	0.47674	5.32902
C	-2.94167	-3.78340	-1.60040
H	-2.69803	-4.11018	-2.61985
H	-2.92690	-4.64108	-0.91457
H	-3.93576	-3.31888	-1.58994
C	-0.48222	4.59552	-1.94684
H	0.01334	5.35277	-1.32440
H	-0.13079	4.66995	-2.98414
H	-1.56884	4.74444	-1.91433
N	-2.51315	-1.67089	-0.63719
N	-1.23182	2.66456	-0.81716
N	-0.79670	0.31484	2.87349
N	0.34059	0.02779	3.47309
N	-1.99151	-2.75946	-1.16653
N	-0.22347	3.25272	-1.42750

[$L_0Co^{III}OH]^+$ (*S* =1)

81
p_u2.out Energy: -1900823.7042469

C	0.61890	1.34444	-0.85929
N	-0.71670	1.45603	-0.55631
B	-1.52357	0.42073	0.34638
N	-1.44415	-0.99614	-0.36878
C	-0.27383	-1.65545	-0.64640
N	-0.51370	0.22033	1.54680
C	0.77727	-0.16322	1.29086
Co	1.31139	-0.45768	-0.56744
O	1.88501	-0.75504	-2.24784
C	2.30100	3.05616	-1.95968
C	2.60331	4.48981	-1.46417
C	3.40752	2.13077	-1.40951
C	2.32732	3.01163	-3.50476
C	0.19437	-4.03247	-1.66081
C	-0.31443	-5.41647	-1.20023
C	0.23396	-3.95044	-3.20495
C	1.62817	-3.84391	-1.11896
C	2.81490	-0.59367	2.89717

C	3.54417	-0.99714	1.60032
C	3.53166	0.64303	3.48731
C	2.87868	-1.78264	3.88188
H	3.65046	4.73955	-1.70171
H	1.97785	5.25461	-1.94583
H	3.40479	2.12444	-0.30615
H	4.39141	2.49261	-1.74975
H	3.28545	1.09491	-1.75838
H	1.55387	3.65628	-3.95345
H	2.16429	1.98511	-3.87398
H	3.30768	3.35566	-3.87535
H	-1.24881	-5.71990	-1.69355
H	-0.46883	-5.44403	-0.10804
H	0.43988	-6.17933	-1.45410
H	-0.76827	-4.06828	-3.65053
H	0.87855	-4.75009	-3.60857
H	1.63722	-3.80026	-0.01652
H	2.25278	-4.69590	-1.43463
H	2.08321	-2.92628	-1.51819
H	4.58146	-1.29054	1.82926
H	3.05771	-1.85904	1.11173
H	4.59044	0.40126	3.67996
H	3.49291	1.49003	2.78213
H	2.33986	-2.65677	3.47933
H	2.45546	-1.53903	4.86771
H	3.93064	-2.07158	4.04245
H	2.47515	4.56861	-0.37139
H	3.09158	0.97251	4.44153
H	0.64402	-2.97574	-3.51646
C	-3.02137	0.89102	0.62099
C	-3.86867	1.05769	-0.49751
C	-5.19568	1.47090	-0.35887
C	-5.71835	1.73187	0.91546
C	-4.89947	1.57424	2.03742
C	-3.56784	1.15885	1.88996
H	-3.48190	0.86056	-1.50279
H	-5.82619	1.59075	-1.24651
H	-6.75820	2.05634	1.02983
H	-5.29627	1.77528	3.03849
H	-2.94809	1.04267	2.78069
H	3.60212	-0.15103	0.89311
H	1.69815	-0.03658	-2.87364
C	-0.66955	-2.89422	-1.14218
C	1.37793	-0.25047	2.54521
C	0.95314	2.56009	-1.45310
C	0.37588	0.12315	4.89499
H	-0.49956	0.70406	5.21193
H	0.30654	-0.89894	5.29584
H	1.29026	0.60524	5.26086
C	-3.03905	-3.84055	-1.54313
H	-2.78690	-4.22858	-2.53897
H	-3.07715	-4.66575	-0.81793
H	-4.01178	-3.33393	-1.57915
C	-0.53505	4.60590	-1.98998
H	-0.17526	5.37215	-1.28838
H	-0.06568	4.74717	-2.97185
H	-1.62560	4.67860	-2.08824
N	-2.51223	-1.70803	-0.65431
N	-1.22978	2.60781	-0.92978

N	-0.76018	0.36508	2.82815
N	0.37666	0.08954	3.43423
N	-2.04916	-2.84801	-1.13069
N	-0.23349	3.26979	-1.47987

[$L_0Co^{III}OH]^+$ (*S* =2)

81
p_u4.out Energy: -1900808.5216804

C	0.57897	1.26366	-0.98169
N	-0.67222	1.49242	-0.46558
B	-1.44529	0.45953	0.45304
N	-1.40383	-0.90486	-0.36062
C	-0.27130	-1.54301	-0.78966
N	-0.43443	0.25469	1.66381
C	0.84643	-0.23668	1.55647
Co	1.43165	-0.53319	-0.39013
O	3.14439	-0.71176	-0.92968
C	2.20243	2.71747	-2.40593
C	2.24972	4.06137	-3.15469
C	3.35572	2.67950	-1.37416
C	2.39334	1.58144	-3.43907
C	0.13684	-3.68050	-2.21573
C	-0.57520	-5.00757	-2.54013
C	0.61386	-3.01429	-3.52926
C	1.36402	-4.00178	-1.33103
C	2.73764	-0.55104	3.36479
C	3.40898	-1.47295	2.32728
C	3.58694	0.73264	3.51905
C	2.67078	-1.31627	4.70651
H	3.21058	4.12735	-3.69062
H	1.45031	4.14988	-3.90727
H	3.22173	3.45977	-0.60559
H	4.31807	2.86029	-1.88369
H	3.40807	1.69586	-0.88285
H	1.57863	1.58205	-4.18286
H	2.41531	0.60042	-2.94314
H	3.34970	1.71751	-3.97212
H	-1.37341	-4.89026	-3.28739
H	-0.99625	-5.47835	-1.63646
H	0.16102	-5.70825	-2.96621
H	-0.23821	-2.76294	-4.18323
H	1.28079	-3.69959	-4.07983
H	1.05581	-4.43811	-0.36636
H	2.01369	-4.72649	-1.84913
H	1.96876	-3.10557	-1.12280
H	4.39683	-1.78657	2.70314
H	2.80433	-2.37844	2.14896
H	4.60081	0.47198	3.86741
H	3.67571	1.25643	2.55255
H	1.96645	-2.16341	4.64947
H	2.38457	-0.67920	5.55522
H	3.66940	-1.72202	4.93724
H	2.20059	4.92532	-2.47471
H	3.15080	1.43408	4.24968
H	1.16821	-2.08425	-3.31764
C	-2.94336	0.78650	0.90789
C	-3.78419	1.72498	0.27921

```
C         -5.12112        1.88684        0.66879
C         -5.65713        1.10464        1.69633
C         -4.84566        0.15166        2.32590
C         -3.51391       -0.00268        1.93160
H         -3.39252        2.34659       -0.52745
H         -5.74653        2.62950        0.16154
H         -6.70109        1.23117        2.00254
H         -5.25381       -0.47583        3.12560
H         -2.90686       -0.76252        2.43381
H          3.56085       -0.97282        1.36037
H          3.37257       -1.17735       -1.75222
C         -0.72787       -2.66714       -1.47660
C          1.35762       -0.16847        2.85273
C          0.90289        2.44301       -1.65438
C          0.27943        0.73763        5.02116
H         -0.59864        1.38079        5.16064
H          0.17230       -0.17294        5.62751
H          1.18615        1.28090        5.31722
C         -3.15734       -3.43881       -1.94949
H         -3.07278       -3.49352       -3.04311
H         -3.09462       -4.44526       -1.51634
H         -4.11399       -2.97648       -1.67601
C         -0.45498        4.64411       -1.89074
H          0.30798        5.32596       -1.49412
H         -0.47718        4.70296       -2.98622
H         -1.43784        4.91508       -1.48563
N         -2.50390       -1.52260       -0.72580
N         -1.12551        2.69657       -0.73902
N         -0.73113        0.64521        2.88149
N          0.34459        0.39608        3.60136
N         -2.10233       -2.58240       -1.40587
N         -0.18159        3.27242       -1.45867
```

[$L_0Co^{II}O]^-$ (*S* =1/2)

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80
r_u1.out Energy: -1900565.4570046
C         -0.52579       -0.77292       -1.35367
N          0.76927       -1.17925       -1.08214
B          1.61075       -0.53487        0.08702
N          1.40835        1.00222       -0.09616
C          0.14442        1.55006       -0.15684
N          0.77488       -0.88919        1.37647
C         -0.52112       -0.43645        1.55444
Co        -1.38617        0.37056       -0.01013
O         -3.05316       -0.10642        0.04816
C         -2.24901       -1.65935       -3.11913
C         -2.22843       -2.31518       -4.51419
C         -3.23893       -2.40047       -2.19014
C         -2.74065       -0.20174       -3.27962
C         -0.65224        4.00604       -0.46629
C         -0.12825        5.43987       -0.65714
C         -1.53758        3.64107       -1.68197
C         -1.51535        3.96472        0.81720
C         -2.24603       -0.93660        3.46407
C         -2.75128        0.51709        3.31198
C         -3.22065       -1.86684        2.70363
C         -2.23200       -1.28552        4.96551
```

H	-3.20603	-2.15006	-4.99823
H	-1.45618	-1.87244	-5.16771
H	-2.90044	-3.43425	-1.99192
H	-4.23876	-2.45389	-2.66151
H	-3.30911	-1.82619	-1.24394
H	-2.02801	0.39703	-3.87443
H	-2.86229	0.25303	-2.28201
H	-3.71613	-0.19600	-3.79942
H	0.46349	5.55026	-1.58016
H	0.47999	5.78094	0.19601
H	-0.98918	6.12510	-0.73812
H	-0.95288	3.67936	-2.61790
H	-2.38237	4.34740	-1.77063
H	-0.91611	4.24390	1.70166
H	-2.36423	4.66699	0.73613
H	-1.90915	2.94691	0.97666
H	-3.72804	0.62369	3.81837
H	-2.04557	1.23504	3.76674
H	-4.22502	-1.82857	3.16696
H	-3.28523	-1.50650	1.65581
H	-1.47165	-0.70541	5.51768
H	-2.06571	-2.35631	5.15840
H	-3.21635	-1.03619	5.39696
H	-2.07543	-3.40457	-4.47733
H	-2.87249	-2.91595	2.73304
H	-1.93858	2.61965	-1.56948
C	3.17811	-0.90105	0.13801
C	3.91766	-1.18317	-1.02910
C	5.30464	-1.37886	-0.99778
C	6.00159	-1.28936	0.21302
C	5.29439	-0.99450	1.38531
C	3.90818	-0.80104	1.34114
H	3.39663	-1.25913	-1.98687
H	5.84435	-1.60046	-1.92579
H	7.08607	-1.44375	0.24258
H	5.82615	-0.91213	2.34029
H	3.37960	-0.57032	2.27008
H	-2.87557	0.74784	2.24070
N	0.17887	-1.82505	3.15273
N	1.78781	3.04379	-0.35922
N	0.16649	-2.47963	-2.60976
C	0.35175	-3.61247	-3.50908
H	-0.45200	-4.34891	-3.36681
H	0.36661	-3.28607	-4.55845
H	1.31618	-4.07107	-3.25469
C	2.66147	4.20167	-0.51011
H	2.48637	4.69990	-1.47361
H	2.50139	4.92023	0.30570
H	3.69372	3.83037	-0.47283
C	0.37196	-2.73036	4.27956
H	0.37243	-2.18185	5.23187
H	-0.41922	-3.49349	4.29788
H	1.34546	-3.21735	4.13733
N	1.19212	-1.73778	2.30438
N	2.39940	1.87729	-0.21516
N	1.18125	-2.21275	-1.80153
C	-0.89740	-1.62515	-2.41445
C	0.41579	2.92518	-0.33446
C	-0.88938	-1.03921	2.77584

[$L_0Co^{II}O$]$^-$ (*S* =3/2)

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80
r_u3.out Energy: -1900568.5119466
C          -0.59741       -0.69970       -1.31376
N           0.72434       -1.03246       -1.05196
B           1.57442       -0.36539        0.10956
N           1.40880        1.19500       -0.06601
C           0.19945        1.85566       -0.10787
N           0.75454       -0.78315        1.39906
C          -0.57363       -0.44800        1.56370
Co         -1.40047        0.62788        0.04813
O          -3.06435        1.15524        0.10774
C          -2.37296       -1.89311       -2.82348
C          -2.37035       -2.45794       -4.26124
C          -3.13290       -2.85710       -1.88120
C          -3.10987       -0.53601       -2.84638
C          -0.42764        4.31894       -0.55423
C           0.19337        5.71775       -0.70341
C          -1.25654        3.98431       -1.81906
C          -1.38779        4.31873        0.65983
C          -2.36301       -1.20268        3.26874
C          -2.80246        0.26476        3.49033
C          -3.28858       -1.81527        2.18760
C          -2.52280       -1.98101        4.58541
H          -3.39236       -2.40537       -4.67368
H          -1.71093       -1.86911       -4.92234
H          -2.64005       -3.84418       -1.82859
H          -4.16837       -3.01219       -2.23411
H          -3.16869       -2.43655       -0.86274
H          -2.58032        0.18035       -3.49922
H          -3.18466       -0.08037       -1.84228
H          -4.12732       -0.68116       -3.25270
H           0.82696        5.80534       -1.60060
H           0.79078        6.00194        0.17909
H          -0.61598        6.46063       -0.80464
H          -0.61230        3.92842       -2.71445
H          -2.02265        4.76201       -1.99205
H          -0.83597        4.49475        1.60033
H          -2.13789        5.12258        0.54521
H          -1.91442        3.35000        0.72275
H          -3.82745        0.28964        3.90380
H          -2.13169        0.77699        4.20299
H          -4.32986       -1.85436        2.55688
H          -3.25917       -1.18071        1.28386
H          -1.87870       -1.57936        5.38571
H          -2.31178       -3.05620        4.46943
H          -3.56725       -1.89183        4.92925
H          -2.06304       -3.51316       -4.31376
H          -2.97637       -2.84247        1.92798
H          -1.76313        3.01417       -1.67733
C           3.14143       -0.73996        0.14144
C           3.86875       -1.01902       -1.03348
C           5.25467       -1.22215       -1.01588
C           5.96297       -1.14339        0.18926
C           5.26773       -0.85150        1.36936
```

```
C          3.88225       -0.65058        1.33843
H          3.33990       -1.08379       -1.98791
H          5.78503       -1.44044       -1.95004
H          7.04686       -1.30347        0.20825
H          5.80823       -0.77686        2.32008
H          3.36381       -0.42044        2.27322
H         -2.79948        0.80138        2.52438
N          0.16753       -1.89329        3.08205
N          1.94731        3.18808       -0.44394
N          0.10762       -2.50995       -2.40647
C          0.28886       -3.71315       -3.20849
H         -0.50658       -4.43982       -2.98850
H          0.27837       -3.47391       -4.28195
H          1.26157       -4.14404       -2.93762
C          2.90355        4.26011       -0.69826
H          2.73244        4.70321       -1.68960
H          2.82372        5.04276        0.06858
H          3.90606        3.81433       -0.66497
C          0.39536       -2.83885        4.16958
H          0.21547       -2.36329        5.14347
H         -0.26152       -3.71388        4.06513
H          1.44321       -3.15927        4.10560
N          1.20538       -1.65917        2.29140
N          2.46295        1.98189       -0.26725
N          1.14398       -2.12217       -1.68374
C         -0.97983       -1.67709       -2.24649
C          0.57161        3.18406       -0.35509
C         -0.94826       -1.18142        2.69855
```

[$L_0Co^{II}O]^-$ (*S* =5/2)

```
80
r_u5.out Energy: -1900545.1677284
C         -0.58573       -0.68930       -1.36952
N          0.76944       -0.95441       -1.10474
B          1.58594       -0.26326        0.01551
N          1.44982        1.31024       -0.18350
C          0.26495        1.99145       -0.28231
N          0.78193       -0.61179        1.33276
C         -0.53819       -0.22688        1.54301
Co        -1.38064        0.75727       -0.10270
O         -2.83758        1.63303       -0.03993
C         -2.43091       -2.09708       -2.58845
C         -2.39898       -2.37240       -4.11257
C         -3.04284       -3.30749       -1.84364
C         -3.34476       -0.87914       -2.36092
C         -0.31189        4.50197       -0.53791
C          0.35281        5.87023       -0.76399
C         -1.27333        4.20933       -1.71497
C         -1.14052        4.54397        0.76933
C         -2.41345       -1.18397        3.07752
C         -3.03601        0.22971        3.09452
C         -3.22736       -2.07617        2.11006
C         -2.50329       -1.75401        4.50934
H         -3.42593       -2.51268       -4.49445
H         -1.94928       -1.51857       -4.64795
H         -2.44727       -4.22576       -1.97296
H         -4.06212       -3.51594       -2.21524
```

H	-3.10525	-3.09863	-0.76285
H	-2.95327	0.01092	-2.87930
H	-3.42682	-0.60786	-1.29739
H	-4.35602	-1.09437	-2.74919
H	0.94335	5.89867	-1.69451
H	1.00119	6.16753	0.07564
H	-0.43463	6.63754	-0.85290
H	-0.71934	4.11448	-2.66540
H	-2.00028	5.03488	-1.82028
H	-0.48926	4.70693	1.64618
H	-1.87387	5.36975	0.72660
H	-1.68677	3.59331	0.88934
H	-4.07459	0.17122	3.46686
H	-2.46752	0.89704	3.76571
H	-4.27787	-2.16149	2.44221
H	-3.21134	-1.63958	1.09774
H	-1.82360	-1.22338	5.19821
H	-2.28062	-2.83000	4.55989
H	-3.53171	-1.62393	4.88720
H	-1.82641	-3.27449	-4.37535
H	-2.80292	-3.09382	2.04863
H	-1.82859	3.27714	-1.52040
C	3.15115	-0.64207	0.07555
C	3.87887	-0.94424	-1.09262
C	5.26255	-1.16081	-1.06523
C	5.96444	-1.07673	0.14418
C	5.26519	-0.77209	1.31909
C	3.88171	-0.55661	1.27731
H	3.34374	-1.02725	-2.04302
H	5.79698	-1.39732	-1.99286
H	7.04670	-1.24740	0.17094
H	5.80117	-0.70066	2.27281
H	3.35372	-0.32180	2.20665
H	-3.04811	0.68501	2.09159
N	0.06064	-1.94494	2.82064
N	2.03228	3.31509	-0.39878
N	0.02531	-2.71101	-2.11207
C	0.22913	-3.90301	-2.89587
H	-0.69783	-4.48610	-2.97612
H	0.59781	-3.68056	-3.91952
H	0.98584	-4.52260	-2.38755
C	3.02049	4.38460	-0.49326
H	2.92266	4.92153	-1.44648
H	2.90525	5.09271	0.33907
H	4.00999	3.91288	-0.43779
C	0.16901	-3.08612	3.70968
H	0.10861	-2.78536	4.76753
H	-0.62100	-3.82502	3.50020
H	1.14751	-3.54900	3.52294
N	1.14728	-1.65743	2.08245
N	2.51490	2.09047	-0.25294
N	1.15487	-2.19149	-1.53669
C	-1.03879	-1.79992	-2.05339
C	0.65263	3.32529	-0.42605
C	-0.99089	-1.08707	2.53602

[$L_0Co^{II}OH$] (*S* =1/2)

```
81
h_u1.out Energy: -1900915.7125718
C           0.51273       -0.51705        1.55500
N          -0.75678       -1.00085        1.30450
B          -1.59708       -0.60358        0.02372
N          -1.41247        0.94943       -0.06841
C          -0.16128        1.50858       -0.07271
N          -0.73485       -1.15023       -1.18465
C           0.53414       -0.67822       -1.46058
Co          1.34727        0.36331        0.01464
O           3.09662       -0.33605       -0.08719
C           2.16787       -1.01740        3.52905
C           2.04885       -1.25438        5.04934
C           3.15199       -2.03864        2.91128
C           2.71699        0.41282        3.32906
C           0.65766        3.96451       -0.26096
C           0.13555        5.41046       -0.32182
C           1.55294        3.82529        0.99337
C           1.50490        3.69018       -1.52683
C           2.21573       -1.33678       -3.37570
C           2.77639        0.09722       -3.24156
C           3.22122       -2.32671       -2.74219
C           2.04794       -1.63525       -4.88217
H           2.99967       -0.97069        5.53064
H           1.25078       -0.63733        5.49644
H           2.79076       -3.07248        3.05007
H           4.14696       -1.95644        3.38374
H           3.24706       -1.84729        1.83034
H           2.02631        1.16448        3.74699
H           2.85291        0.64183        2.26272
H           3.69265        0.51447        3.83383
H          -0.46092        5.67481        0.56600
H          -0.46594        5.60147       -1.22407
H           0.99705        6.09817       -0.35390
H           0.97519        4.01842        1.91335
H           2.38933        4.54411        0.94902
H           0.89369        3.79799       -2.43927
H           2.34818        4.40011       -1.58739
H           1.91336        2.66606       -1.51423
H           3.70816        0.18109       -3.82811
H           2.05827        0.84150       -3.62675
H           4.18412       -2.29119       -3.28342
H           3.38861       -2.04128       -1.69038
H           1.22651       -1.04555       -5.32516
H           1.87144       -2.69921       -5.09722
H           2.97796       -1.35903       -5.40665
H           1.86714       -2.30747        5.30785
H           2.84574       -3.36465       -2.78761
H           1.97589        2.81002        1.06835
C          -3.15219       -0.99574        0.09071
C          -3.86164       -0.77541        1.29187
C          -5.24026       -0.99070        1.38703
C          -5.96097       -1.43101        0.26912
C          -5.28556       -1.64234       -0.93741
C          -3.90341       -1.42286       -1.02192
H          -3.32460       -0.42449        2.17827
H          -5.75624       -0.81150        2.33697
H          -7.04071       -1.60304        0.33849
H          -5.83679       -1.97895       -1.82267
```

```
H         -3.39915       -1.59583       -1.97507
H          3.00576        0.32546       -2.19095
H          3.61659       -0.26222        0.72589
C          0.91003       -1.41501       -2.59382
C         -0.41698        2.88559       -0.18609
C          0.85120       -1.13157        2.77093
C         -2.66173        4.16211       -0.37708
H         -2.51796        4.85132        0.46562
H         -2.46288        4.68751       -1.32111
H         -3.69385        3.78929       -0.37499
C         -0.41861       -2.88600        4.18813
H          0.41705       -3.59753        4.24631
H         -0.51316       -2.34696        5.14104
H         -1.34887       -3.42971        3.97950
C         -0.29234       -3.34798       -3.82368
H         -0.43906       -2.92382       -4.82707
H          0.59058       -4.00214       -3.82416
H         -1.17841       -3.92884       -3.53695
N         -1.12555       -2.12847       -1.97898
N         -1.18418       -1.87347        2.19551
N         -2.39646        1.82461       -0.17376
N         -1.79002        2.99839       -0.24542
N         -0.13002       -2.29045       -2.83144
N         -0.21064       -1.95486        3.08378
```

[$L_0Co^{II}OH$] (*S* =3/2)

```
81
h_u3.out Energy: -1900917.9067340
C          0.58182       -0.51305        1.47954
N         -0.74070       -0.84960        1.30254
B         -1.57734       -0.39769        0.02659
N         -1.40954        1.17368       -0.08236
C         -0.21235        1.84483       -0.14870
N         -0.72701       -1.03189       -1.15792
C          0.59212       -0.71701       -1.43019
Co         1.37181        0.59630       -0.04270
O          3.17200        1.17294       -0.11256
C          2.38575       -1.28742        3.15692
C          2.55160       -2.09276        4.45675
C          3.31111       -1.87986        2.06462
C          2.81525        0.17574        3.41957
C          0.40329        4.35001       -0.22674
C         -0.22875        5.73606       -0.43907
C          1.16497        4.33646        1.12084
C          1.41814        4.08503       -1.36537
C          2.32771       -1.86014       -3.02153
C          3.07652       -0.50996       -3.01203
C          3.09895       -2.87077       -2.13964
C          2.28130       -2.36373       -4.48096
H          3.59578       -2.00497        4.80014
H          1.90703       -1.71167        5.26569
H          3.00328       -2.90469        1.79422
H          4.35272       -1.91721        2.43007
H          3.28559       -1.24886        1.16019
H          2.15241        0.65957        4.15731
```

H	2.78908	0.75479	2.48295
H	3.84719	0.20018	3.81147
H	-0.89866	6.02533	0.38561
H	-0.78815	5.79350	-1.38725
H	0.57337	6.49145	-0.48461
H	0.47868	4.49748	1.97000
H	1.93079	5.13186	1.13725
H	0.90955	4.02713	-2.34312
H	2.15430	4.90713	-1.40790
H	1.96315	3.14197	-1.19322
H	4.07834	-0.64567	-3.45550
H	2.53455	0.24074	-3.61289
H	4.11957	-3.02546	-2.53187
H	3.17505	-2.49523	-1.10537
H	1.61085	-1.74321	-5.10005
H	1.96531	-3.41357	-4.56708
H	3.29271	-2.30157	-4.91615
H	2.34702	-3.16546	4.31568
H	2.59302	-3.85164	-2.11124
H	1.66722	3.36457	1.25965
C	-3.13919	-0.77220	0.02381
C	-3.89361	-0.85534	1.21138
C	-5.27995	-1.05582	1.19211
C	-5.95826	-1.17002	-0.02662
C	-5.23500	-1.07149	-1.22176
C	-3.85025	-0.87144	-1.19052
H	-3.39038	-0.76386	2.17684
H	-5.83321	-1.11961	2.13586
H	-7.04211	-1.32860	-0.04580
H	-5.75291	-1.14724	-2.18446
H	-3.31190	-0.78955	-2.13884
H	3.20039	-0.10114	-1.99852
H	3.39059	1.89576	0.49491
C	0.95125	-1.65385	-2.40324
C	-0.58481	3.18810	-0.20087
C	0.96951	-1.26303	2.59074
C	-2.93231	4.28811	-0.16536
H	-2.79201	4.93129	0.71436
H	-2.82922	4.88717	-1.07977
H	-3.93082	3.83402	-0.13272
C	-0.36914	-2.94785	4.03864
H	0.29337	-3.81602	3.91991
H	-0.19340	-2.48132	5.01707
H	-1.41497	-3.27252	3.96778
C	-0.37780	-3.61562	-3.44198
H	-0.37556	-3.32426	-4.50187
H	0.40436	-4.36694	-3.26346
H	-1.35655	-4.03555	-3.17689
N	-1.17346	-2.07553	-1.83374
N	-1.17991	-1.73783	2.17698
N	-2.46469	1.97372	-0.08789
N	-1.96383	3.19483	-0.15639
N	-0.15942	-2.45318	-2.58757
N	-0.14502	-1.98486	2.96331

[$L_0Co^{II}OH$] (*S* =5/2)

81

h_u5.out Energy: -1900860.9076644

C	0.54929	-0.47076	1.44066
N	-0.78382	-0.78280	1.28187
B	-1.62022	-0.36979	-0.02044
N	-1.45538	1.22045	-0.11092
C	-0.26341	1.88499	-0.21979
N	-0.81056	-0.96318	-1.18378
C	0.54794	-0.68369	-1.42868
Co	1.32532	0.61402	-0.12453
O	3.00434	1.32360	0.03115
C	2.40136	-1.33029	3.04238
C	2.58964	-2.23683	4.27147
C	3.32930	-1.82833	1.90760
C	2.80956	0.11007	3.43124
C	0.36431	4.40079	-0.35748
C	-0.27801	5.76620	-0.66033
C	1.08717	4.47102	1.00920
C	1.40289	4.09496	-1.46284
C	2.40367	-1.89939	-2.82258
C	3.31876	-0.73993	-2.39454
C	3.00723	-3.21647	-2.27953
C	2.36349	-1.91862	-4.37090
H	3.63788	-2.16569	4.60583
H	1.95476	-1.92846	5.11734
H	3.02876	-2.83156	1.56006
H	4.37145	-1.88441	2.26784
H	3.30156	-1.13746	1.05088
H	2.15990	0.50371	4.23136
H	2.73668	0.77909	2.56104
H	3.85274	0.12420	3.79174
H	-0.95283	6.10464	0.14031
H	-0.83096	5.75838	-1.61387
H	0.52069	6.52095	-0.74908
H	0.37585	4.67755	1.82692
H	1.84852	5.27019	1.00012
H	0.91329	3.98800	-2.44566
H	2.13093	4.92201	-1.52730
H	1.95754	3.16960	-1.24357
H	4.31172	-0.85491	-2.86173
H	2.90381	0.23429	-2.69943
H	4.02844	-3.35916	-2.67395
H	3.06358	-3.18258	-1.17809
H	1.93037	-0.97976	-4.75593
H	1.77494	-2.75431	-4.77646
H	3.38829	-2.01212	-4.77051
H	2.39299	-3.29622	4.04601
H	2.41319	-4.10060	-2.56039
H	1.58899	3.51382	1.22568
C	-3.18007	-0.73695	0.05777
C	-3.89702	-0.58795	1.26293
C	-5.27951	-0.79609	1.32936
C	-5.99129	-1.15509	0.17741
C	-5.30420	-1.29838	-1.03386
C	-3.91982	-1.08944	-1.08834
H	-3.36383	-0.30218	2.17485
H	-5.80510	-0.67516	2.28340
H	-7.07345	-1.32031	0.22406
H	-5.84941	-1.57554	-1.94334
H	-3.39552	-1.21991	-2.03866

```
H          3.46178       -0.71125       -1.30479
H          3.12591        1.97807        0.73850
C          1.01413       -1.69422       -2.24813
C         -0.61386        3.23254       -0.29430
C          0.97850       -1.27747        2.49246
C         -2.95670        4.34321       -0.21056
H         -2.78337        5.00188        0.65151
H         -2.88878        4.92278       -1.14037
H         -3.95262        3.88932       -0.13113
C         -0.32869       -3.03599        3.88534
H          0.32394       -3.90049        3.70051
H         -0.13306       -2.63402        4.88856
H         -1.37779       -3.35093        3.81652
C         -0.26841       -3.61661       -3.40409
H         -0.65907       -3.19688       -4.35468
H          0.65178       -4.17701       -3.61381
H         -1.01804       -4.31928       -3.00591
N         -1.19054       -2.14962       -1.76807
N         -1.19396       -1.71376        2.12321
N         -2.49464        2.02683       -0.11168
N         -1.99083        3.24689       -0.21430
N         -0.03737       -2.59907       -2.40800
N         -0.12887       -2.01115        2.86624
```

3. Thermodynamic cycle for the $L_2Co^{III}O$ oxidant

[$L_2Co^{III}O$] (*S* =0)

```
80
o_u0.out Energy: -2143626.4757109
C         -0.26240        1.53744       -0.42487
N         -0.67666        2.76224       -0.87604
C          0.33713        3.30200       -1.66631
C          1.41193        2.42934       -1.60629
N          1.04679        1.39308       -0.77319
B          1.81034        0.06942       -0.36714
N          1.40682       -0.22949        1.13361
C          0.09631       -0.29052        1.48394
N          0.03018       -0.54467        2.82421
C          1.32878       -0.66381        3.31801
C          2.19042       -0.45766        2.24981
N          1.04263       -0.99067       -1.25334
C         -0.27114       -1.24486       -0.99646
N         -0.69498       -2.18287       -1.90101
C          0.32283       -2.38177       -2.83254
C          1.40546       -1.61795       -2.42644
Co        -1.23481       -0.01759        0.10032
O         -2.73257        0.13779       -0.57752
C         -1.99251        3.46506       -0.56442
C         -1.74798        4.98228       -0.47242
C         -2.98075        3.12148       -1.68518
C         -2.50902        2.99979        0.80427
C         -1.26942       -0.77510        3.57063
C         -1.05956       -0.69178        5.08681
C         -2.27081        0.31111        3.15488
C         -1.77445       -2.17093        3.17955
C         -2.03365       -2.91220       -1.91199
```

C	-2.53954	-3.06901	-0.47065
C	-3.00587	-2.09201	-2.76830
C	-1.84200	-4.32753	-2.48601
H	-2.66022	5.44811	-0.06972
H	-0.91669	5.21520	0.21367
H	-2.60302	3.46557	-2.66309
H	-3.94226	3.62511	-1.49224
H	-3.14008	2.03144	-1.70770
H	-1.72876	3.10312	1.57604
H	-2.85796	1.96369	0.77330
H	-3.35998	3.63889	1.08648
H	-0.59485	0.26111	5.38734
H	-0.46472	-1.52785	5.47930
H	-2.04903	-0.74797	5.56606
H	-1.84796	1.31712	3.29993
H	-3.17673	0.21814	3.77383
H	-1.05295	-2.94970	3.47694
H	-2.73422	-2.37324	3.68152
H	-1.93146	-2.23230	2.09362
H	-3.42819	-3.71898	-0.48686
H	-1.77483	-3.54844	0.16196
H	-3.98058	-2.60588	-2.80652
H	-3.13755	-1.09481	-2.31792
H	-1.01433	-4.85903	-1.98750
H	-1.67756	-4.33737	-3.57058
H	-2.76705	-4.89454	-2.30136
H	-1.55635	5.45292	-1.44461
H	-2.62995	-1.99151	-3.80077
H	-2.58367	0.20256	2.10614
C	3.40075	0.08995	-0.47429
C	4.13304	1.25947	-0.18516
C	5.52954	1.25908	-0.15188
C	6.23297	0.07253	-0.38692
C	5.52969	-1.11181	-0.63299
C	4.13315	-1.09956	-0.66349
H	3.60891	2.19272	0.04478
H	6.07001	2.18491	0.06943
H	7.32758	0.06721	-0.36038
H	6.07030	-2.05060	-0.79000
H	3.60908	-2.04868	-0.81485
H	-2.83504	-2.10927	-0.03330
C	0.29401	4.44613	-2.50374
N	0.33863	5.34227	-3.24547
C	2.59207	2.53146	-2.39101
N	3.50461	2.66259	-3.10067
C	2.59163	-1.42042	-3.18339
N	3.50794	-1.27690	-3.88578
C	0.28863	-3.10913	-4.05007
N	0.34847	-3.64627	-5.08109
C	3.60581	-0.49172	2.37379
N	4.73680	-0.55402	2.64265
C	1.77372	-0.94011	4.63652
N	2.23575	-1.16610	5.68079

[$L_2Co^{III}O$] (*S* =1)

```
80
o_u2.out Energy: -2143627.2360955
C          -0.27897        1.64888       -0.31582
N          -0.66800        2.84121       -0.83869
C           0.32395        3.29866       -1.70447
C           1.36745        2.38814       -1.63803
N           1.00329        1.41236       -0.72935
B           1.75639        0.06308       -0.33858
N           1.38698       -0.23806        1.17149
C           0.08860       -0.30635        1.55682
N           0.04410       -0.56398        2.88951
C           1.35168       -0.67192        3.36200
C           2.19228       -0.46294        2.27651
N           1.00184       -1.02834       -1.22104
C          -0.28024       -1.40820       -0.93180
N          -0.67318       -2.29363       -1.88534
C           0.31544       -2.36973       -2.86470
C           1.36102       -1.56183       -2.44469
Co         -1.21498       -0.03225        0.14007
O          -2.66067        0.12309       -0.62918
C          -1.97036        3.56416       -0.55780
C          -1.66962        5.05532       -0.32401
C          -2.89133        3.33777       -1.76509
C          -2.60747        3.00185        0.71803
C          -1.26444       -0.75250        3.62906
C          -1.04034       -0.88801        5.13691
C          -2.13640        0.48180        3.35863
C          -1.91497       -2.02994        3.07915
C          -1.98125       -3.05958       -1.91210
C          -2.59198       -3.07955       -0.50609
C          -2.91343       -2.34364       -2.89953
C          -1.69992       -4.51427       -2.32823
H          -2.60196        5.55180       -0.01337
H          -0.92745        5.18342        0.48137
H          -2.45454        3.74747       -2.69093
H          -3.85575        3.84212       -1.59145
H          -3.06815        2.25716       -1.88751
H          -1.90325        3.03587        1.56439
H          -2.95066        1.97134        0.56632
H          -3.47928        3.62677        0.96744
H          -0.53687       -0.00607        5.56267
H          -0.47358       -1.79374        5.39718
H          -2.02821       -0.97121        5.61595
H          -1.62941        1.40225        3.69008
H          -3.08657        0.38398        3.90636
H          -1.27788       -2.90833        3.27327
H          -2.89099       -2.18822        3.56446
H          -2.07792       -1.95363        1.99441
H          -3.48431       -3.72456       -0.53074
H          -1.88382       -3.49815        0.22665
H          -3.87871       -2.87369       -2.94442
H          -3.08475       -1.31225       -2.55225
H          -0.93798       -4.96983       -1.67412
H          -1.37946       -4.61491       -3.37346
H          -2.63182       -5.09079       -2.22122
H          -1.31347        5.57568       -1.22291
H          -2.48682       -2.32612       -3.91631
H          -2.38017        0.58601        2.29095
C           3.34583        0.09043       -0.47453
```

```
C          4.07766        1.26330       -0.19837
C          5.47451        1.26950       -0.19438
C          6.17846        0.08705       -0.44818
C          5.47606       -1.09961       -0.68609
C          4.07916       -1.09437       -0.68763
H          3.55211        2.19398        0.03959
H          6.01539        2.19736        0.01732
H          7.27340        0.08709       -0.44497
H          6.01828       -2.03435       -0.86089
H          3.55493       -2.04355       -0.83957
H         -2.90123       -2.07522       -0.19121
C          0.27069        4.41462       -2.57758
N          0.27391        5.29736       -3.33678
C          2.52542        2.42110       -2.46170
N          3.41921        2.50105       -3.20213
C          2.51541       -1.26324       -3.21828
N          3.40584       -1.04034       -3.93311
C          0.25907       -3.04380       -4.11090
N          0.26202       -3.54795       -5.16039
C          3.60982       -0.49264        2.37129
N          4.74635       -0.55202        2.61626
C          1.81080       -0.93585        4.67792
N          2.27388       -1.14814        5.72444
```

[$L_2Co^{III}O$] (*S* =4)

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80
o_u4.out Energy: -2143619.5840003
C         -0.30040        1.67731       -0.39053
N         -0.65952        2.83026       -1.01361
C          0.39561        3.26722       -1.80753
C          1.43587        2.36785       -1.61768
N          1.00562        1.43169       -0.69200
B          1.72183        0.08492       -0.23000
N          1.35478       -0.21530        1.31069
C          0.08221       -0.33742        1.77383
N          0.12151       -0.62846        3.09452
C          1.44885       -0.69778        3.49748
C          2.22307       -0.43013        2.37415
N          0.98316       -0.98334       -1.15599
C         -0.33325       -1.28816       -0.97579
N         -0.70113       -2.13666       -1.97175
C          0.36252       -2.29221       -2.85526
C          1.41494       -1.54341       -2.34708
Co        -1.36055        0.00292        0.35909
O         -3.03640        0.01912        0.17418
C         -2.04024        3.45079       -0.88637
C         -1.99734        4.93739       -1.26306
C         -2.97837        2.67893       -1.82531
C         -2.48749        3.33029        0.57983
C         -1.13763       -0.93334        3.88782
C         -0.84082       -0.97395        5.38992
C         -2.16885        0.17318        3.60943
C         -1.64689       -2.30364        3.41225
C         -2.09606       -2.72722       -2.08718
C         -2.55030       -3.16400       -0.68404
C         -3.00949       -1.63548       -2.66285
C         -2.08713       -3.95882       -3.00151
```

H -2.97032 5.38033 -1.00063
H -1.21844 5.48083 -0.70320
H -2.62705 2.74334 -2.86879
H -3.98833 3.11749 -1.77284
H -3.03934 1.62430 -1.51693
H -1.74442 3.78470 1.25546
H -2.65611 2.28557 0.87001
H -3.44194 3.86707 0.69973
H -0.39736 -0.03128 5.74841
H -0.18843 -1.81355 5.66862
H -1.79574 -1.11694 5.91855
H -1.73574 1.17059 3.78863
H -3.02502 0.03729 4.28890
H -0.90524 -3.09186 3.62310
H -2.58070 -2.55251 3.94153
H -1.85269 -2.29866 2.33048
H -3.51666 -3.68494 -0.77509
H -1.82162 -3.85864 -0.23486
H -4.03032 -2.03613 -2.77482
H -3.04599 -0.77320 -1.98047
H -1.33441 -4.70053 -2.68744
H -1.92770 -3.70317 -4.05793
H -3.07686 -4.43583 -2.93258
H -1.85152 5.09984 -2.33956
H -2.65353 -1.31231 -3.65548
H -2.55904 0.13004 2.58153
C 3.31648 0.08604 -0.33484
C 4.06817 1.25506 -0.09860
C 5.46450 1.23872 -0.09641
C 6.14892 0.03667 -0.30682
C 5.42756 -1.14716 -0.49630
C 4.03161 -1.11879 -0.49749
H 3.55939 2.20141 0.11121
H 6.02040 2.16458 0.08201
H 7.24370 0.01936 -0.30461
H 5.95408 -2.09694 -0.63339
H 3.49183 -2.06472 -0.61073
H -2.69905 -2.30499 -0.01709
C 0.45942 4.36671 -2.70266
N 0.59800 5.23246 -3.46813
C 2.63909 2.37898 -2.37471
N 3.56080 2.44610 -3.08175
C 2.63399 -1.31827 -3.04279
N 3.56925 -1.15799 -3.71634
C 0.42953 -3.01202 -4.07661
N 0.57403 -3.56109 -5.09267
C 3.64304 -0.39674 2.44287
N 4.77541 -0.41042 2.71381
C 1.98965 -0.97010 4.78155
N 2.51530 -1.18557 5.79714

[L$_2$Co^{III}OH]$^+$ (*S* =0)

81
p_u0.out Energy: -2143915.9133867
C -0.28413 -1.23490 -1.12972
N -0.89801 -2.31189 -1.68081

C	0.07460	-3.27801	-1.92006
C	1.27396	-2.78046	-1.43205
N	1.03303	-1.49743	-0.97110
B	1.80473	-0.52769	0.02651
N	1.56151	0.93980	-0.52318
C	0.32320	1.46864	-0.62017
N	0.41562	2.77954	-0.97348
C	1.76748	3.05049	-1.19447
C	2.48129	1.90428	-0.89397
N	0.87709	-0.67080	1.32186
C	-0.41935	-0.24009	1.30426
N	-0.97295	-0.55132	2.50948
C	-0.04267	-1.27294	3.25583
C	1.10850	-1.36411	2.49117
Co	-1.12110	0.30240	-0.46734
O	-1.80778	0.82297	-2.05903
C	-2.40370	-2.49285	-1.81020
C	-2.77670	-3.96819	-1.59869
C	-3.04189	-1.68724	-0.67245
C	-2.84571	-2.00148	-3.19212
C	-0.65886	3.87224	-1.05016
C	-0.13828	5.10296	-0.28174
C	-0.91103	4.17351	-2.53250
C	-1.95301	3.42991	-0.36300
C	-2.33190	-0.14524	3.05640
C	-3.05456	0.75121	2.05321
C	-3.15964	-1.41280	3.32016
C	-2.09608	0.66650	4.34376
H	-3.86990	-4.02530	-1.48368
H	-2.51338	-4.59857	-2.45761
H	-2.64858	-2.00073	0.30484
H	-4.13106	-1.84618	-0.66510
H	-2.94222	-0.59727	-0.83015
H	-2.33037	-2.56506	-3.98671
H	-2.63438	-0.92854	-3.30062
H	-3.92995	-2.16400	-3.30242
H	0.71687	5.59549	-0.76044
H	0.13498	4.83153	0.75099
H	-0.94894	5.84608	-0.23800
H	0.00339	4.50466	-3.04954
H	-1.65629	4.98045	-2.61402
H	-1.75945	3.11513	0.67450
H	-2.62511	4.29991	-0.31782
H	-2.47243	2.63964	-0.91777
H	-4.02008	1.05248	2.48622
H	-2.48283	1.66680	1.84931
H	-4.14848	-1.11763	3.70436
H	-3.31055	-1.98819	2.39357
H	-1.45365	1.53832	4.13927
H	-1.64140	0.07104	5.14800
H	-3.06690	1.03043	4.71465
H	-2.31714	-4.38040	-0.68560
H	-2.69646	-2.07111	4.06934
H	-1.30852	3.27938	-3.03657
C	3.36135	-0.73005	0.26105
C	4.21596	-1.23050	-0.73912
C	5.59900	-1.29658	-0.55365
C	6.16719	-0.82613	0.63465
C	5.34644	-0.26882	1.62224

C	3.96470	-0.21582	1.43017
H	3.81255	-1.53685	-1.70692
H	6.23530	-1.69946	-1.34757
H	7.25089	-0.87298	0.78245
H	5.78477	0.13090	2.54191
H	3.35024	0.25275	2.20626
H	-3.28057	0.23368	1.11067
H	-1.18006	0.91860	-2.79505
C	2.33752	4.23410	-1.73105
N	2.87294	5.15261	-2.20365
C	3.89635	1.81634	-0.99468
N	5.04543	1.92278	-1.14229
C	2.46655	-3.54955	-1.36130
N	3.36352	-4.28870	-1.32433
C	2.24488	-2.15021	2.82838
N	3.10086	-2.85974	3.16893
C	-0.07643	-4.51860	-2.59176
N	-0.11332	-5.53369	-3.15838
C	-0.22895	-1.85258	4.53666
N	-0.33203	-2.35408	5.58159

[$L_2Co^{III}OH]^+$ (*S* =1)

81
p_u2.out Energy: -2143907.9247456

C	-0.43785	-1.40746	-1.00493
N	-0.97821	-2.55036	-1.49589
C	0.01392	-3.52480	-1.52276
C	1.16905	-2.94202	-1.01808
N	0.88146	-1.61322	-0.75913
B	1.72343	-0.50405	0.02854
N	1.47224	0.95193	-0.60362
C	0.28363	1.60337	-0.52298
N	0.44757	2.89248	-0.90150
C	1.77454	3.05085	-1.30291
C	2.41250	1.83834	-1.11088
N	0.92004	-0.49460	1.40612
C	-0.38634	-0.12708	1.39048
N	-0.92520	-0.39751	2.60393
C	0.05291	-0.99467	3.39567
C	1.20203	-1.08031	2.62326
Co	-1.18477	0.37186	-0.35424
O	-1.97106	0.85261	-1.87171
C	-2.41468	-2.68088	-1.99238
C	-2.83120	-4.15437	-2.06479
C	-3.34042	-1.96406	-0.99990
C	-2.47132	-2.03391	-3.38369
C	-0.54120	4.05213	-0.82097
C	0.09708	5.14661	0.05459
C	-0.82392	4.54506	-2.24785
C	-1.84250	3.60565	-0.15407
C	-2.35704	-0.17133	3.04521
C	-3.12564	0.53217	1.92762
C	-2.99048	-1.54393	3.32555
C	-2.34833	0.73171	4.28906
H	-3.90583	-4.18523	-2.30037
H	-2.31481	-4.70160	-2.86468
H	-3.16959	-2.31754	0.02893

H	-4.38513	-2.18402	-1.26722
H	-3.23645	-0.87208	-1.05614
H	-1.78987	-2.54698	-4.08177
H	-2.20379	-0.96869	-3.32251
H	-3.49700	-2.11618	-3.77832
H	0.99927	5.58716	-0.39158
H	0.35000	4.74698	1.05011
H	-0.63275	5.96074	0.18376
H	0.08332	4.89828	-2.76008
H	-1.52949	5.38924	-2.19994
H	-1.65972	3.22802	0.86435
H	-2.49860	4.48488	-0.06904
H	-2.37479	2.84727	-0.74394
H	-4.17856	0.63385	2.23091
H	-2.74616	1.54780	1.74354
H	-4.04350	-1.39979	3.61303
H	-2.95828	-2.17941	2.42598
H	-1.83335	1.68225	4.07530
H	-1.86857	0.25382	5.15515
H	-3.38913	0.95526	4.57082
H	-2.68340	-4.67538	-1.10509
H	-2.49184	-2.07568	4.14916
H	-1.28512	3.75073	-2.85699
C	3.29451	-0.71919	0.12892
C	4.03743	-1.34987	-0.88736
C	5.43048	-1.43289	-0.82940
C	6.12075	-0.85346	0.24012
C	5.41130	-0.17141	1.23571
C	4.01855	-0.09960	1.17111
H	3.53429	-1.75322	-1.77040
H	5.97912	-1.93586	-1.63150
H	7.21280	-0.91401	0.28715
H	5.94473	0.31069	2.06075
H	3.49011	0.46707	1.94524
H	-3.14008	-0.06120	0.99783
H	-1.47972	1.41968	-2.49132
C	2.37204	4.21594	-1.84876
N	2.90433	5.13892	-2.31617
C	3.78084	1.63413	-1.43818
N	4.89066	1.64964	-1.78701
C	2.33827	-3.68474	-0.69654
N	3.21021	-4.40500	-0.42531
C	2.39107	-1.75473	3.01437
N	3.29923	-2.36280	3.41090
C	-0.05655	-4.88011	-1.94066
N	-0.00095	-5.99637	-2.26289
C	-0.09421	-1.46114	4.72657
N	-0.17037	-1.86158	5.81627

[L$_2$Co^{III}OH]$^+$ (*S* =2)

81
p_u4.out Energy: -2143896.7746177

C	-0.42940	-1.26297	-1.05705
N	-0.93528	-2.35233	-1.68313
C	-0.06806	-3.42106	-1.47842
C	1.01876	-2.92863	-0.76997
N	0.80060	-1.57579	-0.57814

B	1.65727	-0.52243	0.24810
N	1.42697	0.92283	-0.42641
C	0.21107	1.51613	-0.57345
N	0.36878	2.71095	-1.18117
C	1.71778	2.88470	-1.45767
C	2.38036	1.76125	-0.97998
N	0.91510	-0.54131	1.65717
C	-0.34313	-0.05614	1.80774
N	-0.73805	-0.27417	3.08683
C	0.25104	-1.00695	3.73425
C	1.28429	-1.18409	2.82462
Co	-1.32312	0.32726	-0.00738
O	-3.07575	0.07466	0.10569
C	-2.22084	-2.39259	-2.49797
C	-1.99720	-3.27083	-3.74069
C	-3.32716	-2.95191	-1.59421
C	-2.55443	-0.97226	-2.97695
C	-0.71964	3.70783	-1.53234
C	-0.36257	5.06077	-0.89329
C	-0.80381	3.78878	-3.06471
C	-2.05667	3.23458	-0.96186
C	-2.06674	0.18138	3.67833
C	-2.43138	1.53835	3.05885
C	-3.11153	-0.89287	3.34621
C	-1.93225	0.36659	5.19668
H	-2.87802	-3.17032	-4.39289
H	-1.11201	-2.93912	-4.30786
H	-3.08159	-3.96822	-1.24444
H	-4.26963	-3.00472	-2.16251
H	-3.47842	-2.29387	-0.72378
H	-1.69485	-0.50575	-3.48459
H	-2.88924	-0.32886	-2.15610
H	-3.38551	-1.03960	-3.69558
H	0.55417	5.50092	-1.30991
H	-0.24462	4.95653	0.19754
H	-1.18317	5.76882	-1.08724
H	0.13342	4.14927	-3.51523
H	-1.60122	4.49513	-3.34398
H	-2.03097	3.17083	0.13740
H	-2.82348	3.97821	-1.22766
H	-2.38184	2.27923	-1.40169
H	-3.31302	1.93665	3.58385
H	-1.60672	2.26131	3.16400
H	-4.08181	-0.59962	3.77857
H	-3.23277	-0.99474	2.25699
H	-1.07235	1.00556	5.45633
H	-1.85686	-0.58489	5.73850
H	-2.84440	0.86637	5.55652
H	-1.89575	-4.33787	-3.50515
H	-2.82378	-1.86667	3.77570
H	-1.04600	2.80145	-3.49085
C	3.22485	-0.78772	0.31590
C	3.91981	-1.45754	-0.71067
C	5.30887	-1.59788	-0.67753
C	6.04196	-1.04713	0.37949
C	5.38015	-0.34148	1.39060
C	3.99143	-0.20786	1.34987
H	3.37919	-1.85758	-1.57380
H	5.82219	-2.12789	-1.48572

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H          7.13106       -1.15440        0.40698
H          5.94843        0.11235        2.20833
H          3.50015        0.37419        2.13712
H         -2.70534        1.44310        2.00272
H         -3.84550        0.63557       -0.09584
C          2.32076        3.98018       -2.12746
N          2.85377        4.85242       -2.68292
C          3.78793        1.60172       -1.10816
N          4.93072        1.66130       -1.31957
C          2.06908       -3.71987       -0.23040
N          2.86072       -4.44247        0.22068
C          2.42984       -1.99345        3.05760
N          3.29903       -2.71450        3.33513
C         -0.26917       -4.78500       -1.81444
N         -0.38281       -5.92330       -2.02623
C          0.24351       -1.56194        5.04077
N          0.32081       -2.07379        6.08247
```

$[L_2Co^{II}O]^-$ (*S* =1/2)

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80
r_u1.out Energy: -2143705.5983735
C         -0.32571       -0.80337       -1.37338
N         -0.81404       -1.64355       -2.34940
C          0.06008       -2.71584       -2.51640
C          1.16051       -2.46687       -1.70777
N          0.94338       -1.25825       -1.07971
B          1.76445       -0.56092        0.07926
N          1.57284        0.99361       -0.09362
C          0.30273        1.50176       -0.15053
N          0.42286        2.86607       -0.29927
C          1.77416        3.20412       -0.33464
C          2.49104        2.02023       -0.20401
N          0.94738       -0.98394        1.36643
C         -0.31842       -0.46987        1.55770
N         -0.80633       -1.07398        2.69488
C          0.06365       -2.08839        3.08936
C          1.16179       -2.02775        2.24234
Co        -1.16203        0.28758       -0.01319
O         -2.77606       -0.28593        0.05727
C         -2.11790       -1.48099       -3.09369
C         -1.92027       -1.88659       -4.56581
C         -3.16182       -2.35453       -2.38307
C         -2.54962       -0.00910       -3.06128
C         -0.78135        3.76816       -0.40987
C         -0.37739        5.23817       -0.55336
C         -1.57611        3.33670       -1.65254
C         -1.61677        3.59676        0.86863
C         -2.10521       -0.74391        3.39050
C         -2.53288        0.68513        3.03133
C         -3.15655       -1.74965        2.89906
C         -1.89897       -0.81126        4.91482
H         -2.83403       -1.62490       -5.12222
H         -1.07697       -1.33613       -5.01657
H         -2.86212       -3.41692       -2.38447
H         -4.13269       -2.27178       -2.90056
H         -3.26040       -1.97922       -1.34850
```

H -1.75546 0.64607 -3.45524
H -2.80116 0.28372 -2.03118
H -3.44102 0.10086 -3.70073
H 0.20690 5.42539 -1.46722
H 0.18531 5.60474 0.31901
H -1.30103 5.83381 -0.62480
H -0.96263 3.44186 -2.56294
H -2.47267 3.96901 -1.75676
H -1.02738 3.87214 1.75903
H -2.50535 4.24671 0.81900
H -1.95367 2.55594 0.97965
H -3.41720 0.94125 3.63793
H -1.73269 1.40850 3.25841
H -4.12268 -1.55102 3.39342
H -3.26395 -1.61262 1.80768
H -1.05235 -0.17605 5.22635
H -1.73582 -1.82974 5.29152
H -2.80909 -0.43035 5.40433
H -1.75743 -2.96329 -4.70710
H -2.85861 -2.78638 3.13352
H -1.89702 2.28861 -1.56565
C 3.33483 -0.87575 0.11023
C 4.06449 -1.05428 -1.08221
C 5.45352 -1.20605 -1.07728
C 6.15603 -1.16320 0.13233
C 5.46044 -0.95139 1.32807
C 4.07129 -0.80090 1.30928
H 3.54120 -1.05893 -2.04421
H 5.99094 -1.34894 -2.02063
H 7.24496 -1.28024 0.14159
H 6.00341 -0.89371 2.27727
H 3.55382 -0.60270 2.25381
H -2.79380 0.73879 1.96406
C 2.38951 4.47391 -0.47067
N 2.97546 5.47543 -0.57760
C 3.91111 1.97613 -0.19451
N 5.06947 2.10145 -0.20317
C 2.22843 -3.38125 -1.50449
N 3.04717 -4.19823 -1.36841
C -0.13550 -3.90946 -3.25393
N -0.24644 -4.92471 -3.81624
C 2.22510 -2.96959 2.24039
N 3.04072 -3.79981 2.28299
C -0.13349 -3.08927 4.07237
N -0.24682 -3.95481 4.84517

[$L_2Co^{II}O]^-$ (*S* =3/2)

80
r_u3.out Energy: -2143706.4960007
C -0.35018 -0.85301 -1.37880
N -0.82243 -1.75936 -2.29143
C 0.13407 -2.74806 -2.50433
C 1.23989 -2.40322 -1.73699
N 0.95203 -1.20445 -1.10729
B 1.74677 -0.47103 0.06370

N	1.55660	1.10942	-0.08627
C	0.31799	1.69819	-0.16463
N	0.50769	3.04177	-0.31100
C	1.87257	3.31704	-0.32154
C	2.52732	2.09948	-0.17826
N	0.93883	-0.97376	1.34179
C	-0.35475	-0.55454	1.53987
N	-0.83072	-1.23599	2.62908
C	0.11207	-2.17435	3.03880
C	1.21419	-2.02025	2.20576
Co	-1.18998	0.41776	-0.03240
O	-2.85563	0.84574	-0.06481
C	-2.24048	-1.71420	-2.81302
C	-2.38325	-2.56890	-4.07831
C	-3.15259	-2.24148	-1.69407
C	-2.58687	-0.25355	-3.14850
C	-0.66142	3.98604	-0.48249
C	-0.18878	5.43768	-0.59740
C	-1.39996	3.57482	-1.76749
C	-1.58093	3.83423	0.74158
C	-2.20065	-0.95873	3.20797
C	-2.32668	0.56405	3.38595
C	-3.25585	-1.47643	2.21720
C	-2.36854	-1.64088	4.56975
H	-3.38640	-2.39190	-4.49643
H	-1.64361	-2.28962	-4.84719
H	-2.88710	-3.27846	-1.42579
H	-4.20157	-2.22771	-2.03423
H	-3.06188	-1.59019	-0.81070
H	-1.83439	0.18052	-3.82828
H	-2.66111	0.35071	-2.22985
H	-3.56574	-0.23332	-3.65580
H	0.44990	5.60444	-1.47851
H	0.34366	5.77649	0.30534
H	-1.08068	6.07313	-0.71358
H	-0.72806	3.63505	-2.64058
H	-2.25015	4.25723	-1.93326
H	-1.01500	3.99035	1.67570
H	-2.37725	4.59542	0.68715
H	-2.05354	2.83772	0.74506
H	-3.30785	0.79255	3.83384
H	-1.53812	0.94558	4.05663
H	-4.25561	-1.38155	2.67389
H	-3.23297	-0.87105	1.29392
H	-1.57402	-1.35651	5.27918
H	-2.40782	-2.73726	4.49072
H	-3.32886	-1.31047	4.99563
H	-2.30399	-3.64648	-3.87687
H	-3.08251	-2.54072	1.98331
H	-1.79093	2.55053	-1.66707
C	3.32356	-0.75826	0.09614
C	4.06153	-0.90307	-1.09616
C	5.44982	-1.05664	-1.08681
C	6.14473	-1.04565	0.12769
C	5.44280	-0.85818	1.32358
C	4.05445	-0.70549	1.30002
H	3.54511	-0.88022	-2.06150
H	5.99256	-1.17560	-2.03031
H	7.23332	-1.16515	0.14071

H	5.98017	-0.82039	2.27684
H	3.53369	-0.52228	2.24552
H	-2.26325	1.07173	2.41262
C	2.54937	4.55803	-0.43548
N	3.17469	5.53742	-0.52266
C	3.94618	2.02484	-0.13943
N	5.10328	2.16331	-0.12580
C	2.37303	-3.24589	-1.57852
N	3.23333	-4.02492	-1.48112
C	0.07272	-3.91697	-3.30466
N	0.10170	-4.90062	-3.92870
C	2.32873	-2.90125	2.20835
N	3.17631	-3.69877	2.25534
C	0.03366	-3.15917	4.05617
N	0.04584	-3.99903	4.86371

[$L_2Co^{II}O]^-$ (*S* =5/2)

80
r_u5.out Energy: -2143685.6780101

C	-0.33694	-0.83228	-1.40258
N	-0.83039	-1.77489	-2.24189
C	0.13145	-2.78147	-2.43320
C	1.25569	-2.38961	-1.67912
N	0.95289	-1.15216	-1.10711
B	1.73093	-0.42767	0.07661
N	1.54644	1.16566	-0.06625
C	0.33689	1.77812	-0.20281
N	0.54202	3.11773	-0.29141
C	1.90617	3.37307	-0.19751
C	2.53312	2.14223	-0.05115
N	0.93566	-0.93566	1.34083
C	-0.31535	-0.47228	1.62067
N	-0.86142	-1.26216	2.57009
C	-0.00187	-2.34768	2.84705
C	1.14588	-2.14536	2.03052
Co	-1.23261	0.47144	-0.02468
O	-2.75631	1.11386	-0.36746
C	-2.23625	-1.71304	-2.79582
C	-2.43133	-2.73182	-3.92534
C	-3.21654	-2.02191	-1.65048
C	-2.46190	-0.30084	-3.36139
C	-0.60030	4.10146	-0.46105
C	-0.08501	5.53962	-0.56622
C	-1.34144	3.72991	-1.75525
C	-1.51059	3.97486	0.77163
C	-2.20103	-1.05542	3.21528
C	-2.74393	0.34070	2.88381
C	-3.16000	-2.13014	2.67467
C	-2.03693	-1.15191	4.74461
H	-3.42746	-2.56196	-4.36314
H	-1.68667	-2.60616	-4.72749
H	-2.98148	-2.99531	-1.18844
H	-4.24386	-2.06611	-2.04850
H	-3.18624	-1.23359	-0.88297
H	-1.72059	-0.07782	-4.14699
H	-2.40185	0.45844	-2.57023

H -3.46836 -0.25031 -3.80846
H 0.57579 5.68633 -1.43447
H 0.43323 5.87002 0.34694
H -0.95872 6.19566 -0.70347
H -0.65878 3.78321 -2.61991
H -2.16430 4.44535 -1.91729
H -0.94244 4.17543 1.69542
H -2.32464 4.71425 0.69624
H -1.96228 2.97421 0.82417
H -3.65240 0.50663 3.48509
H -2.01265 1.12610 3.13371
H -4.16354 -1.98875 3.10805
H -3.23643 -2.04414 1.57770
H -1.30992 -0.40243 5.09957
H -1.70961 -2.14545 5.07939
H -3.00818 -0.94367 5.22115
H -2.40287 -3.77085 -3.56778
H -2.81808 -3.14651 2.92671
H -1.77157 2.72139 -1.68159
C 3.30654 -0.71341 0.08828
C 4.03031 -0.74937 -1.12151
C 5.41718 -0.91027 -1.14077
C 6.12141 -1.02371 0.06345
C 5.43021 -0.96222 1.27899
C 4.04272 -0.80007 1.28530
H 3.49740 -0.64775 -2.07334
H 5.95155 -0.94295 -2.09598
H 7.20938 -1.14992 0.05497
H 5.97622 -1.03325 2.22549
H 3.52454 -0.72871 2.24654
H -3.01690 0.45200 1.82519
C 2.60437 4.60788 -0.22975
N 3.25447 5.57375 -0.24532
C 3.94432 2.04447 0.09711
N 5.09389 2.19213 0.21441
C 2.41535 -3.17737 -1.53236
N 3.31298 -3.92542 -1.47237
C 0.05355 -3.97392 -3.17367
N 0.07544 -4.98602 -3.76251
C 2.20861 -3.05124 1.91495
N 3.04588 -3.87535 1.89574
C -0.26451 -3.44805 3.66621
N -0.45594 -4.39124 4.34266

[$L_2Co^{II}OH$] (*S* =1/2)

81
h_u1.out Energy: -2144039.9907461
C 0.36976 -0.74932 1.48923
N 0.86573 -1.43414 2.55937
C 0.00780 -2.49172 2.86073
C -1.07203 -2.38997 1.99583
N -0.86413 -1.27168 1.21337
B -1.71139 -0.67538 0.01127
N -1.51285 0.89563 0.06987
C -0.24855 1.41105 0.06931
N -0.35091 2.76749 0.12502

C	-1.70127	3.11662	0.16018
C	-2.42548	1.93343	0.12564
N	-0.90590	-1.17411	-1.26198
C	0.31789	-0.62852	-1.53772
N	0.77646	-1.22489	-2.67529
C	-0.09142	-2.25755	-3.02989
C	-1.14105	-2.22725	-2.12325
Co	1.18334	0.20873	-0.00288
O	2.75226	-0.77405	-0.07013
C	2.10380	-1.08368	3.35373
C	1.71925	-1.02207	4.84370
C	3.17538	-2.14886	3.07802
C	2.61753	0.29779	2.93079
C	0.79970	3.73637	0.14340
C	0.70263	4.63543	-1.10054
C	0.73667	4.54868	1.44775
C	2.11891	2.95647	0.10083
C	1.98439	-0.80654	-3.48306
C	2.50987	0.53967	-2.97025
C	3.06738	-1.88498	-3.33168
C	1.54561	-0.62830	-4.94848
H	2.59511	-0.68613	5.42066
H	0.90225	-0.29909	5.00362
H	2.83745	-3.15810	3.36289
H	4.08014	-1.91807	3.66332
H	3.43406	-2.13591	2.00823
H	1.83172	1.06415	3.02696
H	2.99414	0.27041	1.89965
H	3.44978	0.57275	3.59778
H	-0.21147	5.24810	-1.10312
H	0.72154	4.02541	-2.01871
H	1.56368	5.32221	-1.12096
H	-0.17495	5.16100	1.51617
H	1.60006	5.23137	1.49235
H	2.21713	2.37076	-0.82657
H	2.95277	3.67549	0.11725
H	2.23644	2.30622	0.98176
H	3.31597	0.87170	-3.64337
H	1.71874	1.30651	-2.97578
H	3.94984	-1.60441	-3.92916
H	3.36479	-1.95548	-2.27425
H	0.72137	0.10060	-5.02026
H	1.22967	-1.56795	-5.42297
H	2.39886	-0.24235	-5.52796
H	1.41540	-1.99580	5.25288
H	2.72102	-2.87007	-3.68313
H	0.77780	3.87733	2.32122
C	-3.27617	-0.99251	0.02531
C	-3.98817	-1.08899	1.23806
C	-5.37677	-1.24152	1.26203
C	-6.09560	-1.28129	0.06205
C	-5.41779	-1.14888	-1.15498
C	-4.02894	-0.99671	-1.16645
H	-3.45541	-1.02313	2.19234
H	-5.90071	-1.31943	2.22012
H	-7.18412	-1.39948	0.07599
H	-5.97397	-1.15387	-2.09793
H	-3.52868	-0.85714	-2.13036
H	2.92464	0.43230	-1.95922

H	2.62996	-1.73500	-0.10967
C	0.08716	-3.21660	-4.05776
N	0.20710	-4.03583	-4.87692
C	-2.17889	-3.19445	-2.03820
N	-2.97269	-4.04450	-2.00268
C	-3.84596	1.88529	0.14731
N	-5.00334	2.00838	0.17150
C	-2.23953	4.42521	0.21743
N	-2.70846	5.49045	0.26387
C	-2.11450	-3.34787	1.87130
N	-2.91093	-4.19295	1.79699
C	0.21749	-3.52867	3.80350
N	0.36157	-4.40986	4.55138

[$L_2Co^{II}OH$] (*S* =3/2)

81
h_u3.out Energy: -2144034.3342565

C	0.34007	-0.75727	1.50337
N	0.80157	-1.55254	2.50550
C	-0.17013	-2.49554	2.82580
C	-1.26089	-2.23541	2.00617
N	-0.94826	-1.12318	1.24172
B	-1.74338	-0.49115	0.00440
N	-1.55003	1.10473	0.00699
C	-0.33030	1.71690	0.01767
N	-0.52182	3.05917	-0.00062
C	-1.88803	3.32066	-0.02396
C	-2.53157	2.09012	-0.01985
N	-0.92891	-1.10777	-1.22358
C	0.35388	-0.71583	-1.48155
N	0.82498	-1.49151	-2.49498
C	-0.12761	-2.45269	-2.81813
C	-1.22079	-2.22144	-1.99376
Co	1.19201	0.41901	0.03663
O	3.00389	0.82261	-0.09084
C	2.19972	-1.40357	3.07632
C	2.36030	-2.22831	4.35722
C	3.19647	-1.88131	2.00919
C	2.41375	0.08160	3.40998
C	0.64236	4.03220	0.01497
C	0.15387	5.48211	-0.03352
C	1.42187	3.79839	1.31843
C	1.51771	3.74213	-1.21559
C	2.21264	-1.30906	-3.08172
C	2.41938	0.19247	-3.33752
C	3.22570	-1.84575	-2.05955
C	2.34683	-2.06365	-4.40889
H	3.34769	-1.99558	4.78504
H	1.60080	-1.97334	5.11370
H	2.97066	-2.91409	1.69633
H	4.21476	-1.86139	2.43075
H	3.17867	-1.21563	1.13304
H	1.65321	0.43971	4.12272
H	2.37737	0.70532	2.50689
H	3.40900	0.20765	3.86474

H -0.46263 5.74719 0.83878
H -0.40356 5.70382 -0.95654
H 1.04064 6.13450 -0.01917
H 0.77755 3.95937 2.19811
H 2.26937 4.50037 1.36960
H 0.91952 3.79057 -2.14026
H 2.31401 4.50158 -1.27688
H 1.99929 2.75592 -1.13995
H 3.40016 0.33714 -3.81844
H 1.63951 0.58444 -4.01114
H 4.23890 -1.78705 -2.48991
H 3.21182 -1.23845 -1.14321
H 1.56066 -1.78072 -5.12767
H 2.34511 -3.15502 -4.27808
H 3.31734 -1.79240 -4.85235
H 2.33689 -3.31072 4.16638
H 3.01404 -2.89995 -1.81471
H 1.82462 2.77636 1.35579
C -3.31629 -0.77425 -0.00440
C -4.05528 -0.80112 1.19624
C -5.44345 -0.95212 1.19872
C -6.13589 -1.05623 -0.01261
C -5.43281 -0.98470 -1.22021
C -4.04465 -0.83299 -1.21005
H -3.54312 -0.68264 2.15668
H -5.98775 -0.97785 2.14806
H -7.22449 -1.17405 -0.01585
H -5.96892 -1.03544 -2.17321
H -3.52527 -0.73736 -2.16892
H 2.42005 0.76497 -2.40109
H 3.41695 1.39225 0.57517
C -0.06064 -3.51758 -3.75372
N -0.09117 -4.42177 -4.48619
C -2.33870 -3.09461 -1.90141
N -3.18030 -3.89753 -1.86445
C -3.95004 1.99700 -0.04043
N -5.10603 2.13746 -0.05944
C -2.57117 4.56434 -0.04945
N -3.20745 5.53881 -0.07110
C -2.39943 -3.08248 1.91949
N -3.25851 -3.86701 1.89273
C -0.12419 -3.56459 3.75796
N -0.17212 -4.46825 4.49006

[$L_2Co^{II}OH$] (*S* =5/2)

81
h_u5.out Energy: -2143975.4844607
C 0.31538 -0.71900 1.52495
N 0.79834 -1.51135 2.51726
C -0.13009 -2.51254 2.78647
C -1.21404 -2.28650 1.94785
N -0.94316 -1.13989 1.22328
B -1.75712 -0.49206 0.00096
N -1.56556 1.08198 0.02369
C -0.34824 1.70453 0.00581
N -0.50529 3.05888 0.01630
C -1.86841 3.37462 0.05099

C	-2.57397	2.05895	0.06611
N	-0.94728	-1.10492	-1.24345
C	0.32980	-0.71387	-1.50495
N	0.80476	-1.47778	-2.52293
C	-0.15562	-2.42673	-2.86041
C	-1.24775	-2.20024	-2.03248
Co	1.13619	0.44831	0.01553
O	2.94251	0.70715	0.03420
C	2.17417	-1.32678	3.13433
C	2.25800	-2.04119	4.48867
C	3.20311	-1.90858	2.15388
C	2.40169	0.17727	3.35355
C	0.67360	4.00609	0.00409
C	0.21407	5.46801	-0.01361
C	1.49773	3.75905	1.27872
C	1.49664	3.73228	-1.26601
C	2.20655	-1.32595	-3.08796
C	2.48236	0.17314	-3.28495
C	3.17784	-1.94698	-2.07319
C	2.32634	-2.03210	-4.44332
H	3.20855	-1.75292	4.96313
H	1.44068	-1.74011	5.16415
H	2.99751	-2.97302	1.95312
H	4.20996	-1.82773	2.59497
H	3.19934	-1.34537	1.20931
H	1.58892	0.61631	3.95445
H	2.48793	0.71486	2.40149
H	3.35037	0.31345	3.89634
H	-0.36123	5.73573	0.88473
H	-0.37930	5.70714	-0.90866
H	1.11444	6.10166	-0.03201
H	0.87904	3.91180	2.17789
H	2.34503	4.46266	1.31279
H	0.87381	3.85306	-2.16713
H	2.33476	4.44532	-1.32151
H	1.91968	2.71846	-1.26971
H	3.45215	0.28880	-3.79420
H	1.70242	0.63841	-3.90921
H	4.20728	-1.86662	-2.45849
H	3.13073	-1.41330	-1.11319
H	1.55771	-1.69086	-5.15564
H	2.28389	-3.12661	-4.35746
H	3.31068	-1.78024	-4.86693
H	2.26651	-3.13544	4.39152
H	2.94910	-3.01356	-1.91308
H	1.90562	2.73903	1.30767
C	-3.32359	-0.79925	-0.00820
C	-4.05959	-0.91783	1.18725
C	-5.44653	-1.08264	1.17902
C	-6.13919	-1.10756	-0.03627
C	-5.43833	-0.94470	-1.23621
C	-4.05156	-0.78229	-1.21540
H	-3.54938	-0.85684	2.15388
H	-5.98986	-1.17973	2.12435
H	-7.22672	-1.23478	-0.04716
H	-5.97483	-0.93466	-2.19033
H	-3.53150	-0.61954	-2.16531
H	2.55076	0.70048	-2.32570
H	3.35875	1.58301	0.04859

```
C          -0.09695        -3.47437        -3.81582
N          -0.13861        -4.36541        -4.56341
C          -2.38120        -3.05631        -1.96511
N          -3.23238        -3.84949        -1.95952
C          -3.95125         1.97329         0.12918
N          -5.12376         2.11224         0.18648
C          -2.51483         4.59535         0.06897
N          -3.15781         5.58640         0.08650
C          -2.30783        -3.18311         1.80193
N          -3.12623        -4.00590         1.71888
C          -0.04529        -3.60593         3.68705
N          -0.06041        -4.53714         4.38505
```

4. Thermodynamic cycle for the $L_3Co^{III}O$ oxidant

[$L_3Co^{III}O$] (*S* =0)

```
74
o_u0.out Energy: -1806771.4859002
C          -0.33097         1.55460        -0.07505
N          -0.75335         2.84288        -0.25442
C           0.29027         3.60136        -0.77489
C           1.37193         2.78395        -0.89221
N           0.99319         1.54031        -0.41415
B           1.70667         0.16820        -0.34941
N           1.45862        -0.44976         1.03611
C           0.16962        -0.62636         1.40825
N           0.20510        -1.19728         2.64556
C           1.53194        -1.37406         3.03781
C           2.31661        -0.90372         2.02705
N           0.98828        -0.69709        -1.41393
C          -0.34014        -0.94624        -1.20723
N          -0.76533        -1.65579        -2.29622
C           0.28260        -1.78044        -3.20282
C           1.36871        -1.16555        -2.66063
Co         -1.27314        -0.08957         0.23377
O          -2.91404         0.01639         0.00796
C          -2.12033         3.40941         0.04419
C          -2.05729         4.94432        -0.00467
C          -3.10713         2.89952        -1.01665
C          -2.53283         2.97960         1.46049
C          -1.00432        -1.62834         3.42252
C          -0.57599        -2.15681         4.79712
C          -1.93406        -0.41802         3.60493
C          -1.70410        -2.74415         2.62929
C          -2.14823        -2.20343        -2.55331
C          -2.63325        -2.94983        -1.30099
C          -3.07182        -1.02900        -2.90947
C          -2.09355        -3.19617        -3.72543
H          -3.04401         5.33598         0.28709
H          -1.31222         5.35124         0.69921
H          -2.75396         3.16536        -2.02788
H          -4.09046         3.37376        -0.85898
H          -3.22221         1.80738        -0.92986
H          -1.79173         3.32274         2.20212
H          -2.63329         1.88907         1.52487
```

```
H          -3.50796        3.42977        1.70786
H          -0.05500       -1.38524        5.38780
H           0.07013       -3.04609        4.71639
H          -1.47818       -2.45360        5.35412
H          -1.39942        0.41723        4.08667
H          -2.78917       -0.70116        4.23984
H          -1.03106       -3.60736        2.49456
H          -2.60482       -3.08130        3.16757
H          -2.01152       -2.38166        1.63637
H          -3.60356       -3.42582       -1.51652
H          -1.91513       -3.73641       -1.01405
H          -4.07993       -1.41092       -3.14271
H          -3.14382       -0.33944       -2.05439
H          -1.38608       -4.02060       -3.53552
H          -1.83384       -2.70961       -4.67944
H          -3.09592       -3.63438       -3.84924
H          -1.84407        5.32472       -1.01682
H          -2.68974       -0.49577       -3.79696
H          -2.33078       -0.07663        2.63672
C           3.97201        1.28710       -0.01733
C           5.36043        1.31136       -0.01388
C           6.06403        0.20945       -0.50956
C           5.34388       -0.89871       -0.96624
C           3.95606       -0.86197       -0.94341
H           3.39049        2.10730        0.40266
H           5.87537        2.18706        0.38744
H           7.15775        0.20552       -0.51958
H           5.84561       -1.79824       -1.32980
H           3.36112       -1.72276       -1.24819
H           0.19722        4.65279       -1.02313
H           2.35668        3.00644       -1.29498
H           1.82081       -1.81000        3.98866
H           3.40114       -0.86158        1.95162
H           0.18893       -2.28921       -4.15579
H           2.35864       -1.02392       -3.08685
H          -2.77176       -2.25490       -0.46331
N           3.27836        0.23184       -0.51281
```

[$L_3Co^{III}O$] (*S* =1)

```
74
o_u2.out Energy: -1806769.0231200
C          -0.35012        1.64129        0.06001
N          -0.74120        2.90846       -0.23159
C           0.28125        3.58009       -0.89442
C           1.32932        2.71555       -0.99275
N           0.95042        1.53813       -0.36020
B           1.64282        0.14585       -0.31259
N           1.41962       -0.48947        1.07282
C           0.14752       -0.68385        1.49104
N           0.21497       -1.25435        2.71881
C           1.55420       -1.42018        3.07556
C           2.30638       -0.94095        2.04454
N           0.94792       -0.72611       -1.39828
C          -0.35440       -1.10727       -1.20367
N          -0.74696       -1.71009       -2.35528
C           0.27684       -1.64946       -3.29559
C           1.32710       -1.01609       -2.70297
```

Co	-1.25931	-0.13182	0.29816
O	-2.89391	-0.03653	0.10064
C	-2.10366	3.48378	0.03626
C	-2.01357	5.01696	0.03696
C	-3.04682	3.00040	-1.07708
C	-2.58520	3.00068	1.41235
C	-0.98803	-1.64522	3.52467
C	-0.54026	-2.24632	4.86165
C	-1.83157	-0.38448	3.77511
C	-1.78290	-2.68763	2.72124
C	-2.11337	-2.27603	-2.62254
C	-2.61432	-2.98979	-1.35831
C	-3.03987	-1.10826	-2.99789
C	-2.02503	-3.28604	-3.77626
H	-2.99495	5.42566	0.32399
H	-1.26653	5.37872	0.76331
H	-2.67831	3.32449	-2.06545
H	-4.05252	3.42690	-0.92562
H	-3.11908	1.90212	-1.04802
H	-1.85635	3.26301	2.19742
H	-2.74374	1.91357	1.40631
H	-3.54488	3.48807	1.64942
H	0.03653	-1.52445	5.46298
H	0.06127	-3.15927	4.72067
H	-1.43563	-2.52305	5.43960
H	-1.24143	0.38072	4.30613
H	-2.71020	-0.64007	4.38910
H	-1.16339	-3.57635	2.51555
H	-2.67137	-3.00237	3.29208
H	-2.12398	-2.26893	1.76125
H	-3.57301	-3.48551	-1.58171
H	-1.89305	-3.75606	-1.02829
H	-4.05095	-1.48939	-3.21856
H	-3.10296	-0.40204	-2.15557
H	-1.28842	-4.07909	-3.56421
H	-1.76990	-2.80837	-4.73602
H	-3.01069	-3.76012	-3.90353
H	-1.77191	5.42477	-0.95795
H	-2.66288	-0.58653	-3.89419
H	-2.19287	0.04505	2.82743
C	3.90346	1.27840	0.01327
C	5.29162	1.31391	0.00318
C	5.99874	0.22523	-0.51661
C	5.28366	-0.88089	-0.98629
C	3.89580	-0.85639	-0.94918
H	3.31621	2.08863	0.44572
H	5.80405	2.18781	0.41156
H	7.09232	0.23065	-0.53740
H	5.78968	-1.76868	-1.37207
H	3.30194	-1.71311	-1.26840
H	0.19865	4.60709	-1.23615
H	2.29721	2.86266	-1.46661
H	1.87047	-1.85723	4.01739
H	3.38800	-0.89168	1.94042
H	0.19367	-2.05920	-4.29736
H	2.29691	-0.75811	-3.12268
H	-2.78125	-2.26747	-0.54750
N	3.21495	0.22341	-0.48988

[$L_3Co^{III}O$] (*S* =2)

```
74
o_u4.out Energy: -1806766.0662013
C          -0.39085        1.64084       -0.01384
N          -0.75437        2.89284       -0.38690
C           0.31078        3.53946       -1.00146
C           1.35717        2.66471       -0.99910
N           0.92747        1.51230       -0.35078
B           1.59019        0.10648       -0.25771
N           1.34191       -0.54020        1.13152
C           0.08779       -0.75396        1.62283
N           0.24400       -1.32307        2.84007
C           1.59718       -1.47073        3.12933
C           2.28413       -0.98233        2.05924
N           0.93681       -0.73608       -1.40348
C          -0.38297       -1.06349       -1.28992
N          -0.74622       -1.60434       -2.47733
C           0.32362       -1.58148       -3.36028
C           1.37233       -1.01612       -2.69173
Co         -1.40119       -0.17718        0.32333
O          -2.98371       -0.18579        0.90265
C          -2.13361        3.45578       -0.19001
C          -2.12810        4.95195       -0.52744
C          -3.10179        2.70966       -1.12350
C          -2.53227        3.25050        1.28004
C          -0.90666       -1.70392        3.72633
C          -0.37538       -2.35709        5.00736
C          -1.68829       -0.42439        4.06735
C          -1.79693       -2.69697        2.96044
C          -2.12815       -2.12395       -2.75465
C          -2.46170       -3.18252       -1.69059
C          -3.11727       -0.94883       -2.67760
C          -2.16776       -2.75393       -4.15160
H          -3.13039        5.36083       -0.32619
H          -1.40604        5.50799        0.09334
H          -2.75736        2.76235       -2.16996
H          -4.10272        3.16771       -1.06225
H          -3.19132        1.65532       -0.82253
H          -1.81035        3.74490        1.95167
H          -2.58038        2.17771        1.52121
H          -3.52819        3.69018        1.45394
H           0.25720       -1.66729        5.59027
H           0.19663       -3.27556        4.79434
H          -1.23231       -2.63627        5.63996
H          -1.03420        0.30756        4.57086
H          -2.52287       -0.66946        4.74505
H          -1.21595       -3.58088        2.64753
H          -2.61996       -3.03314        3.61244
H          -2.23529       -2.21435        2.07349
H          -3.46997       -3.58784       -1.87434
H          -1.73769       -4.01367       -1.72544
H          -4.12140       -1.29051       -2.97735
H          -3.18642       -0.56102       -1.64901
H          -1.45038       -3.58583       -4.24627
H          -1.96576       -2.01302       -4.94260
H          -3.17616       -3.15963       -4.32658
```

H	-1.90455	5.13683	-1.59113
H	-2.80983	-0.13103	-3.35018
H	-2.10315	0.02280	3.15063
C	3.84771	1.22921	0.13445
C	5.23572	1.26848	0.15240
C	5.95593	0.18850	-0.36740
C	5.25296	-0.91316	-0.86501
C	3.86446	-0.89216	-0.85466
H	3.25013	2.03119	0.56811
H	5.73741	2.13770	0.58346
H	7.04968	0.19653	-0.36594
H	5.76857	-1.79554	-1.25043
H	3.28076	-1.74865	-1.19221
H	0.26141	4.55295	-1.38736
H	2.35260	2.79127	-1.41851
H	1.97420	-1.90175	4.05156
H	3.35946	-0.92653	1.91130
H	0.27718	-1.95684	-4.37802
H	2.37140	-0.79368	-3.05946
H	-2.44541	-2.74286	-0.68088
N	3.17121	0.18018	-0.39690

[$L_3Co^{III}OH]^+$ (*S* =0)

75
p_u0.out Energy: -1807065.4647240

C	-0.39517	-1.18985	-1.00521
N	-0.94877	-2.30014	-1.56984
C	0.04950	-3.25863	-1.72359
C	1.20602	-2.73635	-1.23484
N	0.92448	-1.44828	-0.81220
B	1.69020	-0.47682	0.12191
N	1.54079	0.95655	-0.42904
C	0.31346	1.50557	-0.55634
N	0.48182	2.81822	-0.87613
C	1.84960	3.06705	-0.98325
C	2.50671	1.91007	-0.70161
N	0.91696	-0.55531	1.47010
C	-0.38641	-0.14991	1.42548
N	-0.92142	-0.43994	2.63792
C	0.03156	-1.07084	3.42964
C	1.17341	-1.15896	2.69071
Co	-1.16269	0.38777	-0.29492
O	-2.10539	0.88738	-1.73461
C	-2.38755	-2.55906	-1.97431
C	-2.60925	-4.07720	-2.08355
C	-3.33093	-2.01066	-0.89616
C	-2.64368	-1.90120	-3.33771
C	-0.55034	3.91145	-1.06510
C	0.09397	5.26046	-0.69827
C	-0.98999	3.92350	-2.53618
C	-1.74436	3.67067	-0.13154
C	-2.31584	-0.17431	3.12135
C	-3.10235	0.61297	2.07210
C	-2.99712	-1.52763	3.38300
C	-2.22252	0.66032	4.41052
H	-3.67701	-4.25316	-2.28356

H -2.04913 -4.52711 -2.91812
H -3.06282 -2.40377 0.09785
H -4.36246 -2.32198 -1.12203
H -3.32866 -0.91170 -0.88230
H -1.91895 -2.26053 -4.08661
H -2.57892 -0.80857 -3.25753
H -3.65700 -2.16140 -3.68417
H 0.87649 5.56674 -1.40977
H 0.51736 5.24287 0.31937
H -0.68659 6.03562 -0.73131
H -0.12362 4.05298 -3.20548
H -1.68476 4.76243 -2.70407
H -1.40759 3.46010 0.89717
H -2.36944 4.57655 -0.10652
H -2.37373 2.85185 -0.50182
H -4.11312 0.81257 2.46044
H -2.63830 1.58838 1.85727
H -4.02864 -1.36190 3.73203
H -3.03387 -2.12948 2.46045
H -1.69169 1.60795 4.22170
H -1.70038 0.12021 5.21583
H -3.23710 0.89383 4.76995
H -2.34869 -4.59769 -1.14749
H -2.46778 -2.10775 4.15557
H -1.51154 2.99037 -2.79019
C 3.90106 -1.16542 -0.89937
C 5.28110 -1.30920 -0.90455
C 6.00318 -1.01030 0.25565
C 5.31267 -0.54814 1.38046
C 3.93122 -0.42381 1.32497
H 3.30871 -1.34470 -1.79714
H 5.77747 -1.64173 -1.81894
H 7.09152 -1.11705 0.27598
H 5.83467 -0.27031 2.29878
H 3.36536 -0.02038 2.16428
H -0.12894 -4.23220 -2.16587
H 2.18481 -3.20077 -1.14919
H 2.25069 4.03983 -1.24562
H 3.57457 1.70887 -0.67251
H -0.16798 -1.40300 4.44510
H 2.12307 -1.61688 2.95501
H -3.24428 0.04109 1.14019
H -1.63124 0.90296 -2.58212
N 3.23078 -0.76249 0.21221

[$L_3Co^{III}OH]^+$ (*S* =1)

75
p_u2.out Energy: -1807056.4824530
C -0.47008 -1.36550 -0.96476
N -0.95503 -2.51417 -1.49075
C 0.07834 -3.43202 -1.61908
C 1.21127 -2.83136 -1.15189
N 0.86652 -1.54197 -0.77563
B 1.62399 -0.46789 0.06703
N 1.46488 0.96413 -0.51814
C 0.26840 1.60636 -0.51508
N 0.49446 2.88989 -0.87910

C	1.85166	3.04667	-1.15698
C	2.45488	1.84944	-0.92654
N	0.89172	-0.48899	1.44324
C	-0.41012	-0.09564	1.41863
N	-0.94091	-0.39325	2.62791
C	0.02327	-1.01488	3.41038
C	1.15924	-1.09777	2.65807
Co	-1.23064	0.39271	-0.30057
O	-2.12228	0.88224	-1.76031
C	-2.37327	-2.75048	-1.94432
C	-2.62366	-4.26159	-2.04395
C	-3.34281	-2.14302	-0.91945
C	-2.54120	-2.08264	-3.31808
C	-0.48869	4.03050	-0.97022
C	0.18974	5.29364	-0.40984
C	-0.85906	4.22902	-2.44778
C	-1.73556	3.72731	-0.13156
C	-2.34302	-0.14580	3.10083
C	-3.13032	0.60307	2.02387
C	-2.99788	-1.50834	3.38011
C	-2.27402	0.71337	4.37392
H	-3.67998	-4.42464	-2.30678
H	-2.01832	-4.73458	-2.83338
H	-3.11670	-2.49646	0.09934
H	-4.37146	-2.44480	-1.17075
H	-3.31840	-1.04406	-0.94845
H	-1.83270	-2.50822	-4.04799
H	-2.37266	-0.99828	-3.23360
H	-3.56536	-2.25142	-3.68907
H	1.03018	5.63701	-1.03246
H	0.55358	5.12317	0.61668
H	-0.54771	6.11071	-0.38446
H	0.03617	4.41777	-3.06242
H	-1.53590	5.09240	-2.54898
H	-1.46311	3.46993	0.90500
H	-2.36980	4.62683	-0.10627
H	-2.32987	2.91428	-0.57000
H	-4.15749	0.77377	2.38112
H	-2.69333	1.59085	1.80800
H	-4.03500	-1.35638	3.71840
H	-3.01548	-2.12634	2.46764
H	-1.76164	1.66823	4.17146
H	-1.74531	0.19675	5.19050
H	-3.29542	0.93192	4.72332
H	-2.42719	-4.76961	-1.08531
H	-2.46361	-2.06366	4.16727
H	-1.37943	3.34379	-2.84699
C	3.83281	-1.17959	-0.95294
C	5.21351	-1.31779	-0.96612
C	5.94557	-0.96853	0.17356
C	5.26426	-0.46037	1.28414
C	3.88189	-0.34328	1.23685
H	3.23221	-1.39905	-1.83618
H	5.70226	-1.68654	-1.87065
H	7.03435	-1.07166	0.18819
H	5.79397	-0.14208	2.18475
H	3.32253	0.09350	2.06382
H	-0.05597	-4.43227	-2.01827
H	2.20912	-3.24990	-1.04885

H	2.28232	3.98751	-1.48633
H	3.50378	1.58088	-1.02056
H	-0.16439	-1.34349	4.42945
H	2.11304	-1.55451	2.90992
H	-3.22768	0.01037	1.09703
H	-1.61393	1.31893	-2.46481
N	3.17169	-0.73342	0.14749

[$L_3Co^{III}OH]^+$ (*S* =2)

75
p_u4.out Energy: -1807047.4009226

C	-0.42175	-1.22067	-1.01330
N	-0.85529	-2.32373	-1.66489
C	0.13552	-3.29521	-1.64399
C	1.20194	-2.76630	-0.97808
N	0.86372	-1.46655	-0.62766
B	1.60145	-0.44190	0.28604
N	1.48571	0.99365	-0.31930
C	0.28653	1.57428	-0.57841
N	0.53248	2.79661	-1.10661
C	1.89908	2.99336	-1.18127
C	2.49543	1.86418	-0.68638
N	0.86264	-0.50860	1.65655
C	-0.42355	-0.06403	1.74097
N	-0.87526	-0.39005	2.97379
C	0.10652	-1.09303	3.65545
C	1.18538	-1.18406	2.82419
Co	-1.28913	0.43218	-0.07736
O	-3.07310	0.55156	-0.17252
C	-2.22157	-2.48606	-2.28124
C	-2.22359	-3.72285	-3.18930
C	-3.24088	-2.66291	-1.14528
C	-2.52573	-1.23665	-3.12254
C	-0.53733	3.75011	-1.57057
C	0.11284	5.05565	-2.04225
C	-1.28745	3.08785	-2.73712
C	-1.47745	4.03790	-0.39002
C	-2.26062	-0.10122	3.49411
C	-2.61283	1.35866	3.16852
C	-3.23228	-1.07929	2.81552
C	-2.28114	-0.30326	5.01492
H	-3.20501	-3.78961	-3.68332
H	-1.45310	-3.65439	-3.97485
H	-2.97702	-3.53055	-0.51810
H	-4.24197	-2.83564	-1.57271
H	-3.28954	-1.76152	-0.51795
H	-1.75283	-1.08617	-3.89397
H	-2.58740	-0.33458	-2.49821
H	-3.49893	-1.36404	-3.62261
H	0.78163	4.89565	-2.90326
H	0.67473	5.54876	-1.23243
H	-0.68278	5.74428	-2.36508
H	-0.59862	2.86104	-3.56713
H	-2.07104	3.76774	-3.10721
H	-0.91748	4.43580	0.47169
H	-2.23035	4.78205	-0.69391
H	-2.01708	3.13448	-0.06776

H -3.59119 1.60072 3.61319
H -1.85946 2.04598 3.58686
H -4.25259 -0.91067 3.19640
H -3.24528 -0.92708 1.72677
H -1.53757 0.33439 5.52086
H -2.10938 -1.35387 5.29882
H -3.27803 -0.02473 5.38951
H -2.08009 -4.65661 -2.62215
H -2.94864 -2.12261 3.03188
H -1.77178 2.14901 -2.42589
C 3.83981 -1.18062 -0.67266
C 5.22127 -1.31170 -0.65165
C 5.92679 -0.93196 0.49473
C 5.21826 -0.40038 1.57703
C 3.83683 -0.29235 1.49666
H 3.26188 -1.42449 -1.56412
H 5.73127 -1.69898 -1.53648
H 7.01546 -1.02884 0.53601
H 5.72576 -0.05631 2.48095
H 3.25749 0.15900 2.30200
H 0.02395 -4.27548 -2.09628
H 2.15309 -3.23225 -0.73259
H 2.35654 3.89833 -1.56916
H 3.55480 1.64603 -0.57972
H -0.01831 -1.47050 4.66543
H 2.13543 -1.68535 2.99188
H -2.69255 1.52643 2.08532
H -3.58287 1.25654 -0.60835
N 3.15085 -0.71388 0.40189

[$L_3Co^{II}O]^-$ (*S* =1/2)

74
r_u1.out Energy: -1806847.1216684
C -0.34263 -1.00040 -1.11553
N -0.85021 -1.86655 -2.04341
C 0.12542 -2.79657 -2.39747
C 1.24734 -2.48603 -1.68581
N 0.95372 -1.36351 -0.93170
B 1.72952 -0.57000 0.16825
N 1.51993 0.94505 -0.16071
C 0.28425 1.47615 -0.31386
N 0.46540 2.78620 -0.66998
C 1.83451 3.05395 -0.72363
C 2.48659 1.90082 -0.40502
N 0.91114 -0.86120 1.46734
C -0.40416 -0.51239 1.50027
N -0.90595 -1.02262 2.67031
C 0.10273 -1.71931 3.33339
C 1.22795 -1.62677 2.57250
Co -1.21608 0.37578 0.00755
O -2.56451 1.25450 0.42522
C -2.22399 -1.77747 -2.63368
C -2.42723 -2.90185 -3.65762
C -3.26367 -1.91448 -1.51087
C -2.35239 -0.41361 -3.33240
C -0.60257 3.81085 -0.93935
C 0.04192 5.09830 -1.47501

```
C          -1.56904        3.26022       -2.00051
C          -1.33357        4.10793        0.37951
C          -2.29801       -0.85235        3.21986
C          -2.53407        0.64412        3.47877
C          -3.31138       -1.41645        2.21240
C          -2.43109       -1.62530        4.54115
H          -3.43865       -2.80906       -4.08320
H          -1.70816       -2.83719       -4.49057
H          -3.10135       -2.84174       -0.93702
H          -4.27806       -1.93910       -1.94171
H          -3.20963       -1.05807       -0.82212
H          -1.60505       -0.31760       -4.13783
H          -2.19707        0.40666       -2.61516
H          -3.35820       -0.30494       -3.77030
H           0.60615        4.92290       -2.40620
H           0.70719        5.57199       -0.73478
H          -0.76136        5.81714       -1.70002
H          -1.02263        2.97695       -2.91597
H          -2.30880        4.03508       -2.26099
H          -0.61893        4.46401        1.14167
H          -2.08601        4.89804        0.21493
H          -1.84456        3.19748        0.73284
H          -3.53308        0.78750        3.92444
H          -1.78048        1.03323        4.18520
H          -4.32407       -1.37381        2.64632
H          -3.30642       -0.82022        1.29170
H          -1.74582       -1.24751        5.31747
H          -2.26627       -2.70765        4.40936
H          -3.45792       -1.48872        4.91455
H          -2.34984       -3.89869       -3.19298
H          -3.07817       -2.46768        1.97249
H          -2.10849        2.38719       -1.60932
C           3.98745       -1.11281       -0.87440
C           5.35494       -1.21897       -0.82418
C           6.06593       -1.03032        0.39414
C           5.29241       -0.61004        1.51195
C           3.92566       -0.51072        1.43496
H           3.44793       -1.17616       -1.81926
H           5.88839       -1.42586       -1.75797
H           7.15283       -1.12272        0.44748
H           5.77548       -0.32912        2.45380
H           3.33554       -0.11765        2.26354
H          -0.03881       -3.59475       -3.11396
H           2.21370       -2.98355       -1.66583
H           2.23970        4.02658       -0.97975
H           3.55105        1.68825       -0.33692
H          -0.04334       -2.21993        4.28375
H           2.21642       -2.04713        2.73881
H          -2.48732        1.20124        2.52988
N           3.20904       -0.87292        0.27529
```

[$L_3Co^{II}O]^-$ (*S* =3/2)

```
74
r_u3.out Energy: -1806843.4922917
C          -0.39059       -0.92717       -1.34195
```

N	-0.84690	-1.85394	-2.22736
C	0.10266	-2.86071	-2.38591
C	1.16534	-2.53023	-1.59813
N	0.86917	-1.32130	-0.99034
B	1.66335	-0.56143	0.13705
N	1.53956	0.96416	-0.16436
C	0.32487	1.53643	-0.28770
N	0.52793	2.85350	-0.55249
C	1.90262	3.10325	-0.59481
C	2.53007	1.91573	-0.35052
N	0.85530	-0.83904	1.45902
C	-0.40608	-0.34090	1.62184
N	-0.87416	-0.86245	2.78808
C	0.06975	-1.73414	3.32624
C	1.14100	-1.72737	2.48266
Co	-1.20759	0.38729	-0.06761
O	-2.86316	0.35438	-0.06883
C	-2.20486	-1.85433	-2.86273
C	-2.18256	-2.74874	-4.11128
C	-3.20912	-2.39602	-1.83199
C	-2.56668	-0.41814	-3.27147
C	-0.57450	3.83932	-0.77782
C	0.01673	5.23216	-1.02469
C	-1.37838	3.38686	-2.00859
C	-1.46460	3.86681	0.47594
C	-2.23589	-0.61577	3.36496
C	-2.58370	0.87233	3.20532
C	-3.24078	-1.49477	2.60217
C	-2.23040	-0.97972	4.85717
H	-3.15867	-2.67369	-4.61576
H	-1.40321	-2.42955	-4.82359
H	-2.93223	-3.41838	-1.52198
H	-4.21989	-2.42896	-2.27274
H	-3.22588	-1.73195	-0.95367
H	-1.78911	0.01066	-3.92576
H	-2.68901	0.21400	-2.38067
H	-3.52130	-0.42854	-3.82298
H	0.65354	5.25406	-1.92426
H	0.60408	5.58590	-0.16132
H	-0.80927	5.94316	-1.18268
H	-0.73094	3.34220	-2.90029
H	-2.19939	4.09581	-2.20454
H	-0.87497	4.14389	1.36570
H	-2.27341	4.60426	0.34560
H	-1.92522	2.88212	0.65244
H	-3.54379	1.07578	3.70772
H	-1.80715	1.50726	3.66408
H	-4.25287	-1.35679	3.01891
H	-3.25056	-1.20222	1.54049
H	-1.45316	-0.42266	5.40690
H	-2.08168	-2.05868	5.02576
H	-3.20927	-0.71606	5.28754
H	-2.02587	-3.81141	-3.86443
H	-2.97017	-2.56077	2.69397
H	-1.81656	2.38967	-1.84475
C	3.88616	-1.12655	-0.95631
C	5.25171	-1.26228	-0.93614
C	5.98647	-1.16045	0.27829
C	5.23869	-0.79876	1.43378

C	3.87327	-0.66812	1.38688
H	3.32743	-1.13362	-1.89255
H	5.76524	-1.42607	-1.88949
H	7.07214	-1.27563	0.30679
H	5.74177	-0.59032	2.38397
H	3.30469	-0.32324	2.25093
H	-0.03553	-3.71439	-3.04194
H	2.10298	-3.05766	-1.43969
H	2.32269	4.08485	-0.79003
H	3.58965	1.67552	-0.29447
H	-0.07773	-2.27552	4.25546
H	2.07785	-2.27587	2.54539
H	-2.68878	1.12975	2.14214
N	3.13005	-0.94020	0.21955

[$L_3Co^{II}O]^-$ (*S* =5/2)

74
r_u5.out Energy: -1806840.7684551

C	-0.43730	-1.00871	-1.31008
N	-0.86910	-1.99212	-2.14142
C	0.13051	-2.94360	-2.31304
C	1.19896	-2.52487	-1.57256
N	0.84963	-1.31806	-0.98757
B	1.61755	-0.49891	0.11747
N	1.46642	1.03631	-0.18944
C	0.27690	1.67789	-0.33582
N	0.56784	2.98044	-0.57456
C	1.94955	3.16481	-0.58251
C	2.50772	1.94406	-0.33926
N	0.84098	-0.83265	1.45458
C	-0.44707	-0.42552	1.61722
N	-0.89200	-1.00208	2.76251
C	0.10168	-1.80630	3.30563
C	1.18045	-1.70936	2.47066
Co	-1.34217	0.42533	-0.07532
O	-2.86816	1.07507	-0.39630
C	-2.24395	-2.02907	-2.73666
C	-2.33819	-3.18061	-3.74524
C	-3.26134	-2.23853	-1.60184
C	-2.49981	-0.68840	-3.44492
C	-0.47740	4.02859	-0.80078
C	0.19309	5.39048	-1.01673
C	-1.28953	3.63479	-2.04616
C	-1.38622	4.08119	0.43960
C	-2.27299	-0.79020	3.30399
C	-2.50528	0.72328	3.44837
C	-3.28557	-1.39771	2.31774
C	-2.39997	-1.47098	4.67203
H	-3.33941	-3.16712	-4.20358
H	-1.59556	-3.07680	-4.55379
H	-3.01934	-3.14409	-1.02036
H	-4.27352	-2.35360	-2.02407
H	-3.26803	-1.36634	-0.93056
H	-1.74017	-0.50938	-4.22451
H	-2.47875	0.13920	-2.71914
H	-3.49351	-0.70683	-3.92272

```
H          0.84494        5.39140       -1.90614
H          0.78543        5.70041       -0.13964
H         -0.59012        6.14809       -1.17659
H         -0.62987        3.54204       -2.92579
H         -2.04657        4.40851       -2.25805
H         -0.79431        4.28910        1.34713
H         -2.13381        4.88304        0.31892
H         -1.91937        3.12547        0.56116
H         -3.51138        0.90761        3.85959
H         -1.76041        1.16864        4.12900
H         -4.30201       -1.33327        2.73999
H         -3.27869       -0.84637        1.36449
H         -1.66597       -1.07605        5.39386
H         -2.27839       -2.56438        4.60007
H         -3.40640       -1.27441        5.07335
H         -2.20733       -4.16379       -3.26362
H         -3.05394       -2.45779        2.12101
H         -1.80606        2.67806       -1.87143
C          3.84967       -1.01434       -0.98917
C          5.21692       -1.13236       -0.97736
C          5.95741       -1.02402        0.23314
C          5.21173       -0.67166        1.39274
C          3.84438       -0.55889        1.35365
H          3.28655       -1.02245       -1.92281
H          5.72696       -1.28624       -1.93420
H          7.04456       -1.12570        0.25533
H          5.71753       -0.45517        2.33967
H          3.27833       -0.21446        2.21950
H          0.02374       -3.82628       -2.93604
H          2.16882       -2.99553       -1.43049
H          2.42806        4.12374       -0.75594
H          3.55474        1.66076       -0.26339
H         -0.01465       -2.37454        4.22356
H          2.15042       -2.19636        2.53686
H         -2.43411        1.22392        2.46999
N          3.09749       -0.83971        0.19091
```

[L$_3$Co^{II}OH] (*S* =1/2)

```
75
h_u1.out Energy: -1807171.0519584
C          0.35127       -0.63467        1.32670
N          0.85086       -1.27835        2.42357
C         -0.12765       -2.10681        2.96814
C         -1.24631       -1.96213        2.20287
N         -0.95281       -1.02127        1.22363
B         -1.65143       -0.50039       -0.05514
N         -1.48842        1.04150       -0.10090
C         -0.25795        1.61924        0.04088
N         -0.47953        2.96668        0.05269
C         -1.83954        3.22595       -0.10719
C         -2.46709        2.02258       -0.19981
N         -0.91521       -1.20178       -1.22783
C          0.42684       -0.95775       -1.36636
N          0.85943       -1.84524       -2.30945
C         -0.18932       -2.66054       -2.72328
C         -1.29398       -2.27028       -2.03035
```

Co	1.21303	0.38493	-0.04950
O	2.59173	1.13103	-1.06332
C	2.21531	-1.03882	2.99195
C	2.48340	-2.02642	4.13473
C	3.26388	-1.24291	1.88848
C	2.25976	0.40381	3.52318
C	0.57721	4.02607	0.12424
C	-0.05768	5.36532	0.52906
C	1.61374	3.63434	1.18819
C	1.21751	4.14694	-1.26869
C	2.25260	-1.90762	-2.86784
C	2.49481	-0.62500	-3.67986
C	3.25283	-2.01755	-1.70785
C	2.39277	-3.13848	-3.77487
H	3.49876	-1.85006	4.52241
H	1.78157	-1.88933	4.97326
H	3.15755	-2.23421	1.42069
H	4.27571	-1.16038	2.31708
H	3.18216	-0.47480	1.10139
H	1.50418	0.55221	4.31264
H	2.05955	1.12130	2.71236
H	3.25463	0.62373	3.94366
H	-0.60176	5.28396	1.48475
H	-0.74323	5.75341	-0.24112
H	0.74341	6.11041	0.65451
H	1.13247	3.48802	2.16899
H	2.36611	4.43370	1.28115
H	0.46517	4.46096	-2.01174
H	2.02493	4.89786	-1.25378
H	1.63272	3.17557	-1.57713
H	3.49827	-0.66027	-4.13769
H	1.74980	-0.53596	-4.48944
H	4.26772	-2.16596	-2.11254
H	3.25684	-1.09349	-1.11577
H	1.73207	-3.08593	-4.65570
H	2.19252	-4.07693	-3.23095
H	3.42880	-3.18012	-4.14551
H	2.43033	-3.07212	3.78928
H	3.00809	-2.87569	-1.05967
H	2.13614	2.70547	0.92085
C	-3.93350	-0.75855	1.06584
C	-5.31970	-0.84751	1.06404
C	-5.99803	-0.90746	-0.15700
C	-5.25828	-0.84732	-1.34224
C	-3.87402	-0.75901	-1.27300
H	-3.37241	-0.66256	1.99492
H	-5.85323	-0.85703	2.01712
H	-7.08910	-0.97930	-0.18492
H	-5.74263	-0.85635	-2.32121
H	-3.26355	-0.66679	-2.17162
H	0.03334	-2.73117	3.84114
H	-2.20036	-2.47697	2.28683
H	-2.25846	4.22655	-0.13670
H	-3.52711	1.81273	-0.31953
H	-0.08682	-3.44849	-3.46211
H	-2.29396	-2.69660	-2.05010
H	2.44128	0.25094	-3.01364
H	2.93432	1.98533	-0.76282
N	-3.21850	-0.75289	-0.08531

[$L_3Co^{II}OH$] (*S* =3/2)

```
75
h_u3.out Energy: -1807177.1344705
C           0.40945       -0.63303        1.51225
N           0.85176       -1.40225        2.53817
C          -0.14103       -2.29004        2.93871
C          -1.22492       -2.05020        2.14663
N          -0.89297       -0.99664        1.30008
B          -1.61452       -0.44975        0.02856
N          -1.51890        1.10208       -0.06080
C          -0.31732        1.74686       -0.10485
N          -0.59502        3.06921       -0.18491
C          -1.97260        3.27159       -0.19229
C          -2.54984        2.03911       -0.11574
N          -0.89676       -1.12878       -1.17626
C           0.40814       -0.79277       -1.42403
N           0.84235       -1.66029       -2.37218
C          -0.15567       -2.57749       -2.68318
C          -1.23665       -2.25685       -1.91686
Co          1.24523        0.47590       -0.01593
O           3.05446        0.93720       -0.17756
C           2.23904       -1.30645        3.10132
C           2.34321       -2.17674        4.35949
C           3.23675       -1.78858        2.03525
C           2.51284        0.16345        3.45920
C           0.47372        4.11923       -0.22328
C          -0.16777        5.50309       -0.37311
C           1.26323        4.04119        1.09433
C           1.39894        3.83157       -1.41801
C           2.23352       -1.64330       -2.93271
C           2.55364       -0.21141       -3.39208
C           3.20215       -2.08216       -1.82315
C           2.31891       -2.60507       -4.12421
H           3.34953       -2.05646        4.78992
H           1.60988       -1.87652        5.12639
H           2.97062       -2.79675        1.67610
H           4.25018       -1.82944        2.46803
H           3.25710       -1.09036        1.18384
H           1.77002        0.53856        4.18270
H           2.47904        0.79177        2.55622
H           3.51662        0.25611        3.90490
H          -0.82375        5.74778        0.47864
H          -0.74844        5.58371       -1.30702
H           0.62974        6.26157       -0.40745
H           0.60082        4.20504        1.96068
H           2.05429        4.80870        1.10610
H           0.82079        3.78424       -2.35604
H           2.14511        4.63827       -1.50884
H           1.93677        2.88043       -1.27469
H           3.55235       -0.19146       -3.85890
H           1.81469        0.13356       -4.13484
H           4.22867       -2.13466       -2.22252
H           3.19198       -1.35330       -0.99972
H           1.59753       -2.33989       -4.91513
```

H	2.15205	-3.65276	-3.82419
H	3.33040	-2.54361	-4.55504
H	2.20681	-3.24692	4.13253
H	2.92762	-3.07768	-1.43515
H	1.73791	3.05245	1.19563
C	-3.85600	-0.70991	1.22363
C	-5.23870	-0.83241	1.26983
C	-5.95131	-0.97526	0.07530
C	-5.24912	-0.96170	-1.13381
C	-3.86609	-0.83627	-1.11301
H	-3.26806	-0.55293	2.12809
H	-5.74329	-0.80246	2.23810
H	-7.04052	-1.07474	0.08544
H	-5.76200	-1.03549	-2.09535
H	-3.28638	-0.77799	-2.03436
H	-0.01986	-3.01150	3.74096
H	-2.18451	-2.56201	2.13410
H	-2.43969	4.24997	-0.25181
H	-3.60672	1.78477	-0.09942
H	-0.03907	-3.37313	-3.41256
H	-2.19907	-2.75940	-1.85391
H	2.56309	0.48063	-2.53644
H	3.40521	1.57073	0.46677
N	-3.17576	-0.75066	0.05113

[$L_3Co^{II}OH$] (*S* =5/2)

75
h_u5.out Energy: -1807132.6979396

C	0.40433	-0.64090	1.52575
N	0.84717	-1.34329	2.59649
C	-0.15191	-2.20845	3.02408
C	-1.22499	-2.01448	2.20196
N	-0.88216	-1.02078	1.30158
B	-1.67253	-0.53057	0.02912
N	-1.51386	1.04547	-0.06202
C	-0.32129	1.68266	-0.09737
N	-0.57057	3.01491	-0.16504
C	-1.93897	3.21699	-0.17388
C	-2.52689	1.97719	-0.11000
N	-0.88102	-1.16106	-1.17940
C	0.40480	-0.80447	-1.44208
N	0.85116	-1.61869	-2.42936
C	-0.14419	-2.52790	-2.76024
C	-1.21971	-2.24763	-1.96530
Co	1.24509	0.44622	-0.02736
O	3.02636	0.69741	-0.03367
C	2.23045	-1.24799	3.17758
C	2.26158	-1.95839	4.53715
C	3.20506	-1.92785	2.20282
C	2.58421	0.23573	3.36756
C	0.50296	4.06420	-0.19141
C	-0.13755	5.45180	-0.30358
C	1.30329	3.95795	1.11733
C	1.40317	3.80369	-1.40991
C	2.23588	-1.58236	-3.01305
C	2.57494	-0.12913	-3.38283

```
C          3.20950       -2.12998       -1.95759
C          2.28032       -2.45439       -4.27445
H          3.26286       -1.82937        4.97625
H          1.52555       -1.52972        5.23716
H          2.91981       -2.97995        2.03672
H          4.22507       -1.90492        2.62007
H          3.21991       -1.40122        1.23765
H          1.82726        0.74326        3.98779
H          2.66632        0.75270        2.40125
H          3.56055        0.31462        3.87220
H         -0.78178        5.67738        0.56169
H         -0.72685        5.55542       -1.22924
H          0.66273        6.20728       -0.32922
H          0.64730        4.10229        1.99122
H          2.09054        4.72837        1.13687
H          0.81438        3.80401       -2.34151
H          2.17162        4.59002       -1.47830
H          1.92013        2.83503       -1.32605
H          3.55820       -0.10063       -3.87937
H          1.82198        0.28366       -4.07417
H          4.23327       -2.14337       -2.36580
H          3.20822       -1.49402       -1.06096
H          1.54757       -2.11964       -5.02707
H          2.10512       -3.51893       -4.05008
H          3.28420       -2.37474       -4.71931
H          2.08185       -3.04160        4.44487
H          2.93451       -3.15861       -1.67093
H          1.78818        2.97277        1.21006
C         -3.89093       -0.74479        1.24002
C         -5.25660       -0.87643        1.25914
C         -5.99582       -1.08274        0.06232
C         -5.25735       -1.01863       -1.15087
C         -3.89167       -0.88530       -1.14824
H         -3.33026       -0.50730        2.14442
H         -5.76628       -0.78901        2.22422
H         -7.08136       -1.20041        0.06960
H         -5.76763       -1.04542       -2.11921
H         -3.33189       -0.75516       -2.07473
H         -0.04019       -2.88137        3.86824
H         -2.19587       -2.50340        2.20246
H         -2.39958        4.19894       -0.22444
H         -3.57992        1.70498       -0.09682
H         -0.02881       -3.28975       -3.52456
H         -2.18933       -2.73642       -1.91355
H          2.63413        0.51033       -2.49054
H          3.46042        1.56638        0.00675
N         -3.14037       -0.86926        0.04880
```

5. Thermodynamic cycle for the $L_4Co^{III}O$ oxidant

[$L_4Co^{III}O$] (*S* =0)

```
83
o_u0_opt.out      Energy: -2326435.7453302
```

C	1.28135	-0.59586	1.44445
N	1.63045	-1.36471	2.51130
C	0.55842	-2.19114	2.83909
C	-0.49495	-1.84719	2.01087
N	-0.05233	-0.79947	1.21272
B	-0.66308	-0.04209	-0.00275
N	-0.20663	1.44674	0.02848
C	1.13704	1.69342	0.04324
N	1.30742	3.03943	0.06609
C	0.06009	3.65912	0.06355
C	-0.89358	2.65802	0.03912
N	-0.04485	-0.74758	-1.24500
C	1.28830	-0.52716	-1.46466
N	1.64410	-1.25146	-2.55994
C	0.57902	-2.07269	-2.92137
C	-0.47826	-1.76771	-2.08294
Co	2.30773	0.15962	0.01149
O	3.60539	-0.90293	-0.01585
C	2.95234	-1.32951	3.27368
C	2.63784	-1.34290	4.78066
C	3.76991	-2.55003	2.83433
C	3.70355	-0.02579	2.96720
C	2.62976	3.78080	0.08758
C	2.68590	4.62102	1.37382
C	3.78571	2.77828	0.09298
C	2.71429	4.64378	-1.18180
C	2.96447	-1.17205	-3.32081
C	3.70318	0.12406	-2.95779
C	3.79376	-2.40311	-2.93627
C	2.64792	-1.12304	-4.82663
H	3.58321	-1.21468	5.32954
H	1.96863	-0.50922	5.05040
H	3.25681	-3.49364	3.08337
H	4.74134	-2.54398	3.35432
H	3.94177	-2.49884	1.74727
H	3.05200	0.85355	3.10302
H	4.11898	-0.02067	1.95250
H	4.53971	0.05634	3.67829
H	2.58858	3.97422	2.26111
H	1.90419	5.39404	1.41073
H	3.65918	5.13383	1.42307
H	3.76912	2.13639	0.98604
H	4.72909	3.34543	0.11883
H	1.93298	5.41729	-1.22164
H	3.68846	5.15705	-1.20076
H	2.63633	4.01283	-2.08238
H	4.53895	0.24485	-3.66383
H	3.04378	1.00273	-3.05427
H	4.76374	-2.36597	-3.45767
H	3.96783	-2.39799	-1.84838
H	1.97259	-0.28331	-5.05976
H	2.21095	-2.05268	-5.21361
H	3.59164	-0.96511	-5.37060
H	2.19510	-2.28514	5.12848
H	3.28831	-3.33954	-3.22490
H	3.80439	2.16213	-0.81824
C	-2.92266	0.03332	1.16773
C	-4.31525	0.10221	1.21324
C	-5.04274	0.12969	0.00059

C	-4.31832	0.12425	-1.21400
C	-2.92533	0.05745	-1.17301
H	4.11775	0.08829	-1.94331
N	-2.25104	-0.03168	-0.00440
C	0.53963	-3.26977	3.76169
N	0.46155	-4.18895	4.47046
C	-1.75635	-2.48786	1.92271
N	-2.79473	-3.00565	1.82677
C	0.57158	-3.11607	-3.88381
N	0.50432	-4.00859	-4.62693
C	-1.73416	-2.42125	-2.01636
N	-2.76862	-2.94931	-1.93483
C	-2.29661	2.85538	0.02807
N	-3.44944	3.01608	0.01916
C	-0.20747	5.05257	0.08106
N	-0.47363	6.18500	0.09372
C	-4.97918	0.19783	-2.48171
N	-5.50908	0.25404	-3.51343
C	-6.47009	0.19288	0.00291
N	-7.63071	0.24499	0.00480
C	-4.97314	0.15510	2.48352
N	-5.50078	0.19523	3.51715
H	-2.34233	0.11438	-2.09253
H	-2.33719	0.06655	2.08713

[$L_4Co^{III}O$] (*S* =1)

83
o_u2_opt.out Energy: -2326433.8551336

C	-1.27521	-0.52518	-1.55194
N	-1.58594	-1.30572	-2.61497
C	-0.50916	-2.14154	-2.89970
C	0.51163	-1.80151	-2.02970
N	0.04552	-0.74704	-1.25015
B	0.63696	-0.01824	0.00145
N	0.16517	1.46533	0.00549
C	-1.17804	1.69747	0.00443
N	-1.37533	3.03438	0.00753
C	-0.13853	3.67621	0.01079
C	0.83202	2.69049	0.00980
N	0.04361	-0.75425	1.24769
C	-1.27757	-0.53335	1.54864
N	-1.59025	-1.31929	2.60709
C	-0.51437	-2.15728	2.88889
C	0.50782	-1.81328	2.02211
Co	-2.30845	0.11397	-0.00082
O	-3.52645	-0.99293	-0.00467
C	-2.89128	-1.27437	-3.39677
C	-2.55110	-1.21933	-4.89649
C	-3.68646	-2.53144	-3.01980
C	-3.67997	-0.00867	-3.03717
C	-2.72228	3.72695	0.00693
C	-2.82416	4.57737	-1.26888
C	-3.82896	2.66838	0.00341
C	-2.82805	4.57263	1.28555
C	-2.89668	-1.29128	3.38725
C	-3.68451	-0.02363	3.03270

C	-3.69183	-2.54623	3.00319
C	-2.55847	-1.24345	4.88766
H	-3.49005	-1.10903	-5.46048
H	-1.91036	-0.35077	-5.12149
H	-3.14663	-3.45361	-3.29042
H	-4.64588	-2.53048	-3.56152
H	-3.88551	-2.52515	-1.93650
H	-3.06777	0.89882	-3.16589
H	-4.06008	-0.05457	-2.00903
H	-4.54104	0.05712	-3.71995
H	-2.70855	3.94531	-2.16455
H	-2.07262	5.38041	-1.30118
H	-3.81720	5.05209	-1.30431
H	-3.79804	2.04480	-0.90379
H	-4.80199	3.18320	0.00305
H	-2.07672	5.37561	1.32326
H	-3.82124	5.04716	1.31961
H	-2.71523	3.93727	2.17925
H	-4.54646	0.03907	3.71467
H	-3.07222	0.88304	3.16667
H	-4.65197	-2.54748	3.54364
H	-3.88944	-2.53464	1.91966
H	-1.91768	-0.37623	5.11758
H	-2.06914	-2.15615	5.25369
H	-3.49810	-1.13539	5.45095
H	-2.06092	-2.13010	-5.26616
H	-3.15276	-3.46991	3.27011
H	-3.80038	2.04130	0.90827
C	2.89786	0.10280	-1.16895
C	4.28988	0.18461	-1.21261
C	5.01627	0.20360	0.00084
C	4.29111	0.17593	1.21486
C	2.89906	0.09381	1.17221
H	-4.06336	-0.06448	2.00389
N	2.22654	0.01457	0.00169
C	-0.46253	-3.20705	-3.83615
N	-0.37553	-4.11024	-4.56424
C	1.77026	-2.44137	-1.90417
N	2.80702	-2.95744	-1.78439
C	-0.46978	-3.22775	3.81975
N	-0.38442	-4.13487	4.54312
C	1.76595	-2.45378	1.89465
N	2.80214	-2.97065	1.77336
C	2.23224	2.90618	0.01377
N	3.38319	3.07984	0.01735
C	0.09456	5.07559	0.01485
N	0.32425	6.21600	0.01806
C	4.95084	0.23927	2.48372
N	5.48012	0.28771	3.51616
C	6.44310	0.27774	0.00040
N	7.60330	0.33867	0.00004
C	4.94818	0.25617	-2.48177
N	5.47626	0.31107	-3.51451
H	2.31167	0.14106	-2.08781
H	2.31408	0.12440	2.09206

[$L_4Co^{III}O$] (*S* =2)

```
83
o_u4.out Energy: -2327548.5303866
C          1.27538       -0.38033        1.62002
N          1.58769       -1.02486        2.76332
C          0.48520       -1.78208        3.15481
C         -0.52147       -1.54516        2.23404
N         -0.02807       -0.62011        1.32515
B         -0.66227       -0.03293        0.00623
N         -0.10743        1.43956       -0.16783
C          1.22301        1.69376       -0.17538
N          1.41467        3.02147       -0.34319
C          0.16745        3.62925       -0.46319
C         -0.78746        2.63356       -0.34687
N         -0.03637       -0.90373       -1.14910
C          1.26571       -0.72589       -1.49494
N          1.57533       -1.59923       -2.47531
C          0.47489       -2.42544       -2.69315
C         -0.52802       -2.00454       -1.83648
Co         2.37072        0.08694       -0.00436
O          3.21367       -1.32346        0.14244
C          2.90522       -0.96175        3.52930
C          2.58402       -0.59288        4.98795
C          3.58446       -2.33254        3.40293
C          3.80097        0.13423        2.94286
C          2.73101        3.78186       -0.40467
C          2.71304        4.85844        0.69415
C          3.89676        2.83237       -0.13583
C          2.86179        4.37918       -1.81444
C          2.88024       -1.68546       -3.25848
C          3.80108       -0.52618       -2.86843
C          3.54815       -3.02536       -2.91933
C          2.53375       -1.55506       -4.75181
H          3.53257       -0.49485        5.53802
H          2.05215        0.37105        5.03919
H          2.98743       -3.13571        3.86217
H          4.55626       -2.29968        3.92019
H          3.75704       -2.57419        2.34191
H          3.27894        1.10317        2.89115
H          4.19471       -0.13689        1.95225
H          4.66978        0.25449        3.60738
H          2.55986        4.40020        1.68463
H          1.94059        5.62298        0.53258
H          3.68612        5.37341        0.69655
H          3.84343        2.39731        0.87302
H          4.82813        3.41842       -0.17119
H          2.06394        5.10218       -2.04053
H          3.82247        4.91241       -1.88684
H          2.84622        3.58249       -2.57612
H          4.64384       -0.50527       -3.57559
H          3.28404        0.44508       -2.93067
H          4.51693       -3.08207       -3.44012
H          3.72702       -3.09544       -1.83431
H          2.02583       -0.59735       -4.95094
H          1.90312       -2.37576       -5.12121
H          3.46984       -1.57902       -5.33079
H          1.98873       -1.35689        5.50616
H          2.94525       -3.88808       -3.24117
H          4.00358        2.05980       -0.91268
C         -2.86890        0.29783        1.19126
```

```
C         -4.23676        0.37462        1.23902
C         -5.03231        0.18693        0.04681
C         -4.28120        0.04083       -1.18029
C         -2.91221       -0.02557       -1.16302
H          4.22788       -0.66218       -1.86387
N         -2.17903        0.00052        0.01872
C          0.40676       -2.68414        4.24756
N          0.29456       -3.45271        5.11315
C         -1.78153       -2.19719        2.17945
N         -2.79000       -2.77504        2.14397
C          0.39430       -3.52770       -3.58322
N          0.28279       -4.44883       -4.28434
C         -1.77892       -2.64360       -1.63095
N         -2.77903       -3.21217       -1.46142
C         -2.18833        2.85283       -0.40660
N         -3.32030        3.11185       -0.46487
C         -0.09972        5.00485       -0.68567
N         -0.37445        6.11831       -0.87872
C         -4.94884       -0.01073       -2.44535
N         -5.49306       -0.05653       -3.47216
C         -6.43848        0.20803        0.06984
N         -7.60850        0.22405        0.08905
C         -4.85881        0.66482        2.49538
N         -5.36612        0.89558        3.51611
H         -2.27234        0.49814        2.08164
H         -2.35070       -0.06545       -2.09620
```

[L$_4$Co^{III}OH]$^+$ (*S* =0)

```
84
p_u0_opt.out     Energy: -2326706.7896995
C         -1.25909       -0.80591       -1.33184
N         -1.76671       -1.85082       -2.02597
C         -0.71066       -2.67525       -2.40137
C          0.44302       -2.14125       -1.85575
N          0.08664       -0.95347       -1.22205
B          0.70735       -0.06637       -0.09269
N          0.37804        1.42712       -0.37602
C         -0.91419        1.83167       -0.37678
N         -0.96014        3.18261       -0.49347
C          0.34785        3.63461       -0.66449
C          1.18688        2.54284       -0.57288
N         -0.08741       -0.53137        1.18079
C         -1.42922       -0.24269        1.24691
N         -1.91365       -0.83286        2.37077
C         -0.90186       -1.58461        2.96390
C          0.23522       -1.41900        2.19741
Co        -2.22677        0.51180       -0.41488
O         -2.99182        1.20280       -1.89003
C         -3.25737       -2.15733       -2.18333
C         -3.47878       -3.67591       -2.22550
C         -3.94257       -1.61913       -0.92242
C         -3.76626       -1.48826       -3.46320
C         -2.15530        4.14915       -0.37195
C         -1.75303        5.27473        0.59909
C         -2.47133        4.67060       -1.77791
C         -3.36518        3.43569        0.23123
```

C	-3.29873	-0.68164	2.99878
C	-4.13813	0.29797	2.18370
C	-3.97674	-2.05936	3.03223
C	-3.10292	-0.09686	4.40920
H	-4.55932	-3.85729	-2.12053
H	-3.17507	-4.12041	-3.18197
H	-3.49846	-2.04927	-0.01392
H	-5.01052	-1.88559	-0.93342
H	-3.95975	-0.51331	-0.89677
H	-3.20978	-1.85398	-4.34109
H	-3.67293	-0.39607	-3.39257
H	-4.82892	-1.74477	-3.59937
H	-0.97811	5.94443	0.20624
H	-1.42006	4.86114	1.56481
H	-2.64311	5.89540	0.78238
H	-1.61207	5.18944	-2.23132
H	-3.30250	5.39009	-1.71183
H	-3.11067	2.97770	1.20105
H	-4.14196	4.19054	0.42386
H	-3.79113	2.69218	-0.45188
H	-5.11539	0.40788	2.67683
H	-3.67488	1.29339	2.14846
H	-4.98025	-1.94559	3.47048
H	-4.09179	-2.47264	2.01837
H	-2.56656	0.86443	4.36072
H	-2.56110	-0.77443	5.08402
H	-4.09414	0.08129	4.85388
H	-2.96792	-4.19274	-1.39696
H	-3.42976	-2.78758	3.64800
H	-2.78079	3.84096	-2.43165
C	3.04447	-0.38450	-1.03833
C	4.43414	-0.46628	-0.95038
C	5.05760	-0.25140	0.30017
C	4.23883	0.07559	1.40821
C	2.85536	0.11464	1.24268
H	-4.34297	-0.06236	1.16679
H	-2.40568	1.47022	-2.61899
N	2.27239	-0.16444	0.05083
C	-0.99681	-2.40781	4.11638
N	-1.01159	-3.10373	5.04784
C	1.46868	-2.10032	2.36394
N	2.47544	-2.67059	2.48546
C	2.59965	2.58322	-0.67816
N	3.75852	2.63992	-0.75980
C	0.77785	4.95145	-0.97741
N	1.21141	5.98773	-1.27730
C	1.72399	-2.74820	-1.89523
N	2.76196	-3.27332	-1.91993
C	-0.74718	-3.82359	-3.23551
N	-0.67717	-4.75121	-3.93251
C	4.79762	0.36481	2.69388
N	5.24317	0.59657	3.74080
C	6.47717	-0.32705	0.43461
N	7.63218	-0.38871	0.54462
C	5.19073	-0.74675	-2.13219
N	5.79690	-0.97844	-3.09504
H	2.20883	0.40498	2.07186
H	2.55525	-0.44528	-2.00934

[$L_4Co^{III}OH$]$^+$ (*S* =1)

```
84
p_u2_opt.out     Energy: -2326693.6804305
C          -1.33448       -1.08761       -1.19269
N          -1.74196       -2.21305       -1.81949
C          -0.64293       -3.04928       -1.98437
C           0.44620       -2.41333       -1.41471
N           0.00974       -1.16463       -0.97542
B           0.64238       -0.06867       -0.03142
N           0.36217        1.41346       -0.48983
C          -0.89587        1.93403       -0.45165
N          -0.83965        3.25900       -0.70308
C           0.48629        3.59472       -0.96588
C           1.24042        2.44764       -0.82607
N          -0.13501       -0.31369        1.30924
C          -1.47053       -0.03462        1.28419
N          -2.02420       -0.50773        2.42292
C          -1.03935       -1.15417        3.16467
C           0.13778       -1.06799        2.44393
Co         -2.25472        0.56686       -0.44922
O          -2.91762        1.02226       -2.02817
C          -3.16198       -2.48176       -2.33016
C          -3.42473       -3.99273       -2.38614
C          -4.16604       -1.85601       -1.35705
C          -3.25777       -1.84609       -3.72347
C          -1.96875        4.29601       -0.65010
C          -1.54237        5.39743        0.33629
C          -2.18072        4.83438       -2.07173
C          -3.25375        3.65586       -0.12792
C          -3.47893       -0.39952        2.86156
C          -4.27452        0.36555        1.80617
C          -4.04336       -1.82195        3.00224
C          -3.51511        0.38245        4.18424
H          -4.49935       -4.13873       -2.57228
H          -2.89333       -4.48840       -3.20840
H          -4.00759       -2.22028       -0.33030
H          -5.17971       -2.15246       -1.66573
H          -4.15108       -0.75873       -1.39307
H          -2.51999       -2.28978       -4.41183
H          -3.09635       -0.75919       -3.66130
H          -4.26395       -2.03088       -4.13249
H          -0.67145        5.97407       -0.00344
H          -1.32528        4.96923        1.32807
H          -2.37724        6.10701        0.44239
H          -1.28090        5.31806       -2.48024
H          -2.98268        5.58841       -2.04849
H          -3.11075        3.23774        0.88069
H          -4.01569        4.44573       -0.05042
H          -3.64895        2.88873       -0.80790
H          -5.32049        0.43609        2.14117
H          -3.91602        1.39764        1.68446
H          -5.11004       -1.75271        3.26540
H          -3.95501       -2.37501        2.05352
H          -3.07075        1.38282        4.05777
H          -2.99340       -0.13928        4.99953
H          -4.56532        0.50432        4.49130
```

H	-3.17926	-4.48922	-1.43327
H	-3.54659	-2.39940	3.79500
H	-2.49024	4.02977	-2.75811
C	2.95239	-0.54212	-0.97969
C	4.34253	-0.64154	-0.91469
C	4.99957	-0.31618	0.29340
C	4.21452	0.14414	1.37833
C	2.82980	0.20996	1.23511
H	-4.30974	-0.16535	0.84065
H	-2.46197	1.69274	-2.56814
N	2.21136	-0.18372	0.09479
C	-1.19419	-1.80000	4.41880
N	-1.26410	-2.34190	5.44511
C	1.36741	-1.69531	2.77084
N	2.37208	-2.22280	3.02732
C	2.64552	2.40044	-1.00574
N	3.79906	2.41121	-1.15465
C	0.99570	4.86276	-1.35170
N	1.47115	5.86788	-1.69144
C	1.72165	-3.00852	-1.23816
N	2.75055	-3.52933	-1.08177
C	-0.56258	-4.32476	-2.60465
N	-0.37404	-5.35937	-3.10021
C	4.80786	0.54424	2.61795
N	5.28098	0.86539	3.62853
C	6.42014	-0.41235	0.40415
N	7.57590	-0.49010	0.49410
C	5.06661	-1.05267	-2.07802
N	5.64648	-1.39005	-3.02574
H	2.21314	0.61926	2.03572
H	2.43445	-0.70281	-1.92522

$[L_4Co^{III}OH]^+$ (*S* =2)

84
p_u4.out Energy: -2327813.7361380

C	-1.30914	-0.88936	-1.29531
N	-1.67921	-1.97742	-2.01455
C	-0.65822	-2.91816	-1.96830
C	0.36693	-2.36912	-1.21768
N	-0.02883	-1.08070	-0.86763
B	0.60304	-0.05864	0.13824
N	0.35754	1.42830	-0.31654
C	-0.89220	1.94071	-0.49365
N	-0.79197	3.23509	-0.86868
C	0.55221	3.56781	-0.95308
C	1.27669	2.44154	-0.60479
N	-0.14944	-0.38324	1.48351
C	-1.47196	-0.05978	1.57775
N	-1.95598	-0.58738	2.72273
C	-0.95800	-1.33382	3.33376
C	0.17108	-1.22985	2.53847
Co	-2.38016	0.57019	-0.19335
O	-3.91949	0.97919	-0.94741
C	-3.01507	-2.08532	-2.76062
C	-3.00865	-3.28595	-3.71161
C	-4.12349	-2.26545	-1.71427
C	-3.17504	-0.79943	-3.58457

C	-1.99987	4.12743	-1.18656
C	-1.56343	5.58052	-1.38989
C	-2.63032	3.58938	-2.47844
C	-2.95656	4.06081	0.01183
C	-3.36114	-0.41183	3.28529
C	-4.13214	0.58334	2.42057
C	-4.05282	-1.78274	3.26072
C	-3.23282	0.16076	4.70715
H	-3.93733	-3.23936	-4.30063
H	-2.16839	-3.25240	-4.42286
H	-3.92323	-3.13991	-1.07445
H	-5.08018	-2.42941	-2.23473
H	-4.23878	-1.37302	-1.08600
H	-2.36100	-0.70949	-4.32191
H	-3.19416	0.09711	-2.95379
H	-4.13152	-0.84664	-4.12817
H	-0.93741	5.71340	-2.28374
H	-1.05091	5.99461	-0.50766
H	-2.47658	6.17446	-1.54774
H	-1.90821	3.63095	-3.30983
H	-3.49521	4.21934	-2.74007
H	-2.44374	4.34656	0.94404
H	-3.78511	4.76491	-0.16005
H	-3.40031	3.06547	0.12907
H	-5.11504	0.75353	2.88550
H	-3.62336	1.55839	2.35574
H	-5.08095	-1.66783	3.63764
H	-4.09941	-2.17595	2.23189
H	-2.68614	1.11744	4.69602
H	-2.73375	-0.52811	5.40293
H	-4.24460	0.34364	5.10051
H	-3.01199	-4.24910	-3.18199
H	-3.54538	-2.51982	3.90110
H	-2.98785	2.55842	-2.35678
C	2.90698	-0.57718	-0.81289
C	4.29415	-0.70308	-0.74949
C	4.95677	-0.41538	0.46670
C	4.18023	0.02943	1.56268
C	2.79691	0.12887	1.41923
H	-4.33553	0.18696	1.41505
H	-4.84898	1.03643	-0.65971
N	2.17285	-0.21800	0.26736
C	-1.06410	-2.10589	4.52028
N	-1.09963	-2.76332	5.47848
C	1.38807	-1.93360	2.72978
N	2.37555	-2.52948	2.88165
C	2.69298	2.41044	-0.57297
N	3.85598	2.44095	-0.56436
C	1.16739	4.79653	-1.31748
N	1.78124	5.74216	-1.60016
C	1.54407	-3.04060	-0.80013
N	2.49848	-3.59954	-0.43801
C	-0.60590	-4.23278	-2.50585
N	-0.45558	-5.32183	-2.88338
C	4.78096	0.38629	2.81175
N	5.26070	0.67356	3.82940
C	6.37539	-0.53690	0.57397
N	7.52997	-0.63427	0.66017
C	5.01337	-1.10647	-1.91917

```
N          5.58946       -1.43775       -2.87135
H          2.18644        0.52619        2.23136
H          2.38226       -0.73427       -1.75616
```

[L$_4$Co^{II}O]$^-$ (*S* =1/2)

```
83
r_u1_opt.out      Energy: -2326545.6036514
C          1.36114       -0.24174        1.34771
N          1.84960       -0.90294        2.43391
C          0.83686       -1.68072        2.99133
C         -0.30940       -1.44458        2.25193
N          0.02076       -0.50407        1.28940
B         -0.70911       -0.02767       -0.01574
N         -0.33023        1.47833       -0.26428
C          0.96717        1.88650       -0.25322
N          0.99095        3.24983       -0.35107
C         -0.32227        3.69720       -0.47925
C         -1.14784        2.58847       -0.41839
N         -0.01242       -0.92593       -1.09961
C          1.33010       -0.76639       -1.30045
N          1.75078       -1.80020       -2.09954
C          0.67520       -2.65675       -2.31904
C         -0.41935       -2.12253       -1.66268
Co         2.27241        0.54995       -0.23924
O          3.54636        1.04785       -1.15932
C          3.27162       -0.86435        2.95337
C          3.23352       -0.55324        4.46019
C          3.92219       -2.22350        2.65561
C          4.04196        0.25704        2.25537
C          2.24474        4.12583       -0.33441
C          1.87528        5.58561       -0.03995
C          3.17204        3.63584        0.78899
C          2.90519        4.01677       -1.71486
C          3.16344       -1.96853       -2.67008
C          3.44558       -0.74903       -3.55867
C          4.15099       -2.10277       -1.50045
C          3.26178       -3.23516       -3.52757
H          4.26778       -0.45175        4.82411
H          2.70677        0.39709        4.64559
H          3.40840       -3.05135        3.16907
H          4.96779       -2.20984        3.00172
H          3.91661       -2.42004        1.57144
H          3.53103        1.22388        2.37326
H          4.20129        0.06242        1.18470
H          5.03661        0.33699        2.72052
H          1.29280        5.69161        0.88974
H          1.33912        6.06586       -0.86929
H          2.81592        6.14136        0.09299
H          2.63239        3.58076        1.74881
H          3.99749        4.35635        0.89838
H          2.21734        4.36744       -2.50263
H          3.80411        4.65489       -1.73287
H          3.20372        2.97489       -1.90963
H          4.45310       -0.85393       -3.99346
H          2.71582       -0.70227       -4.38452
H          5.14776       -2.33754       -1.90649
```

```
H          4.23447       -1.17033       -0.93110
H          2.58372       -3.21510       -4.39383
H          3.10240       -4.15721       -2.94862
H          4.28789       -3.27433       -3.92414
H          2.75732       -1.34525        5.05415
H          3.84965       -2.92640       -0.83220
H          3.61457        2.66151        0.55459
C         -2.92494        0.11910        1.19489
C         -4.29367        0.07011        1.26513
C         -5.08503       -0.22637        0.09050
C         -4.33825       -0.34094       -1.14377
C         -2.96858       -0.27879       -1.14316
H          3.41566        0.17852       -2.96845
N         -2.22962       -0.14860        0.02393
C         -0.82756        5.01025       -0.67463
N         -1.35843        6.03050       -0.85023
C         -2.56117        2.65343       -0.51425
N         -3.71264        2.79528       -0.60404
C         -1.54431       -2.12858        2.39931
N         -2.53173       -2.73018        2.52979
C          0.94639       -2.60542        4.06127
N          0.98779       -3.39201        4.91799
C         -1.66672       -2.78048       -1.50187
N         -2.65416       -3.38180       -1.36970
C          0.59824       -3.88995       -3.02093
N          0.39930       -4.90592       -3.55155
C         -5.01293       -0.49789       -2.39532
N         -5.56523       -0.63110       -3.41056
C         -6.48577       -0.33317        0.13510
N         -7.65272       -0.42328        0.17274
C         -4.92159        0.33619        2.52301
N         -5.43485        0.54636        3.54566
H         -2.33406        0.40064        2.06682
H         -2.41206       -0.30072       -2.08052
```

[$L_4Co^{II}O]^-$ (*S* =3/2)

```
83
r_u3_opt.out      Energy: -2326545.6993090
C          1.27266       -0.53399        1.55241
N          1.58283       -1.31399        2.61722
C          0.50430       -2.15143        2.89704
C         -0.51225       -1.80899        2.02063
N         -0.04344       -0.75817        1.24588
B         -0.67568       -0.02731       -0.00032
N         -0.15895        1.45903        0.00177
C          1.18043        1.69543        0.00260
N          1.37549        3.03371        0.00416
C          0.13356        3.66955        0.00421
C         -0.83069        2.67530        0.00261
N         -0.04285       -0.75467       -1.24819
C          1.27352       -0.52980       -1.55307
N          1.58441       -1.30676       -2.61988
C          0.50605       -2.14333       -2.90286
C         -0.51115       -1.80323       -2.02630
Co         2.30616        0.10942        0.00083
O          3.55314       -0.96717       -0.00024
```

C	2.88486	-1.28363	3.39696
C	2.54919	-1.24088	4.89832
C	3.68647	-2.53428	3.01058
C	3.67050	-0.01309	3.04595
C	2.71536	3.73172	0.00506
C	2.81764	4.58225	-1.27123
C	2.81656	4.58140	1.28199
C	3.82956	2.68078	0.00530
C	2.88698	-1.27424	-3.39866
C	3.67241	-0.00464	-3.04370
C	3.68828	-2.52598	-3.01521
C	2.55235	-1.22739	-4.90012
H	3.48871	-1.13009	5.46154
H	1.90455	-0.37700	5.13039
H	3.14916	-3.46049	3.27260
H	4.64635	-2.53496	3.55183
H	3.88440	-2.51650	1.92705
H	3.05561	0.89147	3.18233
H	4.04554	-0.05073	2.01549
H	4.53353	0.04992	3.72686
H	2.06075	5.38013	-1.30682
H	2.70744	3.94820	-2.16629
H	3.80810	5.06277	-1.30508
H	2.05993	5.37950	1.31739
H	3.80714	5.06158	1.31711
H	3.80148	2.05352	-0.89930
H	4.79939	3.20189	0.00626
H	3.80008	2.05264	0.90922
H	4.53560	0.06043	-3.72421
H	3.05748	0.90026	-3.17755
H	4.64852	-2.52523	-3.55581
H	3.88548	-2.51125	-1.93151
H	1.90768	-0.36302	-5.13027
H	2.06635	-2.14165	-5.26673
H	3.49225	-1.11487	-5.46234
H	2.06273	-2.15604	5.26207
H	3.15107	-3.45142	-3.28017
H	2.70531	3.94681	2.17653
C	-2.91245	0.10842	1.18562
C	-4.28133	0.18619	1.22211
C	-5.05703	0.17738	0.00029
C	-4.28176	0.18810	-1.22180
C	-2.91286	0.11039	-1.18592
H	4.04720	-0.04529	-2.01327
N	-2.20418	-0.01937	-0.00039
C	-0.10561	5.06690	0.00568
N	-0.33520	6.20789	0.00680
C	-2.23077	2.90327	0.00200
N	-3.36735	3.15222	0.00151
C	-1.75807	-2.47522	1.88447
N	-2.76120	-3.05540	1.77962
C	0.45836	-3.22075	3.82797
N	0.37723	-4.12657	4.55422
C	-1.75715	-2.46970	-1.89313
N	-2.76047	-3.05004	-1.79094
C	0.46073	-3.21015	-3.83669
N	0.38003	-4.11408	-4.56533
C	-4.92476	0.30175	-2.49495
N	-5.45137	0.39006	-3.52859

C	-6.46187	0.21565	0.00058
N	-7.63255	0.24702	0.00081
C	-4.92390	0.29787	2.49565
N	-5.45018	0.38463	3.52959
H	-2.33009	0.17732	-2.10480
H	-2.32931	0.17350	2.10439

[$L_4Co^{II}O]^-$ (*S* =5/2)

83
r_u5_opt.out Energy: -2326529.7339181

C	-1.36417	-0.43606	-1.57114
N	-1.78231	-1.34393	-2.48466
C	-0.78602	-2.29148	-2.68899
C	0.28882	-1.91603	-1.89839
N	-0.06488	-0.73098	-1.26730
B	0.63350	0.01592	-0.06368
N	0.21965	1.54448	-0.06463
C	-1.06248	1.97582	0.11616
N	-1.06609	3.32930	0.05686
C	0.22548	3.77893	-0.19412
C	1.03361	2.65682	-0.27841
N	0.03401	-0.72765	1.20149
C	-1.29053	-0.60472	1.49977
N	-1.57091	-1.47832	2.50009
C	-0.42895	-2.21137	2.80356
C	0.57607	-1.75459	1.96360
Co	-2.42859	0.43635	0.06752
O	-4.02183	0.84414	0.41127
C	-3.15065	-1.35769	-3.13946
C	-2.96271	-1.51883	-4.65772
C	-3.94375	-2.51930	-2.52231
C	-3.86360	-0.02602	-2.87594
C	-2.33908	4.14624	0.23351
C	-2.03401	5.64633	0.24008
C	-3.26853	3.81421	-0.94453
C	-2.95686	3.74846	1.58288
C	-2.96297	-1.59644	3.10740
C	-3.39536	-0.18863	3.54530
C	-3.89576	-2.17156	2.02871
C	-2.95137	-2.52437	4.32519
H	-3.95078	-1.46191	-5.14002
H	-2.33513	-0.70659	-5.05955
H	-3.47031	-3.49425	-2.72110
H	-4.95692	-2.54034	-2.95397
H	-4.03098	-2.38172	-1.43160
H	-3.24022	0.83303	-3.17061
H	-4.15728	0.09943	-1.82414
H	-4.78342	-0.01091	-3.48116
H	-1.64107	6.00247	-0.72383
H	-1.34126	5.92929	1.04796
H	-2.98252	6.17528	0.42067
H	-2.77513	4.03939	-1.90458
H	-4.17833	4.43133	-0.86861
H	-2.25322	3.95398	2.40657
H	-3.86813	4.34566	1.74711
H	-3.23817	2.68708	1.59282

```
H          -4.38724       -0.25367        4.02055
H          -2.68424        0.22500        4.27928
H          -4.89264       -2.33625        2.46824
H          -4.01377       -1.47353        1.18665
H          -2.24921       -2.18373        5.10229
H          -2.72897       -3.56838        4.05976
H          -3.96093       -2.50829        4.76374
H          -2.52015       -2.48389       -4.94013
H          -3.51654       -3.13770        1.65706
H          -3.57272        2.75817       -0.92455
C           2.90010       -0.20494       -1.24379
C           4.27117       -0.23822       -1.24670
C           5.01930       -0.07076       -0.01711
C           4.22543        0.23094        1.15169
C           2.85583        0.24296        1.08589
H          -3.47525        0.48970        2.68527
N           2.16256       -0.05676       -0.08269
C           0.71205        5.10288       -0.36162
N           1.20208        6.14651       -0.51690
C           2.42065        2.72376       -0.56753
N           3.54554        2.87200       -0.82719
C           1.47078       -2.67810       -1.70428
N           2.41029       -3.34586       -1.54620
C          -0.85582       -3.46738       -3.48031
N          -0.87502       -4.45529       -4.09473
C           1.87449       -2.32153        1.87300
N           2.91308       -2.84393        1.82569
C          -0.24101       -3.25712        3.74621
N           0.01103       -4.12195        4.48225
C           4.85104        0.52929        2.40395
N           5.36309        0.76598        3.42124
C           6.42249       -0.14086        0.02468
N           7.59145       -0.20069        0.05884
C           4.94596       -0.41114       -2.49571
N           5.49847       -0.55659       -3.50932
H           2.25586        0.49863        1.96056
H           2.34578       -0.25274       -2.18051
```

[L$_4$Co^{II}OH] (*S* =1/2)

```
84
h_u1_opt.out      Energy: -2326831.4690037
C          -1.29735       -0.82362       -1.30230
N          -1.83837       -1.86362       -1.98313
C          -0.80257       -2.70353       -2.38050
C           0.37108       -2.18257       -1.86193
N           0.04695       -0.99267       -1.22450
B           0.73967       -0.10232       -0.12370
N           0.38270        1.39824       -0.44282
C          -0.89513        1.82980       -0.39720
N          -0.91792        3.18057       -0.54486
C           0.39275        3.59613       -0.78258
C           1.20744        2.48293       -0.70209
N          -0.07048       -0.51685        1.17126
C          -1.40268       -0.21252        1.26502
N          -1.86688       -0.77728        2.41264
C          -0.84539       -1.52667        2.99433
```

C	0.27237	-1.38415	2.19298
Co	-2.22701	0.52646	-0.38072
O	-3.02959	1.21312	-1.84430
C	-3.33194	-2.15173	-2.10787
C	-3.57601	-3.66782	-2.13413
C	-3.99116	-1.59543	-0.84092
C	-3.85878	-1.48617	-3.38293
C	-2.08088	4.17152	-0.39632
C	-1.62062	5.30821	0.53580
C	-2.44432	4.67500	-1.79832
C	-3.28257	3.49682	0.26547
C	-3.23223	-0.60188	3.06327
C	-4.07810	0.37161	2.24659
C	-3.92632	-1.97063	3.13548
C	-3.00707	0.00586	4.45988
H	-4.65654	-3.83421	-2.00661
H	-3.29561	-4.12464	-3.09182
H	-3.53030	-2.01630	0.06392
H	-5.06015	-1.85748	-0.82864
H	-3.99482	-0.49060	-0.82963
H	-3.32450	-1.86585	-4.26884
H	-3.74725	-0.39498	-3.32087
H	-4.92763	-1.72788	-3.49681
H	-0.84614	5.95155	0.10016
H	-1.25786	4.90525	1.49542
H	-2.48934	5.95190	0.74133
H	-1.59381	5.16894	-2.29413
H	-3.25999	5.41047	-1.71519
H	-3.00493	3.06202	1.23949
H	-4.04381	4.26772	0.45719
H	-3.73509	2.73733	-0.38278
H	-5.04054	0.51070	2.76121
H	-3.59842	1.35713	2.17296
H	-4.91997	-1.83885	3.59112
H	-4.06491	-2.39988	2.13104
H	-2.46300	0.96107	4.38369
H	-2.45651	-0.66439	5.13504
H	-3.98775	0.20056	4.92094
H	-3.05486	-4.18443	-1.31189
H	-3.37353	-2.69370	3.75233
H	-2.79202	3.83814	-2.42314
C	3.07321	-0.49175	-1.04871
C	4.43675	-0.57011	-0.92518
C	5.07880	-0.31158	0.34410
C	4.20303	0.13949	1.39939
C	2.84475	0.18590	1.21399
H	-4.31306	-0.00978	1.24395
H	-2.45505	1.46679	-2.58661
N	2.24166	-0.22608	0.02785
C	-0.87399	-3.85254	-3.21078
N	-0.83723	-4.78252	-3.90777
C	1.63036	-2.83385	-1.92808
N	2.62075	-3.43967	-1.99653
C	1.49690	-2.08824	2.34104
N	2.46921	-2.71122	2.47794
C	-0.92069	-2.32807	4.16269
N	-0.92771	-3.00568	5.10812
C	2.61387	2.49503	-0.88606
N	3.76152	2.57999	-1.05358

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C          0.83730        4.89517       -1.14308
N          1.27215        5.91929       -1.48185
C          5.20894       -0.87317       -2.09107
N          5.83751       -1.12397       -3.03687
C          6.47044       -0.42550        0.52021
N          7.62711       -0.52172        0.66727
C          4.73233        0.56178        2.66105
N          5.16250        0.89965        3.68720
H          2.18958        0.56893        1.99697
H          2.60610       -0.58078       -2.02759
```

[$L_4Co^{II}OH$] (*S* =3/2)

```
84
h_u3_opt.out     Energy: -2326821.1939691
C         -1.31261       -0.71624       -1.44220
N         -1.65049       -1.70656       -2.30695
C         -0.53896       -2.49956       -2.56206
C          0.51397       -1.96188       -1.83984
N          0.02981       -0.82555       -1.19367
B          0.61841        0.03517       -0.01277
N          0.31498        1.56953       -0.15296
C         -0.96805        2.02260       -0.29376
N         -0.93731        3.37660       -0.32603
C          0.37450        3.81056       -0.19090
C          1.16533        2.67995       -0.07666
N         -0.07363       -0.57586        1.24962
C         -1.38404       -0.25145        1.50689
N         -1.80733       -1.07787        2.49576
C         -0.82731       -2.02489        2.77074
C          0.25753       -1.72458        1.96796
Co        -2.34122        0.56380       -0.18445
O         -4.17686        0.78052       -0.22451
C         -3.07747       -1.88776       -2.81499
C         -3.13513       -2.95214       -3.91363
C         -3.94619       -2.31480       -1.62096
C         -3.53500       -0.53985       -3.39081
C         -2.21073        4.20351       -0.46030
C         -1.88949        5.69754       -0.53658
C         -2.90643        3.76602       -1.75762
C         -3.08095        3.92106        0.77517
C         -3.16428       -1.00646        3.17550
C         -3.80512        0.35515        2.88638
C         -4.02158       -2.14570        2.60633
C         -2.96071       -1.13636        4.69481
H         -4.16611       -2.97501       -4.29861
H         -2.47248       -2.71556       -4.76108
H         -3.53624       -3.21719       -1.13862
H         -4.95970       -2.54821       -1.98505
H         -4.03650       -1.50241       -0.88409
H         -2.86190       -0.20408       -4.19611
H         -3.58152        0.22795       -2.60781
H         -4.54875       -0.65498       -3.80541
H         -1.24966        5.94568       -1.39738
H         -1.42866        6.07550        0.38839
H         -2.84089        6.23499       -0.66991
```

H -2.25558 3.93445 -2.63080
H -3.82856 4.35375 -1.88811
H -2.52765 4.14524 1.70179
H -3.97173 4.56850 0.73867
H -3.42690 2.87684 0.79790
H -4.71339 0.43500 3.50443
H -3.12910 1.18059 3.16289
H -5.02631 -2.10737 3.05616
H -4.12286 -2.03776 1.51438
H -2.26632 -0.36350 5.06348
H -2.59464 -2.12415 5.00532
H -3.93375 -0.98546 5.18706
H -2.90894 -3.96034 -3.53706
H -3.58769 -3.13471 2.82742
H -3.18431 2.70388 -1.72194
C 2.91256 -0.03513 -1.10103
C 4.30643 -0.08943 -1.11198
C 5.00089 -0.16006 0.11725
C 4.24708 -0.14189 1.31390
C 2.85511 -0.08755 1.23894
H -4.10297 0.47315 1.83601
H -4.61145 1.32622 -0.89709
N 2.20724 -0.07693 0.05236
C -0.41211 -3.66159 -3.36987
N -0.20325 -4.61826 -3.99725
C 1.81206 -2.52492 -1.75578
N 2.87280 -3.00067 -1.69092
C 1.44419 -2.48969 1.84363
N 2.41622 -3.11908 1.72134
C -0.91364 -3.14797 3.63497
N -0.93527 -4.10164 4.30082
C 2.57168 2.72589 0.08592
N 3.72530 2.80455 0.22236
C 0.89819 5.13138 -0.16382
N 1.42081 6.16968 -0.12869
C 4.99840 -0.06987 -2.36467
N 5.55400 -0.05902 -3.38428
C 6.42801 -0.21817 0.15011
N 7.58859 -0.26359 0.17675
C 4.87882 -0.16393 2.59802
N 5.38507 -0.18431 3.64290
H 2.25413 -0.01080 2.14555
H 2.35341 0.06914 -2.03257

[L$_4$Co^{II}OH] (*S* =5/2)

84
h_u5_opt.out Energy: -2326798.7602106
C -1.26103 -0.64907 -1.53887
N -1.52695 -1.51027 -2.55085
C -0.38379 -2.25749 -2.81264
C 0.60347 -1.80556 -1.95172
N 0.05414 -0.76699 -1.21232
B 0.65638 -0.00428 0.03424
N 0.18864 1.52509 0.01441

C	-1.10917	1.90175	-0.08479
N	-1.19118	3.25137	-0.08234
C	0.09263	3.76179	0.03505
C	0.95920	2.67636	0.10307
N	-0.03735	-0.73507	1.24667
C	-1.34772	-0.49607	1.53728
N	-1.71479	-1.32636	2.53890
C	-0.66521	-2.19873	2.80576
C	0.38311	-1.83893	1.97506
Co	-2.40317	0.35897	-0.07969
O	-4.15217	0.12631	-0.28219
C	-2.88926	-1.62782	-3.23484
C	-2.76181	-2.36535	-4.57268
C	-3.81289	-2.40817	-2.28900
C	-3.39157	-0.20374	-3.51514
C	-2.51836	3.99959	-0.20852
C	-2.29513	5.51342	-0.19878
C	-3.15397	3.58870	-1.54486
C	-3.39225	3.60437	0.99031
C	-3.03021	-1.30035	3.30966
C	-3.81106	-0.03324	2.95020
C	-3.82565	-2.55422	2.92220
C	-2.69604	-1.25596	4.81112
H	-3.73478	-2.29215	-5.08222
H	-2.00696	-1.90713	-5.23158
H	-3.40670	-3.41350	-2.09096
H	-4.79870	-2.52402	-2.76733
H	-3.95602	-1.87703	-1.33809
H	-2.68056	0.34312	-4.15502
H	-3.55676	0.36719	-2.59509
H	-4.35711	-0.26732	-4.04002
H	-1.67544	5.84980	-1.04333
H	-1.86006	5.86753	0.74763
H	-3.28034	5.99239	-0.30502
H	-2.48225	3.81203	-2.38875
H	-4.09100	4.14972	-1.68380
H	-2.87613	3.80769	1.94189
H	-4.32320	4.19153	0.96356
H	-3.67915	2.54298	0.96447
H	-4.67212	0.03814	3.63194
H	-3.19769	0.87356	3.07878
H	-4.79046	-2.54655	3.45335
H	-4.02442	-2.56471	1.83790
H	-2.06678	-0.38182	5.04490
H	-2.19518	-2.16406	5.17290
H	-3.63871	-1.16217	5.37180
H	-2.54583	-3.43520	-4.44941
H	-3.29788	-3.48105	3.19713
H	-3.40672	2.51860	-1.57468
C	2.88272	0.18657	-1.12275
C	4.25258	0.20900	-1.16432
C	5.03301	0.04482	0.03965
C	4.27018	-0.02331	1.26774
C	2.89978	-0.03692	1.24482
H	-4.20427	-0.06458	1.92674
H	-4.84654	0.77022	-0.51181
N	2.17520	-0.03021	0.05931
C	-0.19004	-3.32527	-3.72948
N	0.07223	-4.21413	-4.43170

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C           1.88945       -2.38952       -1.80653
N           2.91366       -2.93193       -1.70955
C           1.60560       -2.54610        1.83066
N           2.57773       -3.17446        1.71885
C          -0.66977       -3.30474        3.69533
N          -0.62838       -4.23798        4.38807
C           2.36296        2.80987        0.26097
N           3.49738        3.02116        0.40552
C           0.52512        5.11379        0.09226
N           0.97963        6.18230        0.14892
C           4.89182        0.41728       -2.42838
N           5.41239        0.58205       -3.45515
C           6.43918        0.01678        0.02586
N           7.60915       -0.00755        0.01420
C           4.92986       -0.04825        2.53739
N           5.46834       -0.07239        3.56804
H           2.33252       -0.01588        2.17511
H           2.29654        0.35734       -2.02658
```

Transition states for HAA by the $L_1Co^{III}O$ oxidant

$L_1Co^{III}O$ + CHD (*S*=0, closed-shell singlet)

```
88
chd_ts_u0_closed_freq.out Energy: -1941557.0065351
C           0.57543        1.47788       -0.44505
N           0.30086        2.72060       -0.96049
C           1.49629        3.34809       -1.29848
C           2.50731        2.49519       -0.97116
N           1.93433        1.36799       -0.42266
B           2.61884        0.02703        0.04762
N           1.94692       -0.32930        1.41057
C           0.60263       -0.42854        1.47570
N           0.29103       -0.71993        2.77602
C           1.47111       -0.79454        3.51696
C           2.50176       -0.54886        2.65651
N           2.06391       -1.02289       -0.97933
C           0.71883       -1.20291       -1.03729
N           0.48746       -2.06957       -2.07233
C           1.69819       -2.38269       -2.68528
C           2.67520       -1.71623       -2.00526
Co         -0.48862       -0.08547       -0.03435
O          -2.16112        0.27207       -0.31223
C          -1.04946        3.36203       -1.15965
C          -0.86777        4.83602       -1.55689
C          -1.78248        2.62238       -2.28934
C          -1.82928        3.30335        0.16304
C          -1.09518       -0.87485        3.32786
C          -1.02251       -1.32299        4.79347
C          -1.81006        0.48349        3.23438
C          -1.83648       -1.94141        2.50785
C          -0.85332       -2.55022       -2.54605
C          -1.67119       -3.02451       -1.33583
C          -1.55409       -1.38783       -3.26816
```

C	-0.66607	-3.72779	-3.51389
H	-1.86728	5.28855	-1.65031
H	-0.31200	5.40580	-0.79371
H	-1.19288	2.66182	-3.22128
H	-2.75873	3.10138	-2.47353
H	-1.96003	1.57962	-1.99580
H	-1.26375	3.80639	0.96596
H	-2.03490	2.26176	0.43986
H	-2.79481	3.82114	0.03929
H	-0.52957	-0.57279	5.43300
H	-0.49893	-2.28734	4.90187
H	-2.04961	-1.45302	5.16872
H	-1.27101	1.24624	3.82122
H	-2.83705	0.39441	3.62440
H	-1.27112	-2.88782	2.49325
H	-2.82885	-2.12659	2.94808
H	-1.99511	-1.59958	1.47555
H	-2.63012	-3.44492	-1.67910
H	-1.12550	-3.80011	-0.77362
H	-2.53109	-1.72013	-3.65603
H	-1.72446	-0.55483	-2.57182
H	-0.10680	-4.55502	-3.04606
H	-0.15420	-3.42886	-4.44284
H	-1.66028	-4.10730	-3.79691
H	-0.36498	4.95174	-2.53095
H	-0.94266	-1.03625	-4.11623
H	-1.87744	0.81295	2.18728
C	4.21571	0.07194	0.25592
C	4.85315	1.21794	0.77886
C	6.21564	1.22795	1.10240
C	6.98749	0.07344	0.92705
C	6.37466	-1.09050	0.44955
C	5.01062	-1.08689	0.13028
H	4.27140	2.12575	0.96662
H	6.67352	2.13943	1.50182
H	8.05397	0.07641	1.17626
H	6.95808	-2.01034	0.33328
H	4.55644	-2.02626	-0.19848
H	1.54794	4.33849	-1.73652
H	3.58028	2.61063	-1.09730
H	1.49264	-1.01674	4.57871
H	3.57453	-0.51531	2.83193
H	1.78014	-3.04959	-3.53710
H	3.74631	-1.68542	-2.18554
H	-1.90181	-2.18684	-0.66517
H	-3.17630	-0.13067	-0.59921
C	-4.50537	-0.71449	-0.92868
C	-4.88190	-1.56701	0.27548
C	-5.15406	0.55579	-1.06487
H	-4.28486	-1.26568	-1.85309
C	-5.18896	-0.69792	1.47738
H	-4.07431	-2.28523	0.51159
H	-5.77127	-2.21528	0.05826
C	-5.67747	1.22093	0.02350
H	-5.11483	1.06374	-2.03825
C	-5.60032	0.58805	1.32792
H	-5.14585	-1.15020	2.47593
H	-6.07745	2.23584	-0.06917
H	-5.86824	1.17667	2.21515

$L_1Co^{III}O$ + CHD (*S*=0, open-shell singlet)

```
88
chd_ts_u0_open.out        Energy: -1942836.9525274
C          0.54650        1.49905       -0.42691
N          0.29745        2.75548       -0.92030
C          1.50073        3.36138       -1.27041
C          2.49591        2.48039       -0.96954
N          1.90397        1.35967       -0.42550
B          2.56852        0.00103        0.02189
N          1.90455       -0.36820        1.38539
C          0.55966       -0.46504        1.45877
N          0.25931       -0.77057        2.75890
C          1.44463       -0.85552        3.49135
C          2.46856       -0.60250        2.62541
N          2.00081       -1.03035       -1.01704
C          0.65452       -1.21439       -1.06882
N          0.42296       -2.05959       -2.12204
C          1.63007       -2.35100       -2.75323
C          2.60807       -1.69533       -2.06467
Co        -0.53895       -0.08951       -0.04281
O         -2.19645        0.30469       -0.37699
C         -1.04243        3.42128       -1.08951
C         -0.84261        4.90669       -1.43120
C         -1.79060        2.73013       -2.24006
C         -1.81887        3.32007        0.23271
C         -1.12293       -0.94847        3.30923
C         -1.04624       -1.38527        4.77793
C         -1.86889        0.39244        3.20569
C         -1.83781       -2.03544        2.49235
C         -0.91846       -2.53238       -2.59691
C         -1.73252       -3.01758       -1.38860
C         -1.62033       -1.36055       -3.30329
C         -0.73720       -3.70035       -3.57757
H         -1.83518        5.37935       -1.49586
H         -0.26799        5.43647       -0.65313
H         -1.20320        2.79079       -3.17245
H         -2.76006        3.22984       -2.40626
H         -1.98145        1.68091       -1.97467
H         -1.24428        3.78218        1.05370
H         -2.03528        2.26992        0.46706
H         -2.77804        3.85523        0.13418
H         -0.56610       -0.62195        5.41179
H         -0.50686       -2.33980        4.89475
H         -2.07159       -1.52998        5.15279
H         -1.33992        1.17494        3.77536
H         -2.88876        0.28675        3.61011
H         -1.26481       -2.97727        2.50688
H         -2.83936       -2.22177        2.91119
H         -1.96813       -1.71418        1.44920
H         -2.69928       -3.42112       -1.73031
H         -1.19133       -3.80813       -0.84302
H         -2.59975       -1.68632       -3.69123
H         -1.78311       -0.53478       -2.59592
H         -0.17292       -4.53092       -3.12171
H         -0.23188       -3.39186       -4.50702
H         -1.73271       -4.07886       -3.85773
```

```
H         -0.34812        5.05245       -2.40553
H         -1.01170       -1.00229       -4.15071
H         -1.95626        0.70710        2.15518
C          4.16870        0.02040        0.22201
C          4.82745        1.15041        0.75317
C          6.19122        1.13488        1.07144
C          6.94335       -0.03039        0.88205
C          6.30940       -1.17926        0.39553
C          4.94435       -1.14986        0.08186
H          4.26141        2.06589        0.95141
H          6.66567        2.03483        1.47775
H          8.01069       -0.04744        1.12708
H          6.87714       -2.10741        0.26782
H          4.47314       -2.07795       -0.25524
H          1.56830        4.35627       -1.69655
H          3.56936        2.57267       -1.11072
H          1.47392       -1.08864        4.55067
H          3.54262       -0.57266        2.79364
H          1.70875       -2.99697       -3.62146
H          3.67781       -1.65435       -2.25165
H         -1.94297       -2.18714       -0.70254
H         -3.26107       -0.16318       -0.65686
C         -4.51191       -0.69551       -0.92683
C         -4.86566       -1.58226        0.26111
C         -5.23602        0.55084       -1.03836
H         -4.33131       -1.23541       -1.86726
C         -5.22061       -0.76284        1.48065
H         -4.03662       -2.27635        0.48753
H         -5.72969       -2.25092        0.01889
C         -5.77747        1.16162        0.06480
H         -5.23761        1.07449       -2.00327
C         -5.67662        0.50881        1.36161
H         -5.16927       -1.24130        2.46622
H         -6.23698        2.15302       -0.00671
H         -5.97573        1.06765        2.25710
```

$L_1Co^{III}O$ + CHD (*S*=1)

```
88
chd_ts_u2.out     Energy: -1942837.3627931
C          0.74853       -1.15955       -1.29856
N          0.63740       -2.21174       -2.15388
C          1.84861       -2.89598       -2.21737
C          2.71585       -2.23342       -1.39791
N          2.04101       -1.14879       -0.86217
B          2.52015       -0.14063        0.26290
N          2.02845        1.29847       -0.15462
C          0.72688        1.56388       -0.42645
N          0.64936        2.88058       -0.74796
C          1.91950        3.45429       -0.67568
C          2.77636        2.45839       -0.30429
N          1.69480       -0.57773        1.54322
C          0.33528       -0.47107        1.56918
N         -0.07304       -1.02884        2.73977
C          1.02466       -1.53402        3.43145
C          2.12474       -1.25985        2.67035
Co        -0.49319        0.02382       -0.23341
```

O	-2.19992	-0.28762	-0.44412
C	-0.62757	-2.61134	-2.85120
C	-0.30472	-3.62745	-3.95549
C	-1.57302	-3.23809	-1.81270
C	-1.26555	-1.35907	-3.47470
C	-0.63487	3.55960	-1.09949
C	-0.36881	5.03015	-1.44030
C	-1.24796	2.84179	-2.31411
C	-1.57740	3.46229	0.11202
C	-1.50505	-1.11267	3.17322
C	-2.14994	0.27062	2.99344
C	-2.22173	-2.15277	2.29604
C	-1.57134	-1.52574	4.64937
H	-1.23216	-3.86138	-4.50150
H	0.42389	-3.22421	-4.67873
H	-1.09672	-4.10878	-1.33014
H	-2.49934	-3.57791	-2.30627
H	-1.83961	-2.48966	-1.05081
H	-0.55872	-0.86013	-4.15908
H	-1.57902	-0.65660	-2.68849
H	-2.15999	-1.65279	-4.04923
H	0.30797	5.13247	-2.30472
H	0.05982	5.57767	-0.58470
H	-1.32372	5.51259	-1.70181
H	-0.54882	2.85239	-3.16683
H	-2.17963	3.34730	-2.61765
H	-1.12529	3.93842	0.99796
H	-2.53193	3.96691	-0.11038
H	-1.79330	2.40909	0.34941
H	-3.19149	0.24442	3.35187
H	-1.59758	1.03746	3.56243
H	-3.26857	-2.26229	2.62662
H	-2.22553	-1.81681	1.24730
H	-1.01794	-0.82286	5.29460
H	-1.18053	-2.54351	4.81365
H	-2.62521	-1.52269	4.96938
H	0.08391	-4.57557	-3.54891
H	-1.72613	-3.13569	2.37418
H	-1.49003	1.79654	-2.06561
C	4.12118	-0.05877	0.47199
C	5.01139	-0.18230	-0.61621
C	6.38793	0.03803	-0.48057
C	6.92093	0.41046	0.75894
C	6.05833	0.58060	1.84793
C	4.68374	0.35678	1.69772
H	4.62384	-0.43186	-1.60878
H	7.04517	-0.07267	-1.35004
H	7.99679	0.58228	0.87121
H	6.45509	0.89866	2.81830
H	4.03396	0.53954	2.55902
H	2.00941	-3.77698	-2.83085
H	3.75247	-2.45967	-1.16235
H	2.11838	4.50009	-0.88934
H	3.85048	2.48802	-0.13860
H	0.95298	-2.03234	4.39344
H	3.16803	-1.50407	2.85290
H	-2.17455	0.54889	1.93028
H	-3.20767	0.50350	-0.48860
C	-4.30448	1.14885	-0.67860

```
C          -5.19358        0.09996       -1.34126
C          -4.71447        1.58609        0.65139
H          -3.98571        1.95598       -1.35482
C          -5.79550       -0.85406       -0.33930
H          -4.61482       -0.45454       -2.10301
H          -6.02521        0.58303       -1.90823
C          -5.47433        0.78373        1.45370
H          -4.31428        2.52820        1.04419
C          -5.93836       -0.50768        0.96217
H          -6.17637       -1.81678       -0.70101
H          -5.71041        1.08070        2.48109
H          -6.42029       -1.19648        1.66609
```

$L_1Co^{III}O$ + CHD (*S*=2)

```
88
chd_ts_u4.out     Energy: -1942835.7093810
C           0.52421       -0.84237       -1.48884
N           0.25968       -1.67858       -2.52748
C           1.42895       -2.30659       -2.94178
C           2.42909       -1.82786       -2.14315
N           1.86836       -0.90751       -1.27328
B           2.53722       -0.16668       -0.03828
N           2.03940        1.33305       -0.03295
C           0.72777        1.70001       -0.00922
N           0.70696        3.05754       -0.01124
C           2.00941        3.55348       -0.03667
C           2.83766        2.47009       -0.05013
N           1.91471       -0.89950        1.22654
C           0.58006       -0.82783        1.48916
N           0.35036       -1.64359        2.55133
C           1.53250       -2.26610        2.93622
C           2.50444       -1.80507        2.09284
Co         -0.54335        0.08035        0.01891
O          -2.23993        0.57655        0.04189
C          -1.11838       -1.93148       -3.05341
C          -1.03471       -2.71818       -4.36748
C          -1.88526       -2.74438       -1.99782
C          -1.81193       -0.58117       -3.29936
C          -0.55336        3.86578        0.01095
C          -0.20955        5.36055        0.00358
C          -1.37929        3.51117       -1.23750
C          -1.33286        3.51344        1.28952
C          -1.00640       -1.84912        3.14847
C          -1.61589       -0.47249        3.46517
C          -1.87507       -2.59044        2.11988
C          -0.88688       -2.67647        4.43372
H          -2.05258       -2.85189       -4.76625
H          -0.44059       -2.17906       -5.12407
H          -1.37733       -3.70180       -1.79382
H          -2.90943       -2.95631       -2.34646
H          -1.95248       -2.17395       -1.06027
H          -1.21802        0.03977       -3.99078
H          -1.95663       -0.03153       -2.35642
H          -2.80337       -0.75416       -3.74950
H           0.34554        5.65069       -0.90411
H           0.37874        5.65190        0.88972
```

```
H          -1.14722        5.93809        0.02051
H          -0.79549        3.69938       -2.15483
H          -2.28914        4.13427       -1.27019
H          -0.71682        3.70538        2.18472
H          -2.24265        4.13419        1.35317
H          -1.63759        2.45563        1.26761
H          -2.58894       -0.60640        3.96638
H          -0.95442        0.10141        4.13549
H          -2.87991       -2.77758        2.53279
H          -1.98832       -1.97654        1.21479
H          -0.23816       -2.18214        5.17589
H          -0.49784       -3.68923        4.23796
H          -1.88815       -2.78688        4.87887
H          -0.60254       -3.72201       -4.22371
H          -1.42067       -3.55607        1.84229
H          -1.68548        2.45405       -1.20133
C           4.15564       -0.13361       -0.06873
C           4.86717       -0.01027       -1.28147
C           6.25542        0.17258       -1.31608
C           6.98295        0.25680       -0.12343
C           6.30099        0.18045        1.09635
C           4.91243       -0.00240        1.11540
H           4.32640       -0.02649       -2.23258
H           6.76874        0.25992       -2.27995
H           8.06886        0.39797       -0.14440
H           6.85034        0.27405        2.03955
H           4.40799       -0.01178        2.08632
H           1.47324       -3.02409       -3.75560
H           3.48511       -2.08424       -2.13575
H           2.25219        4.61158       -0.04323
H           3.92338        2.42781       -0.07044
H           1.60478       -2.96924        3.76053
H           3.55867       -2.06562        2.05150
H          -1.78052        0.10359        2.54093
H          -3.29483       -0.20737       -0.03802
C          -4.35616       -0.90622        0.00525
C          -5.03697       -0.46425        1.29917
C          -5.05235       -0.55323       -1.23180
H          -3.98856       -1.94197        0.03742
C          -5.76313        0.84891        1.14308
H          -4.29221       -0.40144        2.11263
H          -5.77137       -1.23167        1.64205
C          -5.90036        0.51462       -1.28139
H          -4.80002       -1.09628       -2.15055
C          -6.17908        1.28042       -0.07099
H          -6.00700        1.42021        2.04698
H          -6.35575        0.82701       -2.22739
H          -6.74726        2.21407       -0.15884
```

$L_1Co^{III}O$ + DHA (*S*=0, closed-shell singlet)

```
100
dha_ts_u0_closed_freq.out Energy: -2134154.4444290
C          -1.55040        1.38383       -0.80652
N          -1.31438        2.59738       -1.39198
C          -2.50570        3.31569       -1.44710
C          -3.47562        2.52453       -0.90239
```

N	-2.87903	1.33307	-0.54030
B	-3.39527	0.08934	0.26488
N	-2.83781	-1.15579	-0.49813
C	-1.51787	-1.24767	-0.76740
N	-1.33099	-2.42302	-1.44244
C	-2.56329	-3.06118	-1.58007
C	-3.49916	-2.26431	-0.98740
N	-2.55691	0.17546	1.59658
C	-1.19661	0.12867	1.55444
N	-0.76399	0.30129	2.84524
C	-1.86738	0.50100	3.66936
C	-2.97838	0.43197	2.88317
Co	-0.30497	0.06326	-0.15208
O	1.41363	-0.08297	0.03733
C	0.02521	3.11952	-1.82161
C	-0.16016	4.40327	-2.64275
C	0.84841	3.42307	-0.55974
C	0.71571	2.06155	-2.69708
C	-0.01854	-2.96727	-1.93086
C	-0.26271	-4.23269	-2.76491
C	0.65387	-1.90734	-2.81798
C	0.85036	-3.31532	-0.71146
C	0.65083	0.22309	3.36266
C	1.22004	-1.15394	2.98328
C	1.47140	1.37853	2.76871
C	0.64863	0.35320	4.89413
H	0.82970	4.74179	-2.98636
H	-0.78892	4.23216	-3.53234
H	0.33625	4.17580	0.06299
H	1.84372	3.80469	-0.83621
H	0.99656	2.50922	0.03290
H	0.06358	1.75831	-3.53242
H	0.98923	1.17321	-2.11109
H	1.64785	2.47786	-3.10979
H	-0.90060	-4.03261	-3.64186
H	-0.71352	-5.04291	-2.16905
H	0.70983	-4.59646	-3.13151
H	-0.01877	-1.60010	-3.63583
H	1.57483	-2.32359	-3.25446
H	0.34278	-4.06539	-0.08146
H	1.81726	-3.72420	-1.04492
H	1.05657	-2.41480	-0.11631
H	2.22833	-1.26797	3.41377
H	0.57916	-1.95587	3.38780
H	2.48276	1.37816	3.20719
H	1.57368	1.25690	1.68291
H	0.07172	-0.44981	5.38169
H	0.26493	1.33043	5.23056
H	1.69005	0.27170	5.24221
H	-0.59655	5.22077	-2.04645
H	0.99398	2.34595	2.99978
H	0.93977	-1.02352	-2.23262
C	-4.98831	-0.06966	0.42892
C	-5.88224	0.38381	-0.56382
C	-7.25782	0.12742	-0.49719
C	-7.78336	-0.61389	0.56705
C	-6.91565	-1.11270	1.54569
C	-5.54261	-0.84889	1.46738
H	-5.50159	0.92854	-1.43276

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H          -7.91963        0.50103       -1.28607
H          -8.85828       -0.81546        0.62471
H          -7.30744       -1.71836        2.37004
H          -4.88816       -1.28790        2.22685
H          -2.58111        4.31326       -1.86700
H          -4.53053        2.73186       -0.74492
H          -2.68442       -4.01512       -2.08204
H          -4.57289       -2.39765       -0.87883
H          -1.79171        0.67280        4.73700
H          -4.02483        0.55645        3.14756
H           1.29696       -1.24909        1.89230
H           2.36714       -0.08445       -0.60040
C           3.64024       -0.03612       -1.32779
C           4.21814        1.15074       -0.69148
C           4.19765       -1.32968       -0.92477
H           3.40666        0.06618       -2.39705
C           4.71483        1.04104        0.63672
C           4.27737        2.41211       -1.32349
C           4.69368       -1.47756        0.40004
C           4.24390       -2.44984       -1.78348
C           5.24931        2.16322        1.27741
C           4.57161       -0.29372        1.33702
C           4.80046        3.53048       -0.66695
H           3.90785        2.50711       -2.35055
C           5.21184       -2.70737        0.81808
C           4.74961       -3.67876       -1.34872
H           3.87970       -2.34387       -2.81138
C           5.29189        3.41335        0.64030
H           5.63177        2.06073        2.30043
H           5.27793       -0.37900        2.18088
H           3.55575       -0.32349        1.77392
H           4.83090        4.49768       -1.18140
H           5.59504       -2.80416        1.84140
C           5.23859       -3.81610       -0.04241
H           4.76975       -4.53211       -2.03605
H           5.70685        4.28369        1.15935
H           5.64084       -4.77392        0.30382
```

$L_1Co^{III}O$ + DHA (*S*=1)

```
100
dha_ts_u2.out     Energy: -2135632.8429139
C          -1.24889       -1.48195       -0.80057
N          -0.94289       -2.51741       -1.62624
C          -2.07632       -2.89367       -2.34194
C          -3.09171       -2.08023       -1.92685
N          -2.58121       -1.23525       -0.95510
B          -3.27396        0.00041       -0.24013
N          -2.82485       -0.02943        1.26915
C          -1.51662       -0.03354        1.60976
N          -1.44790       -0.06233        2.96418
C          -2.74299       -0.07655        3.48700
C          -3.59751       -0.05579        2.42151
N          -2.58709        1.26771       -0.90341
C          -1.25603        1.51417       -0.73807
N          -0.95476        2.58467       -1.51957
C          -2.08983        2.98513       -2.21939
```

C	-3.10136	2.15008	-1.83929
Co	-0.25541	-0.00032	0.13337
O	1.45893	0.00792	-0.07965
C	0.43106	-3.10091	-1.78772
C	0.33234	-4.44409	-2.52325
C	1.28471	-2.11178	-2.59840
C	1.04375	-3.32140	-0.39659
C	-0.15692	-0.07735	3.72189
C	-0.44377	-0.10715	5.22713
C	0.63316	-1.33234	3.31166
C	0.63336	1.19281	3.36200
C	0.41608	3.18219	-1.65427
C	1.02402	3.35027	-0.25361
C	1.27764	2.23178	-2.50218
C	0.31079	4.55332	-2.33533
H	1.33778	-4.89097	-2.57238
H	-0.32923	-5.15006	-1.99355
H	0.83709	-1.93254	-3.59101
H	2.29951	-2.52099	-2.73626
H	1.37263	-1.16192	-2.05010
H	0.40035	-3.97505	0.21642
H	1.19104	-2.36119	0.11637
H	2.03477	-3.79198	-0.49936
H	-1.00484	-1.01039	5.51846
H	-1.00568	0.78352	5.55346
H	0.51401	-0.11741	5.77054
H	0.04835	-2.24560	3.51094
H	1.57516	-1.38646	3.88175
H	0.04815	2.09749	3.59613
H	1.57462	1.22466	3.93500
H	0.88970	1.20322	2.29117
H	2.01106	3.83342	-0.33426
H	0.37368	3.97271	0.38406
H	2.28993	2.65287	-2.62165
H	1.37125	1.26121	-1.99243
H	-0.35543	5.23381	-1.77879
H	-0.04574	4.47700	-3.37573
H	1.31376	5.00741	-2.36495
H	-0.02622	-4.32819	-3.55931
H	0.83285	2.08972	-3.50205
H	0.88815	-1.30108	2.24089
C	-4.88784	-0.00331	-0.26778
C	-5.62093	-1.20688	-0.19366
C	-7.01536	-1.22081	-0.06232
C	-7.72539	-0.01720	0.01695
C	-7.02233	1.19270	-0.01427
C	-5.62784	1.19208	-0.14584
H	-5.09390	-2.16581	-0.21267
H	-7.54786	-2.17687	-0.01247
H	-8.81595	-0.02236	0.11795
H	-7.56034	2.14292	0.07355
H	-5.10635	2.15402	-0.12642
H	-2.08553	-3.69886	-3.07014
H	-4.12773	-2.04610	-2.25408
H	-2.95749	-0.09955	4.55108
H	-4.68462	-0.05773	2.39553
H	-2.10275	3.82000	-2.91331
H	-4.13710	2.12466	-2.16823
H	1.17806	2.37113	0.22006

H	2.41425	-0.00891	0.67812
C	3.60603	-0.02132	1.28033
C	4.14659	-1.26632	0.71000
C	4.14829	1.24207	0.75366
H	3.41872	-0.04004	2.36305
C	4.59067	-1.25784	-0.63646
C	4.16775	-2.47861	1.42734
C	4.59249	1.27989	-0.59230
C	4.16963	2.42896	1.51228
C	5.04985	-2.44475	-1.21891
C	4.47025	0.02531	-1.43055
C	4.61987	-3.65949	0.83207
H	3.81657	-2.48714	2.46554
C	5.05270	2.48587	-1.13335
C	4.62232	3.62948	0.95807
H	3.81781	2.40196	2.54995
C	5.06468	-3.64691	-0.49699
H	5.39237	-2.43139	-2.26049
H	5.18876	0.03932	-2.26834
H	3.45918	0.03407	-1.88499
H	4.62561	-4.59285	1.40543
H	5.39539	2.50826	-2.17471
C	5.06783	3.66244	-0.37041
H	4.62811	4.54258	1.56317
H	5.42205	-4.56742	-0.97027
H	5.42584	4.59854	-0.81156

$L_1Co^{III}O$ + DHA (*S*=2)

100
dha_ts_u4.out Energy: -2135629.9062323

C	1.42388	-0.31117	-1.70386
N	1.29818	-0.71993	-2.99285
C	2.55169	-1.01626	-3.51650
C	3.45709	-0.76736	-2.52277
N	2.75599	-0.30646	-1.42079
B	3.27682	-0.03751	0.05847
N	2.62088	1.30831	0.59226
C	1.28019	1.51960	0.64173
N	1.08842	2.75245	1.16874
C	2.31830	3.33291	1.45989
C	3.27360	2.42384	1.09600
N	2.66743	-1.24177	0.88496
C	1.31908	-1.39217	1.02316
N	1.12583	-2.58403	1.64789
C	2.35127	-3.20970	1.86234
C	3.30914	-2.37114	1.37044
Co	0.19469	-0.01493	-0.08527
O	-1.50889	-0.39003	-0.00113
C	-0.02095	-0.85971	-3.69114
C	0.21306	-1.19180	-5.16989
C	-0.81631	-1.98863	-3.01404
C	-0.77963	0.47371	-3.57368
C	-0.27561	3.33504	1.38126
C	-0.14863	4.74391	1.97025
C	-0.99859	3.39464	0.02614
C	-1.04762	2.42243	2.34963

C	-0.22140	-3.14621	1.99561
C	-1.02112	-2.07399	2.75464
C	-0.94072	-3.53154	0.69225
C	-0.04775	-4.38386	2.88597
H	-0.76255	-1.25592	-5.67673
H	0.80620	-0.41139	-5.67515
H	-0.24888	-2.93422	-3.03744
H	-1.77242	-2.14144	-3.54210
H	-1.04042	-1.72674	-1.96912
H	-0.18528	1.30145	-3.99500
H	-1.01370	0.70076	-2.52312
H	-1.73219	0.40904	-4.12488
H	0.39712	5.42206	1.29323
H	0.35718	4.73492	2.95008
H	-1.15863	5.15761	2.11742
H	-0.41659	3.98144	-0.70423
H	-1.98942	3.85811	0.14777
H	-0.52506	2.34501	3.31791
H	-2.05699	2.83138	2.51976
H	-1.15938	1.41474	1.91958
H	-2.00169	-2.48632	3.04653
H	-0.48559	-1.76173	3.66734
H	-1.92181	-3.97974	0.92407
H	-1.11196	-2.63352	0.08130
H	0.50480	-4.14800	3.81095
H	0.46871	-5.20443	2.36101
H	-1.04516	-4.75281	3.17246
H	0.71764	-2.16354	-5.29840
H	-0.34634	-4.26558	0.12158
H	-1.16010	2.38204	-0.37405
C	4.87879	0.14317	0.18673
C	5.62679	0.79490	-0.81721
C	6.98510	1.09642	-0.65635
C	7.64122	0.76760	0.53543
C	6.91650	0.15805	1.56603
C	5.55859	-0.13763	1.39121
H	5.13620	1.10613	-1.74459
H	7.52995	1.59971	-1.46253
H	8.70362	0.99943	0.66611
H	7.40724	-0.08016	2.51605
H	5.01334	-0.57409	2.23352
H	2.71488	-1.36828	-4.53055
H	4.53648	-0.89321	-2.52923
H	2.42989	4.32343	1.89104
H	4.35656	2.49355	1.15877
H	2.45847	-4.17732	2.34271
H	4.38687	-2.50452	1.33057
H	-1.19929	-1.20012	2.11140
H	-2.51768	-0.11922	-0.71171
C	-3.71326	0.05396	-1.20789
C	-4.37408	-1.05326	-0.48630
C	-4.08374	1.41677	-0.77831
H	-3.62733	-0.08424	-2.29532
C	-4.67873	-0.86879	0.88527
C	-4.62128	-2.30535	-1.07978
C	-4.40425	1.62633	0.58647
C	-4.09993	2.51433	-1.65989
C	-5.23897	-1.92243	1.61643
C	-4.30042	0.44770	1.52917

C	-5.16891	-3.35600	-0.33647
H	-4.37326	-2.45155	-2.13737
C	-4.74662	2.90969	1.02694
C	-4.43915	3.79349	-1.20803
H	-3.84638	2.35370	-2.71402
C	-5.48364	-3.16610	1.01614
H	-5.47634	-1.77278	2.67635
H	-4.87888	0.62257	2.45200
H	-3.23561	0.36171	1.82814
H	-5.35455	-4.32428	-0.81379
H	-4.99713	3.06439	2.08303
C	-4.76688	3.99548	0.13937
H	-4.44845	4.63545	-1.90855
H	-5.91725	-3.98272	1.60286
H	-5.03513	4.99396	0.49992

$L_1Co^{III}O$ + Fluorene (*S*=0, closed-shell)

97
fluorene_ts_u0_closed.out Energy: -2110974.6416944

C	-1.03275	-0.70758	-1.29869
N	-0.45861	-1.31630	-2.37900
C	-1.45126	-1.61537	-3.30797
C	-2.63780	-1.19615	-2.77837
N	-2.36635	-0.66473	-1.53339
B	-3.25977	0.04612	-0.45474
N	-2.84982	-0.61020	0.91416
C	-1.56338	-0.65658	1.33563
N	-1.56422	-1.31255	2.53966
C	-2.87536	-1.66630	2.85146
C	-3.66977	-1.22571	1.83561
N	-2.65635	1.49385	-0.41655
C	-1.33682	1.62090	-0.13451
N	-1.02722	2.94669	-0.27527
C	-2.16922	3.63349	-0.67828
C	-3.17794	2.72021	-0.77432
Co	-0.22018	0.10958	0.25018
O	1.30904	0.10085	1.00316
C	0.99430	-1.68333	-2.51673
C	1.22113	-2.40366	-3.85253
C	1.84736	-0.40717	-2.48065
C	1.36334	-2.62441	-1.36113
C	-0.38584	-1.62184	3.43018
C	-0.86199	-2.40451	4.66409
C	0.61199	-2.49304	2.65099
C	0.23892	-0.29619	3.89273
C	0.31431	3.59000	-0.03943
C	0.70015	3.38709	1.43425
C	1.34349	2.95342	-0.98369
C	0.22553	5.09345	-0.33746
H	2.28654	-2.67404	-3.91772
H	0.63652	-3.33528	-3.92640
H	1.49970	0.32052	-3.23250
H	2.89873	-0.66128	-2.68441
H	1.82363	0.05632	-1.48578
H	0.73760	-3.53266	-1.38535
H	1.23454	-2.12474	-0.39097

H	2.42130	-2.91513	-1.43997
H	-1.31978	-3.37054	4.39480
H	-1.57094	-1.82654	5.27912
H	0.01835	-2.61831	5.28995
H	0.12557	-3.42137	2.30668
H	1.45252	-2.76546	3.31004
H	-0.50057	0.30064	4.45343
H	1.09366	-0.50511	4.55743
H	0.60428	0.27538	3.02980
H	1.67690	3.85923	1.62537
H	-0.05233	3.84733	2.09684
H	2.30766	3.47730	-0.89769
H	1.52850	1.90677	-0.71391
H	-0.49520	5.60739	0.31950
H	-0.03780	5.29283	-1.38932
H	1.21657	5.53652	-0.15340
H	0.98532	-1.76006	-4.71630
H	0.99755	3.00671	-2.02939
H	1.01808	-1.94848	1.79055
C	-4.85409	-0.06568	-0.63457
C	-5.45790	-1.20902	-1.19942
C	-6.84870	-1.37007	-1.24052
C	-7.68576	-0.38952	-0.69614
C	-7.11488	0.73647	-0.09169
C	-5.72285	0.88530	-0.05734
H	-4.83457	-2.01666	-1.59400
H	-7.27884	-2.27084	-1.69154
H	-8.77382	-0.50997	-0.72740
H	-7.75516	1.49922	0.36444
H	-5.31033	1.75576	0.46167
H	-1.25150	-2.09551	-4.25998
H	-3.63662	-1.22962	-3.20445
H	-3.14805	-2.19609	3.75698
H	-4.74539	-1.30313	1.69900
H	-2.18728	4.70177	-0.86382
H	-4.21131	2.85788	-1.07998
H	0.79054	2.31731	1.66881
H	2.46767	-0.02037	1.36975
C	3.82962	-0.12986	1.64001
C	4.33283	1.02406	0.89432
H	3.83750	-0.14914	2.73928
C	4.23159	-1.29998	0.85876
C	4.32573	2.39788	1.19447
C	4.82686	0.58657	-0.37917
C	4.11469	-2.67739	1.11994
C	4.77576	-0.86878	-0.39625
C	4.78499	3.31440	0.24298
H	3.95757	2.74798	2.16547
C	5.25922	1.51930	-1.33524
C	4.53321	-3.60073	0.15642
H	3.70079	-3.02370	2.07346
C	5.16757	-1.80616	-1.36483
C	5.23894	2.88312	-1.02137
H	4.78270	4.38491	0.47800
H	5.62004	1.18218	-2.31403
C	5.05098	-3.17233	-1.08440
H	4.45011	-4.67377	0.36311
H	5.57386	-1.47193	-2.32663
H	5.58128	3.61946	-1.75645

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H          5.36279       -3.91289       -1.82870
```

$L_1Co^{III}O$ + Fluorene (*S*=1)

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97
fluorene_ts_u2.out        Energy: -2110968.8996314
C         -0.89473       -0.79022       -1.19407
N         -0.30900       -1.23924       -2.33578
C         -1.25339       -1.27685       -3.35630
C         -2.43639       -0.85903       -2.81670
N         -2.21236       -0.59235       -1.47811
B         -3.18446        0.05480       -0.41086
N         -2.89291       -0.68452        0.93920
C         -1.63998       -0.74224        1.43139
N         -1.68322       -1.43981        2.59737
C         -3.00527       -1.82353        2.83475
C         -3.75338       -1.34911        1.79631
N         -2.64384        1.53068       -0.23448
C         -1.40337        1.76855        0.27764
N         -1.17867        3.10415        0.14871
C         -2.26363        3.69954       -0.48758
C         -3.16889        2.70835       -0.73492
Co        -0.25769        0.11717        0.46339
O          1.41489        0.34466        0.73281
C          1.14502       -1.58665       -2.47910
C          1.35483       -2.39189       -3.76857
C          1.95243       -0.28048       -2.53613
C          1.56536       -2.43798       -1.27426
C         -0.49997       -1.73251        3.47278
C         -0.94918       -2.56781        4.67811
C          0.53378       -2.52207        2.65298
C          0.09158       -0.39788        3.95701
C          0.09507        3.80784        0.51683
C          0.55094        3.32685        1.90283
C          1.14701        3.47203       -0.55263
C         -0.15219        5.32254        0.55929
H          2.41183       -2.69722       -3.81751
H          0.73488       -3.30396       -3.78495
H          1.62982        0.33957       -3.38999
H          3.02450       -0.50704       -2.64592
H          1.82606        0.28502       -1.60148
H          0.92498       -3.33173       -1.18498
H          1.50947       -1.85640       -0.34563
H          2.61016       -2.75878       -1.39545
H         -1.37901       -3.53505        4.36986
H         -1.68261       -2.03052        5.30142
H         -0.06898       -2.77766        5.30547
H          0.08854       -3.44464        2.24515
H          1.38340       -2.79934        3.29784
H         -0.66695        0.19021        4.50004
H          0.93728       -0.59220        4.63694
H          0.46882        0.19514        3.11001
H          1.44878        3.89184        2.20362
H         -0.23758        3.49725        2.65510
H          2.08861        4.00246       -0.34003
H          1.35992        2.39287       -0.54767
H         -0.96325        5.58243        1.26006
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H	-0.39182	5.73590	-0.43392
H	0.76865	5.81818	0.90435
H	1.14230	-1.79834	-4.67289
H	0.79232	3.77524	-1.55251
H	0.92707	-1.91701	1.82293
C	-4.75799	-0.07570	-0.73029
C	-5.28272	-1.20569	-1.39255
C	-6.66104	-1.40019	-1.54777
C	-7.56498	-0.46821	-1.02480
C	-7.07475	0.64350	-0.32976
C	-5.69412	0.82646	-0.18170
H	-4.60451	-1.97198	-1.78073
H	-7.02987	-2.28828	-2.07237
H	-8.64363	-0.61481	-1.14522
H	-7.77006	1.36852	0.10708
H	-5.34458	1.68626	0.39850
H	-1.02663	-1.60083	-4.36723
H	-3.40854	-0.73481	-3.28705
H	-3.30960	-2.39430	3.70590
H	-4.81983	-1.43160	1.60069
H	-2.32089	4.76137	-0.70525
H	-4.13712	2.76015	-1.22642
H	0.81444	2.26037	1.87800
H	2.56792	0.13618	0.96942
C	3.91591	0.01827	1.28899
C	4.48891	1.01117	0.37508
H	3.87639	0.19658	2.37272
C	4.31925	-1.28339	0.75062
C	4.47058	2.41498	0.40977
C	5.05686	0.34163	-0.75514
C	4.12566	-2.58659	1.23817
C	4.95644	-1.09431	-0.51758
C	5.00525	3.13617	-0.66389
H	4.02835	2.93987	1.26386
C	5.57574	1.07456	-1.83239
C	4.55293	-3.67808	0.47381
H	3.63820	-2.74638	2.20592
C	5.36423	-2.19618	-1.28337
C	5.54947	2.47348	-1.78278
H	4.99414	4.23164	-0.63900
H	5.99921	0.55890	-2.70189
C	5.16321	-3.48845	-0.78280
H	4.40541	-4.69548	0.85289
H	5.84147	-2.04809	-2.25877
H	5.95506	3.05772	-2.61572
H	5.48130	-4.35725	-1.36885

$L_1Co^{III}O$ + Fluorene (*S*=2)

97
fluorene_ts_u4.out Energy: -2110966.6862674

C	-0.87314	-0.67459	-1.26175
N	-0.35357	-1.14340	-2.42422
C	-1.36786	-1.31148	-3.35731
C	-2.53174	-0.94620	-2.73751
N	-2.21960	-0.58465	-1.43887
B	-3.14812	0.05642	-0.31668

N	-2.83328	-0.66289	1.06289
C	-1.59478	-0.72649	1.61562
N	-1.70769	-1.43070	2.76840
C	-3.03159	-1.81476	2.95256
C	-3.73043	-1.33201	1.88132
N	-2.63214	1.54671	-0.23437
C	-1.35666	1.84001	0.14778
N	-1.17425	3.16375	-0.10556
C	-2.32223	3.69723	-0.68380
C	-3.22405	2.67786	-0.77464
Co	-0.15641	0.14593	0.49105
O	1.44625	0.58715	0.99298
C	1.10204	-1.45481	-2.60677
C	1.32934	-2.06414	-3.99505
C	1.91263	-0.15710	-2.46532
C	1.51079	-2.46402	-1.52305
C	-0.54403	-1.72961	3.66371
C	-1.02380	-2.53211	4.87868
C	0.48551	-2.55099	2.86740
C	0.07500	-0.39754	4.12053
C	0.11018	3.90364	0.12681
C	0.55571	3.67080	1.57922
C	1.15990	3.36536	-0.85901
C	-0.10777	5.40410	-0.10952
H	2.39849	-2.30654	-4.09960
H	0.75793	-2.99715	-4.13269
H	1.56686	0.60264	-3.18627
H	2.97913	-0.36157	-2.64834
H	1.82893	0.24874	-1.44629
H	0.88666	-3.37175	-1.57923
H	1.40838	-2.02519	-0.51942
H	2.56524	-2.74817	-1.65053
H	-1.46360	-3.49931	4.58395
H	-1.76247	-1.96995	5.47365
H	-0.15989	-2.74142	5.52867
H	0.03036	-3.47293	2.46882
H	1.32510	-2.83155	3.52458
H	-0.67646	0.22437	4.63551
H	0.90345	-0.59539	4.82101
H	0.47793	0.15885	3.25929
H	1.47643	4.24566	1.77568
H	-0.22360	4.00969	2.28301
H	2.11130	3.90799	-0.73434
H	1.35321	2.30199	-0.66157
H	-0.88669	5.81469	0.55469
H	-0.37622	5.62610	-1.15553
H	0.83382	5.93253	0.10756
H	1.06527	-1.36018	-4.80174
H	0.81626	3.49156	-1.89996
H	0.89300	-1.96464	2.02931
C	-4.73602	-0.10206	-0.57589
C	-5.27566	-1.26143	-1.17277
C	-6.65660	-1.47747	-1.26391
C	-7.55075	-0.53770	-0.73845
C	-7.04551	0.60277	-0.10352
C	-5.66234	0.80600	-0.01978
H	-4.60658	-2.03891	-1.55380
H	-7.03440	-2.38949	-1.73877
H	-8.63149	-0.70081	-0.80835

H	-7.73072	1.33449	0.33817
H	-5.30177	1.68713	0.51993
H	-1.20386	-1.67079	-4.36874
H	-3.54225	-0.91407	-3.13578
H	-3.37961	-2.38828	3.80627
H	-4.78845	-1.41827	1.64813
H	-2.42197	4.73768	-0.97639
H	-4.22949	2.68120	-1.18671
H	0.77366	2.60630	1.74878
H	2.57903	0.12746	1.14375
C	3.86994	-0.17246	1.35276
C	4.49705	0.83481	0.47941
H	3.90476	-0.05825	2.44611
C	4.20060	-1.46951	0.74079
C	4.51777	2.23375	0.57078
C	5.04087	0.19136	-0.67246
C	3.93528	-2.77987	1.16441
C	4.87151	-1.25111	-0.50158
C	5.08163	2.97930	-0.47243
H	4.08182	2.73777	1.44003
C	5.59389	0.94520	-1.71591
C	4.33542	-3.85545	0.36095
H	3.41842	-2.95965	2.11275
C	5.25803	-2.33234	-1.30427
C	5.61312	2.34223	-1.61011
H	5.10234	4.07268	-0.40722
H	6.00335	0.45073	-2.60383
C	4.99065	-3.63619	-0.86566
H	4.13336	-4.88089	0.68890
H	5.76953	-2.16224	-2.25810
H	6.04281	2.94415	-2.41785
H	5.29038	-4.49080	-1.48126

$L_1Co^{III}O + Ph_2CH_2$ (*S*=0, closed-shell)

99
ph2ch2_ts_u0_closed.out Energy: -2111718.7042639

C	-1.28865	-0.19138	1.58188
N	-0.97627	-0.36956	2.90297
C	-2.15616	-0.43474	3.64032
C	-3.18897	-0.28595	2.76184
N	-2.64049	-0.11454	1.50669
B	-3.29282	-0.00353	0.08157
N	-2.56262	1.19985	-0.62303
C	-1.21246	1.26606	-0.73470
N	-0.92920	2.42544	-1.40968
C	-2.12674	3.07072	-1.71028
C	-3.13897	2.30264	-1.21741
N	-2.75489	-1.29029	-0.63827
C	-1.40915	-1.42287	-0.72242
N	-1.16719	-2.62656	-1.32490
C	-2.38225	-3.25644	-1.58098
C	-3.36823	-2.42186	-1.13916
Co	-0.18169	-0.13870	0.01776
O	1.49137	0.24197	-0.07003
C	0.40445	-0.42694	3.49665
C	0.30626	-0.67268	5.00898

C	1.18385	-1.58262	2.85187
C	1.09485	0.92277	3.24193
C	0.42819	2.98480	-1.76223
C	0.25843	4.27784	-2.57504
C	1.17586	3.30640	-0.46024
C	1.18548	1.96011	-2.62153
C	0.18403	-3.15741	-1.71421
C	0.80104	-2.18732	-2.73483
C	1.06328	-3.27407	-0.46148
C	0.03140	-4.54406	-2.35320
H	1.32770	-0.71728	5.41763
H	-0.22283	0.14195	5.52975
H	0.63440	-2.53258	2.95767
H	2.16526	-1.68759	3.34184
H	1.37000	-1.38854	1.78845
H	0.51307	1.74459	3.69213
H	1.20912	1.10487	2.16443
H	2.09849	0.91589	3.69701
H	-0.25445	5.06879	-2.00368
H	-0.28011	4.10873	-3.52233
H	1.26288	4.65333	-2.82523
H	0.61321	4.04911	0.13147
H	2.17062	3.72143	-0.68996
H	0.60789	1.71517	-3.52927
H	2.15382	2.38901	-2.92774
H	1.38525	1.04908	-2.04311
H	1.79237	-2.55407	-3.04260
H	0.15713	-2.10122	-3.62626
H	2.02066	-3.75245	-0.71848
H	1.30858	-2.28340	-0.05729
H	-0.41173	-5.27261	-1.65421
H	1.03396	-4.90930	-2.62523
H	-0.57358	-4.51436	-3.27420
H	-0.18831	-1.63045	5.24048
H	0.55919	-3.87142	0.31614
H	1.32800	2.39249	0.12749
C	-4.88150	0.24949	0.03694
C	-5.52251	1.05226	1.00500
C	-6.87858	1.38909	0.91118
C	-7.63941	0.94260	-0.17549
C	-7.02173	0.17987	-1.17307
C	-5.66451	-0.14977	-1.06692
H	-4.94859	1.45552	1.84474
H	-7.33958	2.01131	1.68590
H	-8.70074	1.20145	-0.25280
H	-7.59572	-0.15298	-2.04463
H	-5.20542	-0.70785	-1.88798
H	-2.18091	-0.57963	4.71482
H	-4.26004	-0.30383	2.94273
H	-2.17629	4.01306	-2.24392
H	-4.21490	2.45488	-1.24583
H	-2.46128	-4.23231	-2.04831
H	-4.44521	-2.56442	-1.13659
H	0.93624	-1.18963	-2.29214
H	2.56300	0.13068	0.36094
C	3.91689	-0.05731	0.79614
H	3.84635	-0.19202	1.88553
C	4.37850	1.28989	0.43758
C	4.25011	-1.30776	0.09818

C	4.94853	1.66025	-0.80756
C	4.17199	2.34484	1.36919
C	4.54568	-2.47736	0.84564
C	4.18180	-1.46310	-1.31123
C	5.25836	2.99196	-1.10610
H	5.16756	0.89351	-1.55329
C	4.48440	3.66986	1.07187
H	3.74063	2.10263	2.34652
C	4.78975	-3.70752	0.23109
H	4.58516	-2.40519	1.93889
C	4.44072	-2.69069	-1.92692
H	3.87315	-0.61775	-1.93010
C	5.02355	4.01418	-0.17802
H	5.69632	3.23115	-2.08233
H	4.29988	4.44795	1.82163
C	4.75277	-3.82571	-1.16618
H	5.01781	-4.58376	0.84886
H	4.37931	-2.76611	-3.01871
H	5.26261	5.05533	-0.41784
H	4.95212	-4.78658	-1.65168

$L_1Co^{III}O + Ph_2CH_2$ (*S*=1)

99
ph2ch2_ts_u2.out Energy: -2111715.9297622

C	-1.53814	-0.84377	-1.49761
N	-1.59856	-1.34992	-2.75844
C	-2.91451	-1.32283	-3.21121
C	-3.66840	-0.80928	-2.19608
N	-2.81917	-0.54902	-1.13441
B	-3.14432	0.16332	0.24396
N	-2.34832	-0.61525	1.35429
C	-1.01196	-0.80482	1.26484
N	-0.63814	-1.54714	2.33755
C	-1.76141	-1.82876	3.11596
C	-2.82681	-1.24219	2.49545
N	-2.48318	1.59307	0.10419
C	-1.13215	1.74111	-0.00595
N	-0.90465	3.06382	-0.22521
C	-2.11692	3.74187	-0.30545
C	-3.09936	2.81409	-0.11190
Co	-0.14321	-0.01082	-0.29960
O	1.40867	0.17441	-1.05180
C	-0.41642	-1.81180	-3.55579
C	-0.89924	-2.65688	-4.74301
C	0.34341	-0.57262	-4.05743
C	0.48102	-2.66737	-2.64885
C	0.76045	-2.02825	2.56196
C	0.84808	-2.76314	3.90434
C	1.13086	-2.98119	1.41514
C	1.70165	-0.81454	2.57387
C	0.45187	3.68087	-0.39226
C	1.37760	3.12610	0.69788
C	0.98450	3.31995	-1.78846
C	0.34471	5.20475	-0.24315
H	-0.01921	-3.05096	-5.27514
H	-1.50919	-3.51367	-4.41080

H	-0.31678	0.06391	-4.67130
H	1.19861	-0.88644	-4.67989
H	0.72693	0.00219	-3.19981
H	-0.08666	-3.50625	-2.21270
H	0.90867	-2.05663	-1.84187
H	1.31294	-3.08090	-3.24240
H	0.20752	-3.66003	3.92469
H	0.57330	-2.10787	4.74761
H	1.88755	-3.09360	4.05678
H	0.44936	-3.84829	1.39304
H	2.16434	-3.34040	1.53622
H	1.39989	-0.08698	3.34545
H	2.72940	-1.15228	2.77995
H	1.71225	-0.31004	1.59530
H	2.36621	3.60300	0.62245
H	0.96473	3.32450	1.70147
H	1.97626	3.77964	-1.93637
H	1.09405	2.22746	-1.87302
H	-0.09776	5.48898	0.72644
H	-0.24518	5.66456	-1.05314
H	1.35859	5.63225	-0.29255
H	-1.48094	-2.06445	-5.46805
H	0.30377	3.69287	-2.57317
H	1.07277	-2.46325	0.44604
C	-4.70200	0.16195	0.67089
C	-5.54859	-0.92454	0.36354
C	-6.85612	-1.01136	0.85809
C	-7.35675	-0.01100	1.69934
C	-6.52736	1.05891	2.05489
C	-5.22181	1.13322	1.55298
H	-5.17609	-1.74471	-0.25788
H	-7.48271	-1.86966	0.59206
H	-8.37904	-0.07299	2.08740
H	-6.89430	1.83609	2.73417
H	-4.58779	1.96182	1.88324
H	-3.21742	-1.66997	-4.19406
H	-4.73675	-0.61311	-2.15893
H	-1.72149	-2.40704	4.03393
H	-3.87689	-1.22144	2.77649
H	-2.19564	4.81034	-0.48067
H	-4.17910	2.93863	-0.11469
H	1.52368	2.04544	0.57183
H	2.58533	0.09747	-0.80174
C	3.94467	-0.00096	-0.72369
H	4.08641	0.06809	-1.81415
C	4.21909	-1.37793	-0.25203
C	4.38164	1.23706	-0.04975
C	4.86250	-1.72192	0.95828
C	3.80220	-2.45000	-1.08095
C	4.79097	2.34106	-0.83733
C	4.32267	1.44218	1.35010
C	5.05898	-3.05947	1.32449
H	5.24117	-0.93690	1.61587
C	3.99792	-3.78126	-0.71843
H	3.30498	-2.21600	-2.02694
C	5.14550	3.56471	-0.26435
H	4.82992	2.22657	-1.92659
C	4.69005	2.66096	1.92621
H	3.95288	0.64703	1.99814

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C          4.62531       -4.10052        0.49591
H          5.56503       -3.28675        2.26941
H          3.65395       -4.57943       -1.38560
C          5.10808        3.73287        1.12679
H          5.45809        4.39346       -0.90914
H          4.63055        2.78010        3.01362
H          4.77616       -5.14486        0.78773
H          5.38974        4.68888        1.57986
```

$L_1Co^{III}O + Ph_2CH_2$ (*S*=2)

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99
ph2ch2_ts_u4.out  Energy: -2111713.9799961
C         -1.35298       -1.52215       -0.90958
N         -1.19777       -2.53532       -1.80109
C         -2.42093       -2.84268       -2.38533
C         -3.34065       -2.00076       -1.82488
N         -2.67890       -1.21193       -0.89940
B         -3.21821        0.04593       -0.09374
N         -2.65653       -0.02700        1.38171
C         -1.33321       -0.10980        1.69005
N         -1.24859       -0.10546        3.04465
C         -2.52488       -0.02187        3.59853
C         -3.40041        0.02701        2.55389
N         -2.52869        1.27932       -0.82042
C         -1.17544        1.43543       -0.79992
N         -0.89383        2.48914       -1.60917
C         -2.06488        2.97759       -2.17550
C         -3.08274        2.20585       -1.68744
Co        -0.13443       -0.14665        0.01687
O          1.56708       -0.27014        0.44895
C          0.12787       -3.15042       -2.12711
C         -0.07824       -4.36453       -3.04112
C          0.98507       -2.09276       -2.84389
C          0.80046       -3.59059       -0.81642
C          0.04731       -0.15638        3.79501
C         -0.22778       -0.13684        5.30372
C          0.78013       -1.45379        3.41397
C          0.88286        1.07338        3.39826
C          0.49776        2.98708       -1.85168
C          1.16205        3.25613       -0.49269
C          1.27042        1.90355       -2.62075
C          0.45019        4.27993       -2.67429
H          0.89997       -4.83171       -3.23488
H         -0.72728       -5.12141       -2.57024
H          0.45053       -1.67914       -3.71500
H          1.92619       -2.54483       -3.19684
H          1.23720       -1.27073       -2.15692
H          0.15599       -4.29829       -0.26848
H          1.01207       -2.72160       -0.17427
H          1.75899       -4.08668       -1.03804
H         -0.82476       -1.00700        5.62410
H         -0.74487        0.78553        5.61662
H          0.73479       -0.17697        5.83751
H          0.15390       -2.33346        3.64119
H          1.71618       -1.53456        3.99219
H          0.33769        2.00430        3.63008
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H	1.83188	1.07674	3.96086
H	1.11965	1.04131	2.32407
H	2.17814	3.65193	-0.64445
H	0.57635	3.98996	0.08644
H	2.28754	2.25829	-2.84987
H	1.36433	0.99580	-2.00707
H	0.02304	4.11738	-3.67774
H	1.47902	4.65006	-2.80655
H	-0.12902	5.06657	-2.16263
H	-0.50937	-4.08041	-4.01522
H	0.75814	1.64790	-3.56329
H	1.03689	-1.44592	2.34370
C	-4.83035	0.13492	0.00904
C	-5.62111	-1.02663	0.14192
C	-6.99959	-0.96587	0.38216
C	-7.63523	0.27388	0.51626
C	-6.87131	1.44345	0.43089
C	-5.49349	1.36739	0.19039
H	-5.15066	-2.01314	0.08634
H	-7.57714	-1.89211	0.47506
H	-8.71318	0.32753	0.70249
H	-7.34743	2.42128	0.56232
H	-4.92123	2.29987	0.17504
H	-2.55525	-3.61830	-3.13318
H	-4.40443	-1.91067	-2.02811
H	-2.71858	-0.00562	4.66657
H	-4.48499	0.09495	2.56036
H	-2.09831	3.81776	-2.86264
H	-4.14640	2.25230	-1.90533
H	1.25290	2.32674	0.08859
H	2.61314	-0.19829	-0.21398
C	3.80773	-0.07332	-0.76814
H	3.63590	-0.16211	-1.85199
C	4.49348	-1.26955	-0.22451
C	4.20289	1.30381	-0.36872
C	5.25678	-1.26940	0.96500
C	4.33326	-2.50906	-0.88931
C	4.70462	2.21814	-1.31756
C	4.01887	1.76408	0.95384
C	5.81535	-2.44947	1.46760
H	5.42556	-0.33116	1.49973
C	4.88866	-3.68680	-0.38768
H	3.75188	-2.53848	-1.81586
C	5.02759	3.53219	-0.95989
H	4.84358	1.88827	-2.35322
C	4.34836	3.07280	1.31534
H	3.56544	1.09285	1.68774
C	5.63286	-3.66795	0.80123
H	6.40410	-2.41442	2.39101
H	4.74104	-4.62807	-0.92872
C	4.85627	3.96549	0.36114
H	5.41523	4.22166	-1.71778
H	4.18833	3.40627	2.34653
H	6.06931	-4.59007	1.19860
H	5.10657	4.99359	0.64285

$L_1Co^{III}O$ + 9-Ph-Fluorene (*S*=0, closed-shell)

```
107
phflu_ts_u0_closed.out    Energy: -2255927.7441641
C           1.57534       -1.77165       -0.21029
N           1.14670       -3.05792       -0.38147
C           2.25092       -3.90510       -0.39644
C           3.35965       -3.12234       -0.24725
N           2.92889       -1.81362       -0.16176
B           3.67525       -0.45449        0.08715
N           3.07410        0.53900       -0.96785
C           1.74108        0.75359       -1.06644
N           1.55854        1.63922       -2.09634
C           2.80417        1.96623       -2.62842
C           3.74340        1.27754       -1.92043
N           3.09123        0.00177        1.47034
C           1.74707        0.14296        1.58744
N           1.49166        0.39915        2.90858
C           2.69424        0.38521        3.60954
C           3.68497        0.12671        2.70907
Co          0.56392       -0.14908        0.10809
O          -1.06143        0.36559        0.08332
C          -0.27722       -3.48839       -0.60083
C          -0.32900       -5.00334       -0.84009
C          -1.11091       -3.14485        0.64239
C          -0.81029       -2.75922       -1.84215
C           0.26194        2.23944       -2.57775
C           0.53076        3.15027       -3.78540
C          -0.68753        1.11288       -3.01287
C          -0.33334        3.07714       -1.43782
C           0.14756        0.64101        3.54487
C          -0.47389        1.89454        2.91016
C          -0.73051       -0.60044        3.33264
C           0.32318        0.87471        5.05249
H          -1.37801       -5.28501       -1.02106
H           0.25444       -5.30391       -1.72578
H          -0.64708       -3.55916        1.55280
H          -2.12328       -3.56246        0.53484
H          -1.22632       -2.05853        0.75458
H          -0.19557       -2.99783       -2.72650
H          -0.81062       -1.67076       -1.69064
H          -1.84950       -3.06183       -2.03567
H           0.96944        2.59926       -4.63374
H           1.18268        4.00179       -3.53090
H          -0.43362        3.56345       -4.11953
H          -0.22244        0.49378       -3.79854
H          -1.61127        1.55560       -3.41929
H           0.36766        3.87669       -1.14245
H          -1.27609        3.54178       -1.76669
H          -0.55987        2.44059       -0.57281
H          -1.45772        2.08711        3.36748
H           0.17115        2.77321        3.08004
H          -1.67929       -0.48784        3.87834
H          -0.98265       -0.72554        2.27311
H           0.94757        1.75714        5.26850
H           0.75002       -0.00438        5.56276
H          -0.67213        1.05866        5.48600
H           0.02409       -5.57356        0.03514
H          -0.21485       -1.50488        3.69658
H          -0.96446        0.48042       -2.16080
C           5.27813       -0.45953       -0.04761
```

```
C          5.94532       -1.31147       -0.95286
C          7.32685       -1.22881       -1.16905
C          8.08760       -0.26913       -0.49184
C          7.44723        0.61764        0.38159
C          6.06549        0.52412        0.58888
H          5.37666       -2.04367       -1.53325
H          7.80829       -1.91161       -1.87745
H          9.16828       -0.20171       -0.65606
H          8.02381        1.39286        0.89774
H          5.59144        1.26017        1.24549
H          2.17563       -4.98125       -0.51082
H          4.40593       -3.40845       -0.18544
H          2.93358        2.65320       -3.45701
H          4.82557        1.25527       -2.02118
H          2.76282        0.55909        4.67755
H          4.75399        0.01409        2.86644
H         -0.62073        1.74828        1.83151
H         -2.32520        0.45300       -0.00684
C         -3.66905        0.49910       -0.08481
C         -4.02153       -0.03873        1.25290
C         -3.95329       -0.61639       -1.01396
C         -4.07253        0.57201        2.51632
C         -4.31353       -1.43269        1.14233
C         -3.86401       -0.70073       -2.41462
C         -4.28475       -1.78929       -0.26940
C         -4.37268       -0.19933        3.64532
H         -3.88454        1.64375        2.62465
C         -4.58443       -2.20296        2.28310
C         -4.13199       -1.91628       -3.05400
H         -3.58821        0.17703       -3.00545
C         -4.52945       -3.00932       -0.91745
C         -4.61009       -1.58327        3.53735
H         -4.41400        0.28070        4.62944
H         -4.78815       -3.27573        2.18997
C         -4.46454       -3.06799       -2.31363
H         -4.07334       -1.97521       -4.14642
H         -4.77801       -3.90434       -0.33607
H         -4.82639       -2.17153        4.43543
H         -4.66475       -4.01118       -2.83277
C         -3.90322        1.93192       -0.42712
C         -3.26061        2.94706        0.31596
C         -4.74058        2.33847       -1.48773
C         -3.45445        4.29991        0.02418
H         -2.57167        2.66292        1.11385
C         -4.92218        3.69229       -1.79359
H         -5.26847        1.58158       -2.07443
C         -4.28250        4.68395       -1.03853
H         -2.93674        5.06051        0.61909
H         -5.57917        3.97448       -2.62400
H         -4.42723        5.74310       -1.27615
```

$L_1Co^{III}O$ + 9-Ph-Fluorene (*S*=1)

```
107
phflu_ts_u2_opt.out       Energy: -2254315.8488442
C          1.46323       -1.56402       -0.52701
N          1.04729       -2.84649       -0.70141
```

C	2.13609	-3.70566	-0.60259
C	3.23549	-2.92649	-0.38115
N	2.81540	-1.60896	-0.36896
B	3.63546	-0.30687	-0.01179
N	3.11160	0.81184	-0.97587
C	1.79870	1.11062	-1.03502
N	1.64024	2.10747	-1.94494
C	2.89399	2.43710	-2.46425
C	3.80645	1.62421	-1.85607
N	3.13333	0.07939	1.43740
C	1.84287	0.45519	1.66075
N	1.69921	0.56893	3.00902
C	2.89020	0.21809	3.63632
C	3.77716	-0.09954	2.64849
Co	0.61091	0.14203	0.08910
O	-1.06870	0.17175	0.39467
C	-0.37456	-3.26302	-0.93821
C	-0.40808	-4.70706	-1.45673
C	-1.14067	-3.16273	0.38993
C	-0.97834	-2.33063	-1.99495
C	0.33706	2.77667	-2.27147
C	0.55826	3.82219	-3.37120
C	-0.66200	1.71685	-2.76259
C	-0.18213	3.46019	-0.99777
C	0.43139	0.96022	3.70936
C	-0.14338	2.19633	3.00348
C	-0.55098	-0.22002	3.63610
C	0.73707	1.30245	5.17378
H	-1.45252	-4.96540	-1.69210
H	0.18786	-4.82414	-2.37738
H	-0.68383	-3.81756	1.15171
H	-2.18800	-3.46907	0.24157
H	-1.14342	-2.12332	0.74977
H	-0.37200	-2.34193	-2.91637
H	-1.04476	-1.30226	-1.61850
H	-1.99816	-2.65946	-2.23732
H	0.94281	3.36696	-4.29886
H	1.24734	4.62013	-3.04948
H	-0.40954	4.29303	-3.60384
H	-0.26859	1.17994	-3.64154
H	-1.60654	2.21015	-3.04311
H	0.54780	4.19825	-0.62519
H	-1.13403	3.97401	-1.20378
H	-0.37741	2.71841	-0.20974
H	-1.06216	2.52120	3.51835
H	0.58032	3.02825	3.01760
H	-1.47833	0.02837	4.17728
H	-0.81710	-0.43129	2.58969
H	1.49134	2.10266	5.25756
H	1.08174	0.42425	5.74384
H	-0.19008	1.65797	5.65012
H	-0.05201	-5.43077	-0.70524
H	-0.10912	-1.11965	4.09742
H	-0.89409	0.98871	-1.97174
C	5.23314	-0.41778	-0.18623
C	5.80843	-1.21007	-1.20216
C	7.18539	-1.20168	-1.45827
C	8.03408	-0.37921	-0.70831
C	7.48709	0.44568	0.28147

C	6.10848	0.42785	0.52774
H	5.16833	-1.83653	-1.83125
H	7.59522	-1.83439	-2.25303
H	9.11171	-0.37042	-0.90353
H	8.13496	1.11324	0.85989
H	5.70798	1.11146	1.28297
H	2.05707	-4.78338	-0.70536
H	4.27318	-3.21472	-0.23350
H	3.04065	3.20756	-3.21417
H	4.88473	1.55869	-1.97984
H	3.02498	0.22790	4.71329
H	4.80785	-0.43678	2.72346
H	-0.39932	1.95650	1.96322
H	-2.26430	0.19251	0.07302
C	-3.60741	0.34558	-0.10661
C	-4.04072	-0.43051	1.08564
C	-3.93078	-0.53403	-1.25214
C	-4.03331	-0.10747	2.45130
C	-4.45093	-1.73530	0.68054
C	-3.78522	-0.33792	-2.63564
C	-4.39116	-1.79745	-0.77466
C	-4.41406	-1.07370	3.39054
H	-3.72936	0.88749	2.78718
C	-4.81764	-2.70127	1.62845
C	-4.10939	-1.37389	-3.51922
H	-3.41408	0.61440	-3.02382
C	-4.69547	-2.83721	-1.66508
C	-4.79667	-2.36715	2.98701
H	-4.40832	-0.81956	4.45629
H	-5.11977	-3.70457	1.30788
C	-4.56172	-2.61891	-3.04105
H	-4.00022	-1.21695	-4.59786
H	-5.03891	-3.80690	-1.28801
H	-5.08174	-3.11076	3.73878
H	-4.80300	-3.41923	-3.74845
C	-3.76185	1.82962	-0.16211
C	-3.10130	2.64333	0.78323
C	-4.55230	2.47803	-1.13454
C	-3.23165	4.03384	0.76936
H	-2.44489	2.16870	1.51223
C	-4.66976	3.87306	-1.16268
H	-5.09454	1.88092	-1.87275
C	-4.01282	4.66191	-0.20971
H	-2.69781	4.63308	1.51536
H	-5.29018	4.34630	-1.93200
H	-4.10686	5.75270	-0.23151

$L_1Co^{III}O$ + 9-Ph-Fluorene (*S*=2)

107
phflu_ts_u4.out Energy: -2255919.3871311

C	1.44969	-1.68936	-0.41836
N	1.08623	-2.98663	-0.57932
C	2.21833	-3.78984	-0.60945
C	3.29325	-2.95384	-0.47575
N	2.80922	-1.66027	-0.38852
B	3.58611	-0.31150	-0.07057

N	3.03964	0.82885	-1.03340
C	1.73509	1.19989	-1.10012
N	1.65348	2.22211	-1.98602
C	2.91908	2.50557	-2.48708
C	3.78141	1.62835	-1.88945
N	3.12445	0.02998	1.40273
C	1.82054	0.29950	1.69204
N	1.73178	0.37101	3.04649
C	2.97348	0.10420	3.61577
C	3.83596	-0.12216	2.58287
Co	0.51028	0.08426	0.06095
O	-1.13191	0.37986	0.49953
C	-0.33885	-3.42778	-0.73576
C	-0.38301	-4.92951	-1.04085
C	-1.10003	-3.13363	0.56686
C	-0.95134	-2.64158	-1.90456
C	0.37961	2.96208	-2.26486
C	0.62564	4.01962	-3.34669
C	-0.68688	1.96298	-2.74489
C	-0.07416	3.63278	-0.95799
C	0.46157	0.64581	3.79613
C	-0.16293	1.93346	3.23419
C	-0.48490	-0.55028	3.60249
C	0.77094	0.83135	5.28723
H	-1.43409	-5.22759	-1.17928
H	0.16201	-5.17615	-1.96722
H	-0.62776	-3.64610	1.42195
H	-2.14195	-3.48057	0.47627
H	-1.13094	-2.05198	0.76507
H	-0.36410	-2.79108	-2.82616
H	-0.98891	-1.56585	-1.67749
H	-1.98335	-2.97516	-2.08302
H	0.97318	3.56580	-4.28981
H	1.35886	4.77652	-3.02265
H	-0.32203	4.54148	-3.55239
H	-0.34777	1.42229	-3.64413
H	-1.61444	2.50697	-2.98783
H	0.70498	4.31624	-0.58008
H	-0.99821	4.20737	-1.12875
H	-0.29186	2.87239	-0.19200
H	-1.09350	2.16172	3.78025
H	0.52934	2.78445	3.35101
H	-1.41776	-0.38905	4.16782
H	-0.74929	-0.65563	2.54117
H	1.48023	1.65815	5.45926
H	1.17441	-0.08708	5.74468
H	-0.16640	1.07622	5.81110
H	0.02811	-5.53051	-0.21278
H	-0.01292	-1.48067	3.96181
H	-0.92881	1.23426	-1.95680
C	5.18571	-0.38431	-0.29084
C	5.74879	-1.14086	-1.34085
C	7.11634	-1.09586	-1.64015
C	7.97024	-0.26927	-0.90095
C	7.43486	0.52446	0.11998
C	6.06538	0.46955	0.40834
H	5.10445	-1.76443	-1.96814
H	7.51380	-1.70217	-2.46138
H	9.04067	-0.23148	-1.12949

```
H          8.08410        1.19832        0.68955
H          5.67455        1.13566        1.18355
H          2.18897       -4.86921       -0.72386
H          4.35183       -3.19541       -0.43131
H          3.11711        3.28537       -3.21628
H          4.85544        1.51815       -2.01444
H          3.15731        0.09975        4.68559
H          4.89027       -0.38364        2.60981
H         -0.41130        1.80449        2.17135
H         -2.33037        0.36336        0.08744
C         -3.61724        0.46488       -0.16188
C         -4.10943       -0.26778        1.04034
C         -3.88177       -0.46560       -1.28717
C         -4.15480        0.11248        2.38817
C         -4.50023       -1.58526        0.66729
C         -3.66194       -0.32062       -2.66486
C         -4.37586       -1.70344       -0.78332
C         -4.57071       -0.81807        3.34981
H         -3.86303        1.12160        2.69245
C         -4.90493       -2.51395        1.63549
C         -3.95834       -1.38576       -3.52511
H         -3.26458        0.61602       -3.06587
C         -4.66043       -2.76869       -1.64815
C         -4.93640       -2.12547        2.98041
H         -4.60672       -0.52407        4.40444
H         -5.19388       -3.52961        1.34371
C         -4.45913       -2.60137       -3.02381
H         -3.79519       -1.27150       -4.60213
H         -5.03920       -3.71792       -1.25389
H         -5.25029       -2.84024        3.74837
H         -4.68275       -3.42278       -3.71247
C         -3.80193        1.94462       -0.28388
C         -3.15141        2.81245        0.61935
C         -4.61548        2.52299       -1.27920
C         -3.32014        4.19740        0.54072
H         -2.47512        2.38757        1.36402
C         -4.77191        3.91132       -1.36911
H         -5.14055        1.87562       -1.98732
C         -4.12792        4.75761       -0.45764
H         -2.79799        4.84635        1.25224
H         -5.40974        4.33369       -2.15340
H         -4.25199        5.84342       -0.52662
```

$L_1Co^{III}O$ + 9-tBu-Fluorene (*S*=0, closed-shell)

```
109
tbuflu_ts_u0_closed.out   Energy: -2209621.7404222
C          1.54944       -1.75863       -0.19434
N          1.09266       -3.03661       -0.35533
C          2.17442       -3.91109       -0.34162
C          3.30006       -3.15458       -0.18715
N          2.90159       -1.83498       -0.12598
B          3.68863       -0.49421        0.09188
N          3.13129        0.48168       -1.00154
C          1.80755        0.73733       -1.13671
N          1.68260        1.57899       -2.21221
C          2.94851        1.83645       -2.73163
```

C	3.84641	1.14927	-1.97205
N	3.10643	0.02115	1.45112
C	1.76403	0.18805	1.55019
N	1.50217	0.47273	2.86363
C	2.69626	0.45584	3.57746
C	3.69107	0.16279	2.69245
Co	0.58055	-0.09666	0.05733
O	-1.03976	0.45625	-0.11328
C	-0.33656	-3.43881	-0.58722
C	-0.42258	-4.95730	-0.79168
C	-1.17317	-3.04675	0.63756
C	-0.83367	-2.72597	-1.85255
C	0.42386	2.19808	-2.75847
C	0.75626	3.05191	-3.99194
C	-0.54059	1.07798	-3.18023
C	-0.16387	3.10155	-1.66505
C	0.15129	0.70236	3.48329
C	-0.47750	1.94661	2.84095
C	-0.70341	-0.55098	3.25184
C	0.30365	0.93362	4.99339
H	-1.47615	-5.21599	-0.98032
H	0.16399	-5.29369	-1.66232
H	-0.71859	-3.43485	1.56387
H	-2.18931	-3.45454	0.53971
H	-1.27726	-1.95634	0.71221
H	-0.21294	-3.00230	-2.72176
H	-0.80813	-1.63478	-1.72567
H	-1.87765	-3.00645	-2.05285
H	1.19513	2.45314	-4.80705
H	1.43193	3.88939	-3.75347
H	-0.18404	3.48500	-4.36695
H	-0.04259	0.38921	-3.88336
H	-1.41264	1.51704	-3.69073
H	0.57006	3.87192	-1.37316
H	-1.06813	3.60708	-2.03841
H	-0.44030	2.49910	-0.79006
H	-1.46836	2.12883	3.28558
H	0.15500	2.83348	3.01543
H	-1.64866	-0.47455	3.80781
H	-0.96615	-0.65529	2.19205
H	0.91733	1.82103	5.21968
H	0.73155	0.05713	5.50722
H	-0.69914	1.10787	5.41344
H	-0.09575	-5.51549	0.10138
H	-0.16443	-1.45363	3.58447
H	-0.89905	0.51971	-2.30637
C	5.29272	-0.55409	-0.02458
C	5.94353	-1.44895	-0.90004
C	7.32917	-1.41422	-1.10230
C	8.11196	-0.46087	-0.44150
C	7.48958	0.46790	0.40063
C	6.10347	0.42188	0.59426
H	5.35935	-2.17745	-1.46942
H	7.79672	-2.12959	-1.78746
H	9.19589	-0.43081	-0.59489
H	8.08384	1.23902	0.90267
H	5.64569	1.19034	1.22463
H	2.07280	-4.98651	-0.44057
H	4.33758	-3.46576	-0.10501

H	3.12018	2.47894	-3.58756
H	4.92864	1.08377	-2.04820
H	2.75625	0.65168	4.64226
H	4.75640	0.03637	2.86285
H	-0.61482	1.80051	1.76130
H	-2.23921	0.53696	-0.04699
C	-3.67903	0.54997	0.02222
C	-3.98057	-0.07695	1.33096
C	-3.95020	-0.53237	-0.95805
C	-4.01885	0.43502	2.64515
C	-4.27869	-1.46629	1.15486
C	-3.84690	-0.59888	-2.36650
C	-4.27555	-1.74611	-0.26742
C	-4.29780	-0.40692	3.72682
H	-3.82741	1.49062	2.84335
C	-4.52454	-2.31287	2.24625
C	-4.12080	-1.79218	-3.04235
H	-3.54166	0.26809	-2.95066
C	-4.52815	-2.94478	-0.95150
C	-4.53242	-1.78273	3.53945
H	-4.32020	0.01298	4.73885
H	-4.72474	-3.37803	2.08222
C	-4.46974	-2.96630	-2.34708
H	-4.04646	-1.81425	-4.13556
H	-4.77444	-3.85464	-0.39206
H	-4.73127	-2.42904	4.40098
H	-4.67485	-3.89139	-2.89613
C	-4.08152	2.03781	-0.22499
C	-3.90017	2.45122	-1.69814
H	-4.04409	3.54115	-1.80287
H	-2.88955	2.20851	-2.05572
H	-4.63219	1.95957	-2.35659
C	-3.21129	3.00385	0.61027
H	-3.49833	4.05065	0.40390
H	-3.31694	2.84663	1.69197
H	-2.14751	2.88467	0.36055
C	-5.56823	2.24611	0.14173
H	-5.88926	3.28201	-0.07556
H	-6.20817	1.56046	-0.44137
H	-5.75295	2.05099	1.21066

$L_1Co^{III}O$ + 9-tBu-Fluorene (*S*=2)

109
tbuflu_ts_u4.out Energy: -2209616.5155775

C	1.39249	-1.65498	-0.28777
N	0.97818	-2.94840	-0.27095
C	2.07474	-3.79668	-0.19729
C	3.18378	-2.99778	-0.18193
N	2.75421	-1.68489	-0.26643
B	3.59808	-0.35836	-0.07828
N	3.12888	0.70979	-1.15281
C	1.84681	1.14037	-1.28296
N	1.85130	2.10511	-2.23733
C	3.14340	2.28745	-2.71652
C	3.93803	1.40930	-2.03486
N	3.14538	0.15814	1.34607

C	1.86138	0.54967	1.58240
N	1.77482	0.79100	2.91799
C	2.99040	0.50410	3.53229
C	3.83829	0.09493	2.54470
Co	0.53483	0.21571	-0.03168
O	-1.12776	0.58265	0.37327
C	-0.46315	-3.35404	-0.25959
C	-0.57532	-4.87584	-0.41348
C	-1.07551	-2.91417	1.07821
C	-1.16984	-2.66535	-1.43655
C	0.63595	2.89686	-2.60394
C	0.96484	3.84364	-3.76394
C	-0.47852	1.92587	-3.02483
C	0.21010	3.70399	-1.36523
C	0.53782	1.28152	3.60736
C	0.03831	2.53151	2.86428
C	-0.52076	0.16706	3.57224
C	0.86690	1.64470	5.06147
H	-1.64266	-5.14609	-0.43883
H	-0.11286	-5.22841	-1.35070
H	-0.52454	-3.36233	1.92270
H	-2.12789	-3.22988	1.13520
H	-1.05106	-1.81901	1.17149
H	-0.66246	-2.90010	-2.38727
H	-1.19338	-1.57362	-1.30165
H	-2.21232	-3.00922	-1.49864
H	1.29977	3.29114	-4.65758
H	1.73781	4.57975	-3.48852
H	0.05515	4.40267	-4.03370
H	-0.14429	1.27967	-3.85340
H	-1.35706	2.49927	-3.36171
H	1.02048	4.38030	-1.04523
H	-0.68270	4.30802	-1.59455
H	-0.03530	3.02555	-0.53311
H	-0.85264	2.93421	3.37335
H	0.81742	3.31243	2.85115
H	-1.41290	0.48467	4.13763
H	-0.82648	-0.03595	2.53550
H	1.65328	2.41539	5.12382
H	1.18125	0.76517	5.64733
H	-0.04077	2.04965	5.53600
H	-0.11876	-5.41247	0.43455
H	-0.12924	-0.75593	4.03274
H	-0.79078	1.29317	-2.18045
C	5.19402	-0.54475	-0.26918
C	5.71348	-1.42364	-1.24400
C	7.08216	-1.48994	-1.53338
C	7.98328	-0.65633	-0.86092
C	7.49436	0.25492	0.08209
C	6.12281	0.31033	0.36129
H	5.03337	-2.05935	-1.81949
H	7.44415	-2.18925	-2.29495
H	9.05488	-0.70490	-1.08189
H	8.18216	0.93455	0.59697
H	5.77178	1.06531	1.07117
H	1.99857	-4.87931	-0.16781
H	4.23190	-3.27567	-0.11172
H	3.40373	3.00269	-3.49084
H	5.00738	1.23463	-2.11806

```
H          3.16868        0.61262        4.59752
H          4.87019       -0.23782        2.61627
H         -0.24276        2.27591        1.83254
H         -2.29798        0.36435        0.11429
C         -3.64528        0.27326       -0.03760
C         -4.01544       -0.85449        0.87126
C         -3.92271       -0.27379       -1.40039
C         -3.86809       -1.01803        2.25968
C         -4.50224       -1.95713        0.11084
C         -3.69455        0.25288       -2.68337
C         -4.45232       -1.59338       -1.30022
C         -4.24414       -2.22322        2.86669
H         -3.42929       -0.23149        2.87238
C         -4.87482       -3.16249        0.71913
C         -4.00987       -0.50362       -3.82021
H         -3.24934        1.23816       -2.81260
C         -4.77205       -2.34588       -2.43675
C         -4.75530       -3.29001        2.10777
H         -4.12178       -2.33880        3.94908
H         -5.24365       -3.99769        0.11381
C         -4.55356       -1.79409       -3.70411
H         -3.82168       -0.08153       -4.81337
H         -5.17526       -3.35929       -2.33408
H         -5.03986       -4.22578        2.60017
H         -4.79454       -2.37030       -4.60360
C         -4.09806        1.72884        0.30684
C         -3.71079        2.11252        1.75027
H         -2.64597        1.90694        1.93664
H         -3.89050        3.18991        1.91075
H         -4.31361        1.57265        2.49565
C         -3.43124        2.75623       -0.63158
H         -3.62816        3.78078       -0.27053
H         -2.34302        2.60061       -0.65953
H         -3.82323        2.70017       -1.65768
C         -5.63167        1.82844        0.15996
H         -6.13778        1.11482        0.83309
H         -5.98321        2.84564        0.41232
H         -5.94611        1.60451       -0.87369
```

$L_1Co^{III}O$ + Xanthene (*S*=0, closed-shell)

```
98
xanthene_ts_u0_closed.out Energy: -2158169.6209325
C          1.30370        1.21610       -0.80574
N          0.90339        2.25524       -1.59833
C          1.99877        2.73270       -2.31241
C          3.07746        1.98359       -1.93741
N          2.63937        1.07746       -0.99139
B          3.33239       -0.12519       -0.25838
N          2.86929       -0.01922        1.23361
C          1.55577        0.05441        1.54282
N          1.47253        0.15593        2.90577
C          2.76363        0.13570        3.43395
C          3.62864        0.02576        2.38537
N          2.57233       -1.36970       -0.85057
C          1.22208       -1.47015       -0.71293
N          0.83960       -2.57280       -1.43461
```

C	1.96222	-3.12544	-2.04346
C	3.03487	-2.36555	-1.68383
Co	0.25245	-0.07057	0.19149
O	-1.36854	-0.55481	0.52419
C	-0.49171	2.80561	-1.66838
C	-0.51545	4.05061	-2.56451
C	-1.42181	1.73408	-2.25721
C	-0.92708	3.19514	-0.24879
C	0.21642	0.22646	3.72969
C	0.57892	0.49881	5.19700
C	-0.66018	1.37788	3.21360
C	-0.51337	-1.12276	3.62173
C	-0.54630	-3.15628	-1.56718
C	-1.04394	-3.55082	-0.16858
C	-1.46478	-2.12298	-2.23509
C	-0.49744	-4.41313	-2.45028
H	-1.54082	4.45224	-2.56814
H	0.15414	4.84192	-2.18908
H	-1.04408	1.38382	-3.23227
H	-2.43219	2.14776	-2.39384
H	-1.51409	0.87490	-1.57837
H	-0.24123	3.94665	0.17694
H	-0.94248	2.31926	0.41462
H	-1.94682	3.60707	-0.26539
H	1.12966	1.44659	5.31616
H	1.16959	-0.31941	5.63986
H	-0.35541	0.57803	5.77420
H	-0.09753	2.32600	3.20449
H	-1.53435	1.49707	3.87329
H	0.12833	-1.93822	3.99643
H	-1.43326	-1.09598	4.22945
H	-0.79430	-1.32379	2.57803
H	-2.04967	-3.99361	-0.25156
H	-0.36378	-4.29253	0.28468
H	-2.46796	-2.55659	-2.37454
H	-1.57646	-1.23754	-1.59911
H	0.14000	-5.20339	-2.02052
H	-0.15825	-4.19240	-3.47592
H	-1.52040	-4.81458	-2.52025
H	-0.24598	3.81578	-3.60745
H	-1.06357	-1.82926	-3.22017
H	-1.03591	1.16961	2.20359
C	4.94008	-0.18565	-0.30200
C	5.72615	0.98432	-0.35778
C	7.12306	0.94528	-0.25904
C	7.78091	-0.27704	-0.08181
C	7.02494	-1.45101	0.01813
C	5.62931	-1.39807	-0.08270
H	5.24381	1.96155	-0.45190
H	7.69829	1.87602	-0.31162
H	8.87287	-0.31296	-0.00589
H	7.52276	-2.41249	0.18437
H	5.06655	-2.32892	0.03943
H	1.93887	3.55486	-3.01804
H	4.10618	2.02931	-2.28443
H	2.97121	0.20304	4.49624
H	4.71484	-0.02043	2.36951
H	1.92536	-4.00476	-2.67641
H	4.07899	-2.45885	-1.96939

```
H          -1.12118       -2.66096        0.47081
H          -2.41278       -0.30499        0.92686
C          -3.79451       -0.02952        1.27384
C          -4.06792        1.37335        0.96221
C          -4.36913       -1.00033        0.34258
H          -3.82448       -0.30188        2.33894
C          -4.42768        1.71742       -0.36391
C          -3.96351        2.43425        1.88503
C          -4.67964       -0.57572       -0.97256
C          -4.52484       -2.37301        0.62069
C          -4.66773        3.03541       -0.74971
C          -4.19064        3.76403        1.50869
H          -3.69308        2.19815        2.91974
C          -5.11841       -1.46286       -1.95325
C          -4.95151       -3.27813       -0.35948
H          -4.28116       -2.73062        1.62745
C          -4.54340        4.07211        0.18910
H          -4.95001        3.23401       -1.78823
H          -4.09196        4.56240        2.25186
H          -5.34394       -1.07177       -2.95016
C          -5.24633       -2.82834       -1.65222
H          -5.04954       -4.34042       -0.11152
H          -4.72213        5.10823       -0.11479
H          -5.57889       -3.52855       -2.42498
O          -4.53369        0.74792       -1.34114
```

$L_1Co^{III}O$ + Xanthene (*S*=1)

```
98
xanthene_ts_u2.out        Energy: -2158166.8584789
C          -1.16819       -1.38959       -0.80545
N          -0.80331       -2.37283       -1.66989
C          -1.90850       -2.77375       -2.41534
C          -2.96737       -2.02954       -1.97934
N          -2.50946       -1.20320       -0.96618
B          -3.26960       -0.03726       -0.20614
N          -2.83346       -0.10895        1.30571
C          -1.53046       -0.05858        1.66410
N          -1.47720       -0.14670        3.01686
C          -2.77559       -0.25577        3.51987
C          -3.61707       -0.23107        2.44438
N          -2.64260        1.28895       -0.80820
C          -1.32662        1.59411       -0.62180
N          -1.07491        2.70795       -1.35965
C          -2.22391        3.07818       -2.05322
C          -3.19449        2.17973       -1.71403
Co         -0.25536        0.10066        0.20496
O           1.45535        0.20886       -0.00119
C           0.59525       -2.89651       -1.81754
C           0.56813       -4.21122       -2.60848
C           1.43483       -1.84540       -2.56205
C           1.17467       -3.15141       -0.41836
C          -0.19737       -0.13741        3.79267
C          -0.50335       -0.23383        5.29149
C           0.64983       -1.34257        3.34947
C           0.54792        1.17441        3.49152
C           0.26238        3.38215       -1.45524
```

C	0.84137	3.53171	-0.03976
C	1.18473	2.51214	-2.32535
C	0.09116	4.77017	-2.08724
H	1.59191	-4.61518	-2.65037
H	-0.07623	-4.96435	-2.12441
H	1.00997	-1.64247	-3.56020
H	2.46717	-2.21320	-2.68575
H	1.47467	-0.91581	-1.97464
H	0.53030	-3.84063	0.15322
H	1.28295	-2.20749	0.13281
H	2.17758	-3.59626	-0.50861
H	-1.02653	-1.17121	5.54270
H	-1.11000	0.61841	5.63967
H	0.44613	-0.22041	5.84921
H	0.09904	-2.28607	3.49851
H	1.58017	-1.38222	3.93927
H	-0.07410	2.04721	3.75064
H	1.47943	1.21860	4.07960
H	0.81717	1.23354	2.42514
H	1.79197	4.08572	-0.09139
H	0.14217	4.08101	0.61309
H	2.17739	2.98606	-2.40914
H	1.31703	1.52559	-1.85640
H	-0.61311	5.39537	-1.51291
H	-0.25363	4.71309	-3.13276
H	1.06961	5.27576	-2.09268
H	0.22929	-4.06684	-3.64765
H	0.76384	2.39247	-3.33851
H	0.92562	-1.25752	2.28665
C	-4.88112	-0.12054	-0.25184
C	-5.55363	-1.36112	-0.24031
C	-6.94682	-1.45015	-0.12605
C	-7.71701	-0.28813	-0.00125
C	-7.07519	0.95537	0.03003
C	-5.68125	1.02986	-0.08509
H	-4.97909	-2.29087	-0.29625
H	-7.43121	-2.43274	-0.12538
H	-8.80686	-0.35199	0.08657
H	-7.66100	1.87274	0.15398
H	-5.20865	2.01460	-0.01666
H	-1.86968	-3.54653	-3.17697
H	-4.00018	-2.03172	-2.31829
H	-3.00143	-0.33970	4.57850
H	-4.70209	-0.28992	2.40304
H	-2.27415	3.93746	-2.71480
H	-4.22534	2.11495	-2.05270
H	1.05674	2.54509	0.39391
H	2.47103	0.15184	0.69366
C	3.69204	0.13442	1.20448
C	4.15172	-1.22535	0.88377
C	4.28075	1.19612	0.37339
H	3.57843	0.36522	2.27319
C	4.65149	-1.47534	-0.41415
C	4.03889	-2.32328	1.75635
C	4.75396	0.85200	-0.91293
C	4.27278	2.55918	0.71853
C	5.01161	-2.75910	-0.82913
C	4.39736	-3.61421	1.35472
H	3.65018	-2.14993	2.76523

```
C          5.18382        1.82176       -1.82113
C          4.69991        3.54137       -0.18147
H          3.89689        2.84503        1.70699
C          4.88010       -3.83537        0.05742
H          5.39323       -2.89506       -1.84535
H          4.29366       -4.45090        2.05292
H          5.53747        1.50030       -2.80525
C          5.14916        3.17412       -1.45749
H          4.67350        4.59635        0.10969
H          5.15727       -4.84320       -0.26728
H          5.47899        3.93647       -2.17029
O          4.79403       -0.45915       -1.33152
```

$L_1Co^{III}O$ + Xanthene (*S*=2)

```
98
xanthene_ts_u4.out        Energy: -2158164.0927623
C          1.49246       -0.24112       -1.83060
N          1.44477       -0.48842       -3.16471
C          2.73500       -0.63138       -3.66243
C          3.58171       -0.45189       -2.60373
N          2.80830       -0.18346       -1.48686
B          3.24852       -0.07935        0.03983
N          2.46615        1.13029        0.70814
C          1.11143        1.24017        0.71231
N          0.80971        2.40779        1.32984
C          1.98034        3.04553        1.72663
C          3.01366        2.23992        1.33563
N          2.70667       -1.42280        0.67122
C          1.37016       -1.68652        0.72909
N          1.24938       -2.94850        1.22056
C          2.51100       -3.50004        1.42724
C          3.41742       -2.54502        1.06834
Co         0.17397       -0.26737       -0.25794
O         -1.50689       -0.74508       -0.25014
C          0.16607       -0.65271       -3.92857
C          0.47345       -0.74063       -5.42863
C         -0.52332       -1.94203       -3.45017
C         -0.73635        0.56376       -3.65490
C         -0.59152        2.92647        1.43416
C         -0.59727        4.24911        2.20851
C         -1.11467        3.15115        0.00596
C         -1.45596        1.88626        2.16614
C         -0.06250       -3.62782        1.47902
C         -0.92281       -2.70313        2.35648
C         -0.75277       -3.88861        0.13000
C          0.17893       -4.95538        2.20928
H         -0.47567       -0.81918       -5.98154
H          1.00290        0.15709       -5.78914
H          0.14289       -2.81185       -3.57792
H         -1.44024       -2.11535       -4.03810
H         -0.80587       -1.85364       -2.38948
H         -0.21770        1.50411       -3.90490
H         -1.04712        0.59699       -2.59953
H         -1.64730        0.49189       -4.27194
H         -0.01487        5.03100        1.69338
H         -0.20248        4.12498        3.23075
```

H	-1.63644	4.60502	2.28876
H	-0.44735	3.83034	-0.55088
H	-2.12269	3.58935	0.03387
H	-1.04521	1.67470	3.16786
H	-2.48341	2.26663	2.27896
H	-1.50925	0.94673	1.59385
H	-1.88732	-3.19070	2.57646
H	-0.41153	-2.48722	3.31018
H	-1.69561	-4.43735	0.29474
H	-0.99299	-2.93262	-0.35870
H	0.70580	-4.80661	3.16669
H	0.75099	-5.66967	1.59406
H	-0.79662	-5.41659	2.42989
H	1.07383	-1.63193	-5.67428
H	-0.10625	-4.49482	-0.52750
H	-1.18043	2.19516	-0.53627
C	4.82530	0.20096	0.26868
C	5.56498	1.01769	-0.61322
C	6.88756	1.39461	-0.34711
C	7.51339	0.97609	0.83266
C	6.79238	0.20006	1.74750
C	5.47056	-0.16927	1.46817
H	5.09377	1.40094	-1.52341
H	7.42714	2.02683	-1.06073
H	8.54786	1.26633	1.04519
H	7.25698	-0.11189	2.68927
H	4.92347	-0.73893	2.22548
H	2.96137	-0.83751	-4.70416
H	4.66687	-0.50292	-2.57591
H	2.00040	3.99824	2.24756
H	4.08472	2.37712	1.45979
H	2.67612	-4.50279	1.80900
H	4.50307	-2.59198	1.06401
H	-1.13324	-1.76267	1.82656
H	-2.65336	-0.27444	-0.55683
C	-3.91351	-0.03599	-0.74564
C	-4.47484	-0.66821	0.46463
C	-4.16766	1.41167	-0.85918
H	-4.08156	-0.60005	-1.67678
C	-4.83964	0.14001	1.56178
C	-4.54612	-2.06331	0.63592
C	-4.59622	2.13301	0.27632
C	-3.96193	2.13998	-2.04643
C	-5.24707	-0.41232	2.77961
C	-4.94977	-2.63071	1.84788
H	-4.25056	-2.70575	-0.20050
C	-4.82112	3.51211	0.23116
C	-4.17375	3.52040	-2.10430
H	-3.62101	1.59875	-2.93553
C	-5.29665	-1.80302	2.92586
H	-5.52062	0.26175	3.59671
H	-4.98722	-3.71942	1.95556
H	-5.16036	4.01812	1.13971
C	-4.60636	4.21009	-0.96242
H	-4.00113	4.06033	-3.04066
H	-5.61032	-2.23754	3.88029
H	-4.77565	5.29079	-0.99767
O	-4.80772	1.51457	1.48633

$L_1Co^{III}O$ + MeCN (*S*=2)

```
80
mecn_anderson_ts_u4.out   Energy: -1879693.8950468
C           0.33526        1.57744       -0.76671
N           0.24386        2.64940       -1.59756
C           1.44811        2.83149       -2.27050
C           2.29300        1.85558       -1.82902
N           1.61033        1.10865       -0.88221
B           2.05979       -0.24353       -0.19878
N           1.63700       -0.18688        1.32964
C           0.36869        0.04586        1.75530
N           0.39536        0.03080        3.11104
C           1.69185       -0.21186        3.55036
C           2.46390       -0.34770        2.43054
N           1.16630       -1.33478       -0.93068
C          -0.19165       -1.30855       -0.83722
N          -0.66156       -2.25666       -1.68832
C           0.39895       -2.85825       -2.35257
C           1.53904       -2.26640       -1.88356
Co         -0.96021        0.26959        0.24385
O          -2.61330        0.89114        0.32465
C          -0.99470        3.47383       -1.78034
C          -0.67664        4.69833       -2.64877
C          -2.05837        2.60461       -2.47122
C          -1.47912        3.93550       -0.39618
C          -0.82443        0.23002        3.95695
C          -0.43843        0.18250        5.43956
C          -1.43931        1.59797        3.61520
C          -1.81736       -0.89921        3.63480
C          -2.11912       -2.56429       -1.86299
C          -2.69948       -2.92981       -0.48710
C          -2.81925       -1.32194       -2.43555
C          -2.28581       -3.74747       -2.82386
H          -1.58621        5.31326       -2.73470
H           0.11286        5.32443       -2.20059
H          -1.67980        2.21932       -3.43329
H          -2.96139        3.20637       -2.66873
H          -2.34143        1.76250       -1.82343
H          -0.69296        4.51712        0.11463
H          -1.75917        3.07149        0.22393
H          -2.36760        4.57840       -0.51288
H           0.27670        0.98013        5.70034
H          -0.00580       -0.79187        5.72060
H          -1.34501        0.33287        6.04633
H          -0.70333        2.40475        3.76970
H          -2.30703        1.78708        4.26879
H          -1.36815       -1.88627        3.83433
H          -2.72373       -0.79271        4.25325
H          -2.11765       -0.85387        2.57696
H          -3.76784       -3.17578       -0.58703
H          -2.16735       -3.79424       -0.05594
H          -3.88784       -1.53634       -2.59345
H          -2.75683       -0.48105       -1.72903
H          -1.78319       -4.65483       -2.44959
H          -1.90272       -3.51543       -3.83128
H          -3.35940       -3.97248       -2.92026
```

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H          -0.37219        4.41501       -3.66982
H          -2.36136       -1.02424       -3.39392
H          -1.78584        1.62091        2.56979
C           3.64947       -0.53670       -0.23434
C           4.59328        0.50704       -0.12584
C           5.96595        0.25887       -0.00001
C           6.44132       -1.05693        0.03947
C           5.52630       -2.11403       -0.02394
C           4.15630       -1.85120       -0.14928
H           4.25390        1.54720       -0.10920
H           6.66561        1.09819        0.07747
H           7.51382       -1.25667        0.13583
H           5.87841       -3.14968        0.03471
H           3.46698       -2.70106       -0.15029
H           1.62159        3.62306       -2.99257
H           3.31619        1.64300       -2.12631
H           1.97234       -0.27027        4.59765
H           3.52895       -0.54515        2.34271
H           0.27989       -3.64549       -3.09066
H           2.57267       -2.44163       -2.16916
H          -2.61573       -2.08114        0.20841
H          -3.55112        0.40631        0.68382
C          -4.75535       -0.26486        1.23255
H          -5.28055        0.57406        1.71107
H          -4.35502       -0.99344        1.95072
C          -5.44297       -0.84619        0.14028
N          -5.94915       -1.31826       -0.80606
```

$L_1Co^{III}O$ + THF (*S*=0, open-shell singlet)

```
87
thf_anderson_ts_u0_open.out        Energy: -1942233.9957720
C           0.56092        1.61245       -0.24553
N           0.29121        2.87214       -0.71727
C           1.47098        3.48872       -1.12553
C           2.48161        2.60644       -0.88213
N           1.91874        1.47915       -0.31705
B           2.60321        0.10303        0.03664
N           2.01004       -0.34587        1.40853
C           0.67114       -0.48705        1.53564
N           0.44151       -0.88102        2.82837
C           1.66243       -0.97094        3.50154
C           2.63661       -0.63640        2.60683
N           2.00293       -0.88748       -1.02507
C           0.65843       -1.10849       -1.01746
N           0.39877       -1.89702       -2.10864
C           1.57713       -2.11151       -2.82021
C           2.57163       -1.46864       -2.14259
Co         -0.50230       -0.05558        0.12731
O          -2.24005        0.31463       -0.04833
C          -1.06622        3.50324       -0.82279
C          -0.92078        4.99383       -1.16643
C          -1.85052        2.79166       -1.93734
C          -1.78140        3.36893        0.53090
C          -0.90830       -1.12061        3.42856
C          -0.75328       -1.66741        4.85402
C          -1.67192        0.21496        3.46448
```

C	-1.65997	-2.15050	2.56877
C	-0.95516	-2.37870	-2.53083
C	-1.66876	-2.98478	-1.31381
C	-1.74125	-1.18426	-3.09634
C	-0.80766	-3.45999	-3.61133
H	-1.92532	5.44513	-1.18449
H	-0.32209	5.53335	-0.41344
H	-1.30464	2.85573	-2.89443
H	-2.83532	3.27236	-2.06714
H	-2.01087	1.73978	-1.65944
H	-1.18244	3.83545	1.33184
H	-1.95998	2.30972	0.76162
H	-2.75675	3.88221	0.48207
H	-0.25696	-0.94476	5.52223
H	-0.18964	-2.61498	4.86965
H	-1.75552	-1.86457	5.26579
H	-1.11311	0.96426	4.05019
H	-2.65973	0.07035	3.93328
H	-1.08292	-3.08606	2.48285
H	-2.63664	-2.37796	3.02682
H	-1.84562	-1.75378	1.56011
H	-2.67341	-3.32532	-1.60691
H	-1.09404	-3.83378	-0.90722
H	-2.73269	-1.51852	-3.43841
H	-1.89170	-0.42552	-2.31518
H	-0.18766	-4.30309	-3.26335
H	-0.37745	-3.06192	-4.54487
H	-1.80869	-3.85109	-3.85235
H	-0.47260	5.15323	-2.16096
H	-1.19802	-0.73638	-3.94596
H	-1.82802	0.59630	2.44348
C	4.21269	0.12759	0.16301
C	4.88830	1.24093	0.70766
C	6.26593	1.22485	0.96011
C	7.01644	0.07509	0.68727
C	6.36821	-1.05823	0.18303
C	4.98947	-1.02821	-0.06384
H	4.32505	2.14287	0.96720
H	6.75320	2.11179	1.37986
H	8.09442	0.05766	0.88048
H	6.93626	-1.97470	-0.01115
H	4.50850	-1.94441	-0.41978
H	1.51412	4.48814	-1.54564
H	3.54669	2.70345	-1.07646
H	1.74844	-1.26445	4.54267
H	3.71623	-0.58589	2.72859
H	1.62705	-2.69987	-3.73079
H	3.62886	-1.38398	-2.38079
H	-1.79607	-2.23123	-0.52610
H	-3.15147	-0.40356	-0.13602
C	-4.36610	-1.07267	-0.21400
O	-4.60000	-1.49307	-1.52694
C	-5.33894	0.04841	0.08699
H	-4.29806	-1.93403	0.46984
C	-5.30271	-0.46331	-2.24447
C	-5.39807	0.73362	-1.28848
H	-4.98005	0.71380	0.88907
H	-6.33540	-0.34136	0.38034
H	-4.75477	-0.23516	-3.17572

H	-6.30209	-0.85377	-2.51890
H	-4.51615	1.38404	-1.40703
H	-6.30734	1.33354	-1.45199

$L_1Co^{III}O$ + THF (*S*=1)

87
thf_anderson_ts_u2.out Energy: -1942232.4503794

C	0.47816	1.52887	-0.13387
N	0.13209	2.75603	-0.62739
C	1.25798	3.38855	-1.15060
C	2.31159	2.54619	-0.94848
N	1.83025	1.42716	-0.29464
B	2.57526	0.08134	0.05730
N	2.04351	-0.35439	1.45711
C	0.71237	-0.48440	1.64630
N	0.53398	-0.88146	2.94237
C	1.78322	-1.00047	3.55783
C	2.72031	-0.66977	2.62277
N	2.00141	-0.96064	-0.97829
C	0.67660	-1.29880	-0.96467
N	0.49029	-2.10051	-2.05765
C	1.67776	-2.21320	-2.77576
C	2.61447	-1.48862	-2.09939
Co	-0.49108	-0.16129	0.22980
O	-2.21557	-0.22515	-0.09401
C	-1.25759	3.30813	-0.69527
C	-1.19376	4.82809	-0.91175
C	-1.98670	2.63822	-1.87162
C	-1.98415	3.01599	0.62701
C	-0.79498	-1.14912	3.57402
C	-0.60033	-1.55751	5.03980
C	-1.63881	0.13519	3.50449
C	-1.48232	-2.29129	2.80571
C	-0.82309	-2.66203	-2.50514
C	-1.56388	-3.23594	-1.28794
C	-1.62102	-1.51922	-3.15236
C	-0.58754	-3.78620	-3.52514
H	-2.21725	5.23316	-0.87371
H	-0.59986	5.32432	-0.12591
H	-1.42663	2.78772	-2.81037
H	-2.98677	3.08517	-1.99291
H	-2.10506	1.56161	-1.67829
H	-1.40699	3.39925	1.48512
H	-2.14909	1.93574	0.74460
H	-2.96790	3.51429	0.61812
H	-0.11201	-0.76168	5.62612
H	-0.01004	-2.48396	5.13279
H	-1.58886	-1.74489	5.48764
H	-1.12203	0.96864	4.00899
H	-2.61060	-0.02745	3.99932
H	-0.85118	-3.19569	2.80779
H	-2.44708	-2.53510	3.28077
H	-1.68143	-1.99558	1.76387
H	-2.50579	-3.70278	-1.62111

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H          -0.95071       -4.00431       -0.78727
H          -2.61155       -1.87009       -3.48306
H          -1.77245       -0.71391       -2.42146
H           0.05738       -4.58021       -3.11237
H          -0.14121       -3.41674       -4.46273
H          -1.55970       -4.23529       -3.78316
H          -0.77506        5.09442       -1.89589
H          -1.07981       -1.12176       -4.02828
H          -1.83469        0.41838        2.45903
C           4.18603        0.17447        0.13928
C           4.83305        1.33968        0.60296
C           6.21577        1.38509        0.82295
C           7.00028        0.24763        0.59932
C           6.38189       -0.93461        0.17587
C           4.99827       -0.96553       -0.04042
H           4.24428        2.23559        0.82351
H           6.68046        2.31114        1.17906
H           8.08210        0.27806        0.76795
H           6.97777       -1.84082        0.02095
H           4.54143       -1.91542       -0.33541
H           1.23440        4.37265       -1.60779
H           3.35682        2.66641       -1.22241
H           1.91094       -1.30279        4.59220
H           3.80490       -0.63406        2.69556
H           1.77480       -2.79330       -3.68806
H           3.66066       -1.31486       -2.33852
H          -1.80695       -2.43793       -0.57364
H          -3.19293       -0.45462       -0.73094
C          -4.39337       -0.69449       -1.32110
O          -4.48918        0.00065       -2.53644
C          -5.42140       -0.11028       -0.37048
H          -4.39084       -1.78463       -1.49138
C          -5.29147        1.17798       -2.36079
C          -5.45271        1.35026       -0.84813
H          -5.12761       -0.21991        0.68647
H          -6.41553       -0.58500       -0.49935
H          -4.79362        2.02795       -2.85751
H          -6.27176        1.01854       -2.85451
H          -4.58616        1.89306       -0.43480
H          -6.37184        1.89306       -0.57590
```

$L_1Co^{III}O$ + THF (*S*=2)

```
87
thf_anderson_ts_u4.out    Energy: -1942235.3773659
C           0.60791        1.77097       -0.35122
N           0.47467        2.99474       -0.93207
C           1.71991        3.47789       -1.32506
C           2.63445        2.53278       -0.96145
N           1.94701        1.50364       -0.33609
B           2.49082        0.07811        0.07569
N           1.84698       -0.32545        1.46912
C           0.50641       -0.37004        1.69820
N           0.34334       -0.76236        2.98731
C           1.58614       -0.96815        3.58124
C           2.52206       -0.69173        2.62583
N           1.90368       -0.87702       -1.05045
```

C	0.55784	-1.03657	-1.20216
N	0.38316	-1.78558	-2.32287
C	1.61463	-2.06375	-2.90654
C	2.56023	-1.47907	-2.11208
Co	-0.58896	0.10962	0.06892
O	-2.36332	0.49457	-0.03155
C	-0.84229	3.66576	-1.16737
C	-0.61178	5.10224	-1.65534
C	-1.61007	2.86377	-2.23189
C	-1.62258	3.68766	0.15726
C	-1.00126	-0.98256	3.60447
C	-0.83872	-1.35158	5.08359
C	-1.82529	0.30989	3.47217
C	-1.68909	-2.13136	2.84686
C	-0.96168	-2.23685	-2.80321
C	-1.61586	-3.05200	-1.67595
C	-1.81003	-0.99944	-3.14091
C	-0.79926	-3.11298	-4.05120
H	-1.58935	5.59478	-1.77748
H	-0.02455	5.69042	-0.93023
H	-1.02499	2.79704	-3.16525
H	-2.56896	3.36106	-2.45714
H	-1.82540	1.85188	-1.85663
H	-1.04312	4.20637	0.94004
H	-1.85224	2.66177	0.48344
H	-2.57502	4.22585	0.01469
H	-0.33267	-0.55125	5.64880
H	-0.27598	-2.29067	5.21433
H	-1.83697	-1.49707	5.52562
H	-1.29918	1.15582	3.94605
H	-2.79896	0.18016	3.97406
H	-1.09339	-3.05719	2.91383
H	-2.68798	-2.32381	3.27244
H	-1.80994	-1.86595	1.78549
H	-2.63446	-3.35102	-1.96558
H	-1.01705	-3.95028	-1.44808
H	-2.77216	-1.31800	-3.57303
H	-2.02798	-0.41437	-2.23493
H	-0.18539	-4.00670	-3.85000
H	-0.35128	-2.55380	-4.88956
H	-1.79529	-3.45633	-4.37227
H	-0.10294	5.13185	-2.63306
H	-1.28630	-0.36014	-3.87181
H	-2.01243	0.54861	2.41256
C	4.09701	-0.00834	0.26222
C	4.83624	1.07463	0.78417
C	6.19792	0.96674	1.09445
C	6.86727	-0.24801	0.90631
C	6.15223	-1.35231	0.42851
C	4.79082	-1.22947	0.12274
H	4.33539	2.02707	0.98320
H	6.73541	1.83367	1.49419
H	7.93236	-0.33767	1.14542
H	6.65349	-2.31823	0.30209
H	4.25355	-2.12417	-0.20654
H	1.86990	4.43574	-1.81369
H	3.71121	2.52425	-1.10853
H	1.71784	-1.28409	4.61177
H	3.60650	-0.72813	2.68854

```
H          1.73519       -2.64233       -3.81744
H          3.63925       -1.44728       -2.23752
H         -1.69691       -2.44006       -0.76537
H         -3.18037       -0.47247        0.05608
C         -4.18504       -1.27868        0.07568
O         -4.48677       -1.65485       -1.23852
C         -5.32136       -0.39233        0.55282
H         -3.91160       -2.16080        0.67664
C         -5.39144       -0.69788       -1.81673
C         -5.62147        0.37777       -0.74391
H         -5.02630        0.25942        1.39059
H         -6.19394       -0.99676        0.87096
H         -4.94707       -0.29705       -2.74525
H         -6.32696       -1.22692       -2.08247
H         -4.88227        1.18754       -0.85699
H         -6.63464        0.80780       -0.78628
```

Transition states for HAA by the $L_0Co^{III}O$ oxidant

$L_0Co^{III}O$ + CHD (*S*=0, closed-shell)

```
94
ts_chd_u0.out     Energy: -2046939.8072645
C          0.55746       -1.04936       -1.21502
N          1.91419       -0.99370       -1.01231
B          2.58548       -0.11893        0.11954
N          1.98273        1.31184       -0.11656
C          0.63124        1.52651       -0.16341
N          1.81177       -0.60102        1.40315
C          0.44074       -0.54362        1.42001
Co        -0.55156        0.06661       -0.11835
O         -2.06403        0.18424       -0.98658
C         -0.90056       -2.56265       -2.81487
C         -0.74019       -3.77885       -3.74729
C         -1.83501       -2.98397       -1.65538
C         -1.54921       -1.40950       -3.61569
C         -0.78423        3.71650       -0.47415
C         -0.61684        5.24228       -0.34299
C         -1.40141        3.38799       -1.85434
C         -1.74882        3.25306        0.64138
C         -1.31870       -1.17809        3.23957
C         -1.86633        0.25824        3.41658
C         -2.18338       -1.93925        2.20752
C         -1.42918       -1.91655        4.58586
H         -1.74481       -4.09320       -4.07454
H         -0.16609       -3.54788       -4.65733
H         -1.38694       -3.80314       -1.06622
H         -2.79781       -3.33826       -2.06336
H         -2.04213       -2.13126       -0.99638
H         -0.88757       -1.08409       -4.43797
H         -1.76252       -0.56398       -2.94249
H         -2.50088       -1.75490       -4.05820
H         -0.05109        5.68394       -1.17674
H         -0.13709        5.52758        0.60794
H         -1.61781        5.70397       -0.35713
H         -0.72344        3.69322       -2.67035
H         -2.35586        3.92938       -1.97799
```

H	-1.31933	3.43392	1.64122
H	-2.70069	3.80494	0.56449
H	-1.98110	2.18367	0.54291
H	-2.92062	0.22783	3.73940
H	-1.28091	0.81169	4.17103
H	-3.21910	-2.02526	2.57453
H	-2.23135	-1.40856	1.24492
H	-0.90832	-1.39300	5.40186
H	-1.05225	-2.95027	4.52499
H	-2.49378	-1.97235	4.86659
H	-0.28007	-4.64216	-3.24010
H	-1.78368	-2.95213	2.02932
H	-1.60268	2.30806	-1.93090
C	4.18200	-0.13626	0.08374
C	4.81478	0.23298	-1.12424
C	6.20629	0.27553	-1.24366
C	7.01394	-0.05214	-0.14558
C	6.41158	-0.41714	1.06229
C	5.01371	-0.45688	1.17316
H	4.20330	0.49390	-1.99433
H	6.66485	0.56549	-2.19548
H	8.10543	-0.02108	-0.23359
H	7.03158	-0.67370	1.92850
H	4.56337	-0.74552	2.12474
H	-1.82390	0.81511	2.46836
H	-3.04608	0.67717	-0.78365
C	-4.45333	1.20584	-0.66846
C	-5.18118	0.18248	-1.53523
C	-4.67274	1.16892	0.74395
H	-4.29856	2.19533	-1.12263
C	-5.45350	-1.09596	-0.76743
H	-4.58397	-0.04082	-2.44400
H	-6.14887	0.58203	-1.93748
C	-5.14359	0.04301	1.38709
H	-4.36160	2.03441	1.34376
C	-5.46106	-1.12711	0.59055
H	-5.70936	-1.99740	-1.33914
H	-5.21140	-0.00169	2.47858
H	-5.70436	-2.06525	1.10697
C	0.50867	2.91680	-0.33711
C	0.40173	-2.04100	-2.20344
C	0.09647	-1.06167	2.67930
N	1.80863	3.37507	-0.39989
N	1.68969	-2.44992	-2.49467
N	1.29801	-1.37212	3.27994
N	2.69761	2.40670	-0.26114
N	2.59693	-1.82091	-1.76989
N	2.33387	-1.09837	2.50465
C	2.35888	4.71200	-0.61594
H	2.00810	5.11695	-1.57461
H	2.07392	5.38754	0.20071
H	3.45042	4.60271	-0.64035
C	2.22410	-3.41579	-3.45485
H	1.87520	-4.42980	-3.22301
H	1.92870	-3.14432	-4.47644
H	3.31674	-3.37301	-3.36448
C	1.61486	-1.92810	4.59412
H	1.26031	-1.25815	5.38872
H	1.15918	-2.91937	4.71336

```
H          2.70717       -2.01624        4.64845
```

$L_0Co^{III}O$ + CHD (*S*=1)

```
94
ts_chd_u2.out    Energy: -2046936.4826001
C          0.55937       -1.22542       -1.44992
N          1.88851       -1.03765       -1.15877
B          2.46032       -0.10362       -0.01250
N          1.88481        1.34661       -0.29209
C          0.54524        1.58272       -0.48704
N          1.66659       -0.52803        1.29401
C          0.29523       -0.65703        1.32875
Co        -0.63477       -0.09779       -0.38771
O         -2.26451       -0.03987       -1.04543
C         -0.68116       -2.71637       -3.18104
C         -0.41001       -3.86719       -4.16579
C         -1.64755       -3.22581       -2.08370
C         -1.35836       -1.54684       -3.93490
C         -0.85712        3.74990       -0.61540
C         -0.70866        5.27938       -0.67734
C         -1.57696        3.26427       -1.89583
C         -1.72220        3.37371        0.61204
C         -1.35234       -1.06942        3.31190
C         -1.87471        0.33300        3.70269
C         -2.29642       -1.68957        2.25861
C         -1.35389       -1.99330        4.54861
H         -1.37415       -4.22161       -4.56650
H          0.20033       -3.55361       -5.02681
H         -1.18118       -4.02838       -1.48625
H         -2.56052       -3.63220       -2.55367
H         -1.94310       -2.39957       -1.41829
H         -0.68447       -1.12672       -4.70199
H         -1.64255       -0.75652       -3.22093
H         -2.27292       -1.90558       -4.44022
H         -0.10253        5.60237       -1.53929
H         -0.27124        5.69898        0.24212
H         -1.70915        5.72815       -0.79399
H         -0.97263        3.48180       -2.79356
H         -2.54567        3.78466       -1.99910
H         -1.23550        3.68106        1.55366
H         -2.70699        3.86905        0.55163
H         -1.88644        2.28485        0.64262
H         -2.88786        0.26002        4.13409
H         -1.21634        0.81380        4.44710
H         -3.29941       -1.82680        2.69357
H         -2.41037       -1.04790        1.37255
H         -0.87568       -1.53754        5.42799
H         -0.85631       -2.95494        4.33550
H         -2.39693       -2.21124        4.83231
H          0.07711       -4.72717       -3.67744
H         -1.92003       -2.67170        1.92508
H         -1.76972        2.18042       -1.84445
C          4.05658       -0.23465        0.05992
C          4.89846        0.57169       -0.73311
C          6.28549        0.38195       -0.76359
C          6.87362       -0.63446       -0.00161
```

```
C          6.05779       -1.46139        0.77989
C          4.67212       -1.26322        0.80290
H          4.46452        1.36899       -1.34183
H          6.90978        1.03019       -1.38865
H          7.95861       -0.78475       -0.02100
H          6.50237       -2.26820        1.37322
H          4.05802       -1.92766        1.41662
H         -1.92851        0.98367        2.81463
H         -3.29354        0.55826       -0.57736
C         -4.44790        1.09829       -0.33912
C         -5.41472        0.16563       -1.06398
C         -4.60607        1.18488        1.10716
H         -4.30177        2.06652       -0.84279
C         -5.78173       -1.03555       -0.22709
H         -4.97257       -0.15274       -2.02627
H         -6.35573        0.69889       -1.34194
C         -5.18851        0.17478        1.81814
H         -4.16757        2.03892        1.63642
C         -5.69620       -1.00118        1.12422
H         -6.18878       -1.91926       -0.73346
H         -5.23368        0.21230        2.91152
H         -6.01517       -1.86594        1.71832
C          0.45173        2.97616       -0.49347
C          0.56024       -2.16281       -2.48631
C          0.02088       -0.90243        2.67620
N          1.73516        3.43755       -0.28966
N          1.89310       -2.43031       -2.72603
N          1.24131       -0.85090        3.31837
N          2.60354        2.44803       -0.16042
N          2.69440       -1.75439       -1.92214
N          2.23654       -0.62432        2.48093
C          2.28107        4.78911       -0.19004
H          2.08521        5.35243       -1.11191
H          1.84066        5.31808        0.66596
H          3.36372        4.68894       -0.04191
C          2.55273       -3.29693       -3.70043
H          2.26230       -4.34424       -3.54634
H          2.29502       -2.98782       -4.72240
H          3.63328       -3.18704       -3.54410
C          1.58983       -0.98896        4.72881
H          0.99359       -0.29123        5.33350
H          1.41586       -2.01851        5.07197
H          2.65471       -0.74205        4.82660
```

$L_0Co^{III}O$ + fluorene (*S*=0, closed-shell)

```
103
ts_fluorene_u0.out        Energy: -2215077.4727932
C         -0.95040       -0.73190       -1.20359
N         -2.30838       -0.66342       -1.38033
N         -2.82695       -0.67927        1.00482
C         -1.50657       -0.64122        1.37813
N         -2.63865        1.46662       -0.17316
C         -1.31978        1.66168        0.13465
Co        -0.16997        0.18096        0.25306
O          1.45921        0.54864       -0.19249
C          0.92238       -2.03973       -2.52577
```

C	1.03792	-3.14306	-3.59559
C	1.77111	-0.82597	-2.97091
C	1.48770	-2.61735	-1.20663
C	-0.24600	-1.73327	3.40397
C	-0.55692	-1.87977	4.90934
C	0.35800	-3.04893	2.85843
C	0.78833	-0.59603	3.25119
C	0.07956	3.85275	0.55944
C	0.77412	3.20787	1.78311
C	1.01024	3.75580	-0.67272
C	-0.16065	5.33751	0.89509
H	2.09194	-3.46232	-3.64172
H	0.43912	-4.03456	-3.34712
H	1.38008	-0.39855	-3.91135
H	2.81338	-1.14747	-3.14446
H	1.77110	-0.05911	-2.17931
H	0.88957	-3.48050	-0.86547
H	1.50750	-1.85690	-0.41546
H	2.52717	-2.95145	-1.35550
H	-1.11965	-2.79411	5.14575
H	-1.11680	-1.01011	5.29334
H	0.39249	-1.94034	5.46633
H	-0.36214	-3.88198	2.93127
H	1.25796	-3.32549	3.43467
H	0.36394	0.37508	3.55489
H	1.66735	-0.80336	3.88354
H	1.15225	-0.49855	2.21573
H	1.69198	3.77067	2.02487
H	0.11541	3.22316	2.66835
H	1.94311	4.31462	-0.48480
H	1.27197	2.70301	-0.86480
H	-0.85442	5.46775	1.74216
H	-0.52949	5.91655	0.03568
H	0.80292	5.78469	1.18923
H	0.76550	-2.79518	-4.60347
H	0.52379	4.18706	-1.56520
H	0.64796	-2.93300	1.80106
C	-5.11758	0.60232	-2.02937
C	-6.43945	0.71285	-2.46899
C	-7.49004	0.28965	-1.64308
C	-7.19957	-0.23778	-0.38096
C	-5.87000	-0.34506	0.05242
H	-4.31264	0.94115	-2.68977
H	-6.65325	1.13135	-3.45860
H	-8.52801	0.37337	-1.98302
H	-8.01220	-0.56912	0.27495
H	-5.66551	-0.76145	1.04079
H	1.06793	2.17159	1.57001
H	2.49540	0.55523	0.44498
C	3.72261	0.53311	1.07889
C	4.48694	1.35177	0.13654
H	3.49077	0.88614	2.09256
C	4.13856	-0.84713	0.82114
C	4.55650	2.74539	-0.03313
C	5.17488	0.49543	-0.78352
C	3.80614	-2.05250	1.46319
C	4.95817	-0.88118	-0.35389
C	5.28840	3.27289	-1.10271
H	4.03511	3.41140	0.66321

```
C          5.89220        1.03680       -1.86165
C          4.27542       -3.26325        0.94378
H          3.18072       -2.04516        2.36042
C          5.40421       -2.10435       -0.87777
C          5.94850        2.42655       -2.01799
H          5.34761        4.35936       -1.23425
H          6.40874        0.37878       -2.57016
C          5.06403       -3.29469       -0.22462
H          4.01822       -4.20250        1.44657
H          6.02075       -2.12698       -1.78388
H          6.51018        2.86106       -2.85202
H          5.41181       -4.25487       -0.62066
B         -3.26235        0.03124       -0.33329
N         -2.44993        3.54298       -0.03346
N         -3.32298        2.58285       -0.28267
N         -3.58270       -1.39248        1.81219
N         -2.76167       -1.82529        2.75210
N         -2.73537       -1.33127       -2.42724
N         -1.64971       -1.86475       -2.95879
C         -1.46757       -1.38582        2.56341
C         -0.50312       -1.55859       -2.25164
C         -1.18803        3.05675        0.24929
C         -3.34109       -2.67926        3.78490
H         -2.76597       -3.61195        3.86618
H         -3.35107       -2.16148        4.75406
H         -4.36935       -2.90795        3.47728
C         -1.86717       -2.62920       -4.18694
H         -1.27204       -2.20801       -5.00740
H         -1.60725       -3.68505       -4.04101
H         -2.93486       -2.54193       -4.42413
C         -2.97087        4.90596       -0.13311
H         -2.90004        5.42145        0.83290
H         -2.42050        5.46862       -0.89877
H         -4.02409        4.81760       -0.42777
C         -4.79817        0.06723       -0.76178
```

Transition states for HAA by the $L_2Co^{III}O$ oxidant

$L_2Co^{III}O$ + CHD (*S*=0, closed-shell)

```
94
ts_chd_u0.out    Energy: -2290045.2275054
C          0.52801       -1.11845       -1.15324
N          0.08790       -2.12440       -1.97070
C          1.09985       -3.07239       -2.10510
C          2.20040       -2.58818       -1.41363
N          1.84547       -1.36052       -0.89270
B          2.53566       -0.45651        0.20191
N          2.12395        1.02952       -0.13469
C          0.82268        1.37177       -0.33263
N          0.77546        2.70670       -0.64844
C          2.07675        3.20417       -0.62412
C          2.91749        2.14786       -0.30972
N          1.71830       -0.90854        1.48752
C          0.37252       -0.68498        1.56852
N         -0.08142       -1.35385        2.68232
C          0.97631       -2.07064        3.23526
C          2.09694       -1.80328        2.46552
```

Co	-0.49540	0.09411	-0.02552
O	-2.04755	0.58066	0.55535
C	-1.29167	-2.24071	-2.57741
C	-1.16920	-2.71721	-4.03532
C	-2.10047	-3.22309	-1.71724
C	-1.95447	-0.86168	-2.58637
C	-0.49834	3.50173	-0.89326
C	-0.18776	4.87330	-1.50482
C	-1.36601	2.72448	-1.89252
C	-1.18825	3.68914	0.46652
C	-1.50511	-1.29454	3.23774
C	-1.83272	0.18323	3.49710
C	-2.44823	-1.96333	2.22617
C	-1.61386	-2.04824	4.56933
H	-2.16772	-2.68005	-4.49759
H	-0.50026	-2.05390	-4.60802
H	-1.64123	-4.22524	-1.70878
H	-3.12085	-3.31615	-2.12234
H	-2.17257	-2.85496	-0.68097
H	-1.30988	-0.11056	-3.06669
H	-2.22179	-0.52272	-1.57485
H	-2.89132	-0.92879	-3.15952
H	0.39866	4.79431	-2.43409
H	0.32281	5.54717	-0.80322
H	-1.15010	5.34388	-1.75896
H	-0.81964	2.55674	-2.83486
H	-2.27238	3.31018	-2.11205
H	-0.53588	4.25639	1.15108
H	-2.12101	4.25906	0.32707
H	-1.43633	2.71759	0.91474
H	-2.86007	0.25521	3.88979
H	-1.14061	0.59939	4.24874
H	-3.46753	-1.97420	2.64306
H	-2.48573	-1.40419	1.28440
H	-0.93219	-1.65392	5.33885
H	-1.46584	-3.13275	4.46237
H	-2.64032	-1.89783	4.93816
H	-0.81121	-3.75075	-4.12717
H	-2.13530	-3.00538	2.04403
H	-1.68899	1.76141	-1.48503
C	4.92625	-0.74975	-0.82230
C	6.32072	-0.70137	-0.75311
C	6.94951	-0.41048	0.46296
C	6.17513	-0.14971	1.59882
C	4.78202	-0.19942	1.51742
H	4.45851	-0.94087	-1.79339
H	4.19839	0.04675	2.41070
H	-1.78867	0.75705	2.56339
H	-3.00938	1.13063	0.29973
C	-4.32380	1.67199	-0.01255
C	-4.75587	0.96106	-1.28193
C	-4.92600	1.23773	1.21711
H	-4.10576	2.74347	-0.11489
C	-5.05632	-0.49631	-1.02998
H	-3.99839	1.07883	-2.07726
H	-5.67276	1.44430	-1.70425
C	-5.43562	-0.03309	1.34439
H	-4.85935	1.88672	2.09891
C	-5.40634	-0.93249	0.20668

H	-5.06123	-1.18595	-1.88177
H	-5.80560	-0.39447	2.30909
H	-5.67023	-1.98549	0.36098
C	2.55417	4.51984	-0.85974
N	3.05388	5.55773	-1.02699
C	4.32931	2.28887	-0.22775
N	5.45437	2.58817	-0.21088
C	3.40394	-3.31146	-1.19606
N	4.34023	-3.98252	-1.03227
C	1.02597	-4.34382	-2.72771
N	1.02014	-5.41101	-3.19353
C	3.33731	-2.48233	2.61381
N	4.28560	-3.13226	2.79401
C	1.01368	-2.97407	4.33057
N	1.17176	-3.73698	5.19534
H	6.65793	0.10456	2.54772
H	8.04222	-0.37063	0.52112
H	6.91835	-0.88145	-1.65242
C	4.12401	-0.53166	0.31559

$L_2Co^{III}O$ + CHD (*S*=1)

94
ts_chd_u2.out Energy: -2290049.5412251

C	0.41895	-1.03136	-1.14543
N	-0.01086	-2.05669	-1.92614
C	0.98174	-3.03087	-1.99625
C	2.06331	-2.54820	-1.27486
N	1.72005	-1.28826	-0.81394
B	2.46816	-0.37075	0.25421
N	2.14653	1.15993	-0.09920
C	0.88613	1.65372	-0.28814
N	0.98357	2.95405	-0.67296
C	2.32974	3.30667	-0.70909
C	3.05564	2.17910	-0.35465
N	1.70435	-0.80525	1.58850
C	0.36804	-0.55971	1.72597
N	-0.06889	-1.25254	2.81396
C	0.98376	-1.99556	3.33683
C	2.09158	-1.73288	2.54223
Co	-0.50821	0.32829	0.07712
O	-2.01867	1.10641	0.38773
C	-1.36492	-2.14888	-2.58656
C	-1.16639	-2.49213	-4.07341
C	-2.18208	-3.22135	-1.84951
C	-2.06639	-0.79195	-2.49250
C	-0.22104	3.82978	-0.98945
C	0.21727	5.17006	-1.58841
C	-1.09116	3.08909	-2.01863
C	-0.97669	4.07053	0.32547
C	-1.52524	-1.25716	3.24448
C	-1.94908	0.19913	3.48164
C	-2.33481	-1.90922	2.11263
C	-1.72030	-2.05803	4.53506
H	-2.14941	-2.49347	-4.56979
H	-0.53216	-1.73516	-4.56348
H	-1.71459	-4.21640	-1.92167

H	-3.18847	-3.28609	-2.29259
H	-2.29093	-2.95446	-0.78582
H	-1.43623	0.01955	-2.88723
H	-2.35783	-0.54009	-1.46357
H	-2.98705	-0.83796	-3.09339
H	0.81028	5.04627	-2.50852
H	0.77485	5.79188	-0.87318
H	-0.69513	5.72508	-1.85598
H	-0.50184	2.82841	-2.91344
H	-1.91507	3.75253	-2.32759
H	-0.32292	4.56760	1.06187
H	-1.83887	4.72927	0.12849
H	-1.35373	3.11786	0.72668
H	-3.00540	0.21418	3.79549
H	-1.33957	0.65345	4.28075
H	-3.38044	-2.02620	2.43371
H	-2.34288	-1.27587	1.21502
H	-1.11793	-1.66265	5.36778
H	-1.50816	-3.12983	4.40549
H	-2.77928	-1.96758	4.82263
H	-0.72077	-3.48405	-4.23134
H	-1.92827	-2.90333	1.86347
H	-1.53602	2.18480	-1.58424
C	4.80379	-0.81622	-0.85547
C	6.19912	-0.86818	-0.83089
C	6.88593	-0.61308	0.36158
C	6.16954	-0.28583	1.51789
C	4.77478	-0.23535	1.48102
H	4.29223	-0.98316	-1.80902
H	4.23893	0.06054	2.38903
H	-1.86471	0.78764	2.55708
H	-3.34851	1.02549	0.38594
C	-4.59355	1.16034	0.30405
C	-5.02705	0.58968	-1.04219
C	-5.15219	0.48518	1.47651
H	-4.65491	2.25950	0.34694
C	-5.18744	-0.90699	-1.00815
H	-4.32748	0.89931	-1.83784
H	-6.00770	1.03116	-1.33801
C	-5.55668	-0.81594	1.40777
H	-5.15805	1.01168	2.43797
C	-5.46298	-1.54888	0.15238
H	-5.15174	-1.46178	-1.95244
H	-5.91630	-1.33606	2.30198
H	-5.63181	-2.63154	0.15956
C	2.93834	4.55051	-1.02155
N	3.52986	5.52542	-1.25518
C	4.47621	2.19986	-0.30115
N	5.61809	2.42854	-0.31615
C	3.22921	-3.30659	-0.98084
N	4.12045	-4.01951	-0.75417
C	0.89572	-4.30616	-2.60883
N	0.85678	-5.36998	-3.08075
C	3.32259	-2.43210	2.67165
N	4.25903	-3.10031	2.84802
C	1.01409	-2.88232	4.44496
N	1.13831	-3.62492	5.33262
H	6.69972	-0.05879	2.44820
H	7.97995	-0.65255	0.38509

```
H          6.75309       -1.09880       -1.74642
C          4.05579       -0.53192        0.30520
```

$L_2Co^{III}O$ + fluorene (*S*=0, closed-shell)

```
103
ts_fluorene_u0.out        Energy: -2458177.8667837
C          0.25022       -1.11704       -0.99903
N         -0.23392       -2.13162       -1.77449
C          0.74258       -3.12083       -1.87743
C          1.86109       -2.65727       -1.20181
N          1.55544       -1.39750       -0.72931
B          2.30588       -0.44362        0.28355
N          1.92906        1.02821       -0.14258
C          0.63442        1.41121       -0.25902
N          0.60299        2.72820       -0.63665
C          1.91929        3.16736       -0.76438
C          2.74563        2.09754       -0.45705
N          1.49892       -0.76175        1.61399
C          0.15603       -0.52430        1.68126
N         -0.30569       -1.09102        2.84649
C          0.75649       -1.73799        3.47062
C          1.87727       -1.55013        2.67819
Co        -0.72456        0.18060        0.09939
O         -2.28482        0.69337        0.60026
C         -1.60206       -2.22094       -2.42062
C         -1.42268       -2.62466       -3.89538
C         -2.42695       -3.25081       -1.63377
C         -2.28392       -0.85047       -2.38870
C         -0.65945        3.57508       -0.76555
C         -0.33924        4.96501       -1.32657
C         -1.61467        2.87769       -1.74559
C         -1.24604        3.72620        0.64624
C         -1.75517       -1.07898        3.34513
C         -2.17646        0.38471        3.53404
C         -2.60456       -1.85214        2.32666
C         -1.88675       -1.78576        4.70005
H         -2.40842       -2.60236       -4.38523
H         -0.76286       -1.91057       -4.41495
H         -1.95877       -4.24798       -1.64833
H         -3.42721       -3.34210       -2.08608
H         -2.54888       -2.92905       -0.58689
H         -1.64305       -0.07071       -2.82903
H         -2.57439       -0.54813       -1.37456
H         -3.20710       -0.90951       -2.98575
H          0.13696        4.92096       -2.31838
H          0.27835        5.56670       -0.64468
H         -1.29714        5.49474       -1.44410
H         -1.13135        2.73964       -2.72648
H         -2.50646        3.50931       -1.88245
H         -0.51335        4.21301        1.31142
H         -2.14671        4.35648        0.60231
H         -1.53644        2.75302        1.06222
H         -3.23518        0.41157        3.83878
H         -1.56903        0.85584        4.32513
H         -3.64561       -1.89108        2.67952
H         -2.61608       -1.36240        1.34883
```

H	-1.28407	-1.31287	5.49023
H	-1.65909	-2.86067	4.64876
H	-2.94243	-1.69428	4.99924
H	-1.02159	-3.63860	-4.02446
H	-2.23100	-2.88513	2.22618
H	-1.96050	1.91012	-1.36759
C	4.67545	-0.92461	-0.73634
C	6.07147	-0.90184	-0.68540
C	6.72135	-0.48313	0.48108
C	5.96677	-0.06807	1.58384
C	4.57230	-0.09403	1.52141
H	4.19542	-1.21111	-1.67693
H	4.00537	0.27131	2.38426
H	-2.09312	0.94356	2.59562
H	-3.33801	0.96689	0.25349
C	2.42582	4.43670	-1.14912
N	2.95575	5.42742	-1.45215
C	4.16365	2.17496	-0.51293
N	5.29726	2.41582	-0.62254
C	3.03008	-3.42358	-0.94439
N	3.93271	-4.12822	-0.73950
C	0.61677	-4.40456	-2.46620
N	0.56266	-5.48002	-2.90867
C	3.12079	-2.20187	2.90315
N	4.06899	-2.82461	3.16152
C	0.80607	-2.49514	4.67166
N	0.98645	-3.13403	5.62741
H	6.46602	0.28711	2.49084
H	7.81524	-0.46286	0.52397
H	6.65379	-1.20030	-1.56288
C	3.89207	-0.55472	0.37467
C	-4.70571	1.17024	-0.15542
C	-5.03261	2.22932	0.79668
H	-4.62393	1.34268	-1.23487
C	-5.24920	-0.06237	0.41411
C	-4.83688	3.61853	0.73972
C	-5.58092	1.63875	1.98067
C	-5.29436	-1.37244	-0.08829
C	-5.72281	0.20511	1.73843
C	-5.15956	4.40230	1.85401
H	-4.43784	4.08303	-0.16827
C	-5.88612	2.43160	3.09449
C	-5.80534	-2.39796	0.71522
H	-4.93513	-1.58893	-1.09860
C	-6.22107	-0.83162	2.53808
C	-5.67113	3.81460	3.02770
H	-5.01166	5.48696	1.81385
H	-6.29589	1.97813	4.00389
C	-6.26349	-2.13340	2.02078
H	-5.84653	-3.42071	0.32507
H	-6.57902	-0.62748	3.55324
H	-5.91017	4.44556	3.89018
H	-6.65420	-2.95150	2.63476

Transition states for HAA by the $L_3Co^{III}O$ oxidant

$L_3Co^{III}O$ + CHD (*S*=0, closed-shell)

```
88
chd_ts_u0.out     Energy: -1953191.0114453
C           0.59355       -1.03038       -1.24508
N           0.32421       -2.05686       -2.11087
C           1.49669       -2.75294       -2.38646
C           2.50217       -2.14684       -1.69890
N           1.94488       -1.06867       -1.03227
B           2.52413       -0.15318        0.07639
N           2.05748        1.29435       -0.15828
C           0.72537        1.55402       -0.17418
N           0.59461        2.90200       -0.35431
C           1.86253        3.47198       -0.46435
C           2.77370        2.46775       -0.34093
N           1.88198       -0.66133        1.38829
C           0.52706       -0.51116        1.44110
N           0.12250       -1.13600        2.58568
C           1.21813       -1.72351        3.21067
C           2.31428       -1.44297        2.44984
Co         -0.48564        0.13130       -0.09203
O          -2.03674        0.25090       -0.87293
C          -1.01024       -2.40972       -2.72676
C          -0.83567       -3.59258       -3.69168
C          -1.98484       -2.81628       -1.61135
C          -1.51546       -1.18963       -3.51159
C          -0.69772        3.66109       -0.47266
C          -0.41657        5.16855       -0.40237
C          -1.33941        3.31118       -1.82518
C          -1.60945        3.26777        0.69858
C          -1.29062       -1.15965        3.09388
C          -1.76550        0.29384        3.24460
C          -2.16430       -1.92709        2.09097
C          -1.33912       -1.85899        4.45803
H          -1.81845       -3.81495       -4.13534
H          -0.14506       -3.35932       -4.51882
H          -1.57470       -3.65591       -1.02471
H          -2.94043       -3.13750       -2.05762
H          -2.19175       -1.96555       -0.95217
H          -0.79062       -0.91038       -4.29559
H          -1.68644       -0.34680       -2.82620
H          -2.47249       -1.44166       -3.99866
H           0.18143        5.52234       -1.25774
H           0.09331        5.44795        0.53461
H          -1.37934        5.70171       -0.43481
H          -0.66734        3.59302       -2.65331
H          -2.28534        3.86553       -1.94189
H          -1.11433        3.46038        1.66440
H          -2.53982        3.85606        0.65515
H          -1.88553        2.20632        0.64341
H          -2.81409        0.31323        3.58079
H          -1.14138        0.83439        3.97575
H          -3.18653       -2.02735        2.48711
H          -2.24256       -1.38740        1.13638
H          -0.70732       -1.35123        5.20526
H          -1.03778       -2.91725        4.39001
H          -2.37702       -1.83264        4.82455
H          -0.49214       -4.50618       -3.17883
H          -1.75224       -2.93263        1.90448
H          -1.55705        2.23436       -1.87784
C           4.79081       -0.13110       -1.07551
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C          6.16874        0.03536       -1.11347
C          6.86229        0.25759        0.08045
C          6.14093        0.33253        1.27597
C          4.76346        0.15793        1.24851
H          4.20752       -0.26569       -1.98683
H          6.68245        0.00054       -2.07677
H          7.94805        0.38973        0.07658
H          6.63257        0.53585        2.22991
H          4.16024        0.25202        2.15136
H          1.54170       -3.61578       -3.04143
H          3.55192       -2.42288       -1.63629
H          2.02505        4.53381       -0.61557
H          3.86016        2.51242       -0.36506
H          1.14931       -2.28680        4.13566
H          3.34549       -1.75683        2.59353
H         -1.71863        0.82380        2.28264
H         -3.00104        0.75949       -0.64981
C         -4.39213        1.26877       -0.53580
C         -5.06891        0.25075       -1.44217
C         -4.62193        1.18948        0.87356
H         -4.23379        2.26763       -0.96513
C         -5.38152       -1.03652       -0.71590
H         -4.42703        0.04258       -2.32296
H         -6.01320        0.65739       -1.88326
C         -5.09658        0.04153        1.46856
H         -4.32638        2.03913        1.50183
C         -5.41275       -1.10594        0.63917
H         -5.64198       -1.91546       -1.31828
H         -5.19429       -0.03047        2.55624
H         -5.68145       -2.05059        1.12805
N          4.10311       -0.10618        0.09399
```

$L_3Co^{III}O$ + CHD (*S*=1)

```
88
chd_ts_u2.out     Energy: -1953193.8643920
C          0.67137       -1.02286       -1.43799
N          0.49738       -2.03300       -2.32775
C          1.68527       -2.74022       -2.48406
C          2.61286       -2.14027       -1.68581
N          1.99225       -1.05448       -1.07801
B          2.46684       -0.13449        0.08715
N          2.02316        1.33001       -0.16545
C          0.70800        1.62991       -0.33687
N          0.63509        2.96782       -0.53138
C          1.91292        3.52300       -0.48097
C          2.78040        2.49649       -0.25184
N          1.79324       -0.69990        1.37320
C          0.43436       -0.58450        1.49455
N          0.09192       -1.30335        2.59271
C          1.21527       -1.92426        3.12887
C          2.27581       -1.56329        2.35150
Co        -0.50732        0.07885       -0.20806
O         -2.21626       -0.20032       -0.34226
C         -0.81195       -2.37684       -2.98063
C         -0.55767       -3.32383       -4.16128
C         -1.70602       -3.05846       -1.93220
```

C	-1.46367	-1.08110	-3.48933
C	-0.66125	3.68797	-0.74598
C	-0.39220	5.18013	-0.96806
C	-1.34840	3.08683	-1.98373
C	-1.53091	3.48910	0.50663
C	-1.31477	-1.43862	3.10297
C	-1.96201	-0.04540	3.11826
C	-2.08425	-2.37818	2.16074
C	-1.28705	-2.01248	4.52548
H	-1.51393	-3.50878	-4.67492
H	0.14164	-2.88444	-4.89228
H	-1.21328	-3.95783	-1.52508
H	-2.65763	-3.36465	-2.39803
H	-1.93058	-2.35520	-1.11612
H	-0.78771	-0.54730	-4.17834
H	-1.72937	-0.42501	-2.64753
H	-2.38967	-1.33117	-4.03296
H	0.23474	5.35431	-1.85814
H	0.09091	5.64451	-0.09263
H	-1.35337	5.69259	-1.12945
H	-0.69888	3.17283	-2.87061
H	-2.28920	3.62465	-2.18524
H	-1.02246	3.88294	1.40226
H	-2.48949	4.01927	0.38549
H	-1.74805	2.42136	0.66553
H	-2.97815	-0.11701	3.53757
H	-1.37308	0.65443	3.73463
H	-3.11005	-2.52417	2.53855
H	-2.14874	-1.93085	1.15707
H	-0.68337	-1.38793	5.20520
H	-0.90146	-3.04495	4.55084
H	-2.31721	-2.03897	4.91360
H	-0.16795	-4.30234	-3.83605
H	-1.59037	-3.36307	2.10170
H	-1.58960	2.02448	-1.82153
C	4.80853	-0.08343	-0.91963
C	6.18234	0.11387	-0.87395
C	6.79555	0.36185	0.35808
C	5.99931	0.43024	1.50549
C	4.63029	0.22423	1.39412
H	4.28683	-0.23804	-1.86436
H	6.75551	0.08270	-1.80325
H	7.87622	0.51891	0.42035
H	6.42573	0.65318	2.48607
H	3.96956	0.31045	2.25687
H	1.79256	-3.59760	-3.14112
H	3.65029	-2.41960	-1.51638
H	2.11382	4.58214	-0.61027
H	3.86265	2.52480	-0.14936
H	1.18965	-2.55980	4.00879
H	3.31692	-1.86757	2.43297
H	-2.05495	0.35222	2.09774
H	-3.24030	0.63145	-0.26789
C	-4.31651	1.27841	-0.32043
C	-5.26557	0.31240	-1.02517
C	-4.64096	1.57927	1.07499
H	-4.04714	2.15525	-0.92841
C	-5.80553	-0.74314	-0.09424
H	-4.75573	-0.15454	-1.88760

H	-6.13039	0.86282	-1.46546
C	-5.35217	0.69639	1.83338
H	-4.21532	2.47796	1.53619
C	-5.85546	-0.53826	1.24343
H	-6.21916	-1.66021	-0.53032
H	-5.52654	0.88766	2.89760
H	-6.29440	-1.29601	1.90270
N	4.04850	-0.06562	0.20372

$L_3Co^{III}O$ + fluorene (*S*=0, closed-shell)

97

fluorene_ts_u0.out Energy: -2121326.5494847

C	-1.10076	-0.89407	-1.30768
N	-0.65810	-1.45156	-2.47565
C	-1.73927	-1.62782	-3.33291
C	-2.85323	-1.18524	-2.68937
N	-2.45452	-0.76767	-1.43114
N	-2.83326	-0.50758	1.04384
C	-1.53318	-0.54950	1.42467
N	-1.51275	-0.99573	2.71396
C	-2.82219	-1.24354	3.12367
C	-3.64361	-0.93803	2.08196
N	-2.59517	1.47615	-0.45997
C	-1.26329	1.54180	-0.18039
N	-0.87971	2.82100	-0.44641
C	-1.96397	3.54023	-0.93724
C	-3.03121	2.69147	-0.96599
Co	-0.21066	-0.07441	0.18925
O	1.27954	-0.90738	0.38755
C	0.74943	-1.89405	-2.82301
C	0.77426	-2.44982	-4.25526
C	1.69749	-0.68805	-2.75272
C	1.14849	-3.00711	-1.84428
C	-0.29733	-1.23952	3.57433
C	-0.74125	-1.49185	5.02277
C	0.43356	-2.47718	3.03127
C	0.59872	0.00852	3.54544
C	0.47671	3.39186	-0.13763
C	0.63063	3.41080	1.39110
C	1.55856	2.52369	-0.79279
C	0.57326	4.81986	-0.68955
H	1.80900	-2.75301	-4.47740
H	0.13856	-3.34270	-4.37216
H	1.36933	0.10373	-3.44744
H	2.71327	-1.00897	-3.03531
H	1.75564	-0.28874	-1.73468
H	0.44256	-3.85227	-1.91903
H	1.17233	-2.61511	-0.81757
H	2.15961	-3.36609	-2.09209
H	-1.33817	-2.41242	5.12449
H	-1.31237	-0.64240	5.43283
H	0.16098	-1.62034	5.64034
H	-0.22304	-3.36240	3.07879
H	1.32862	-2.67570	3.64365
H	0.03354	0.90401	3.85207

H	1.43745	-0.13058	4.24611
H	1.02941	0.17330	2.54980
H	1.62291	3.80108	1.66313
H	-0.14546	4.04396	1.85300
H	2.53972	3.00730	-0.67803
H	1.64703	1.53891	-0.31042
H	-0.15238	5.50139	-0.21668
H	0.43247	4.84483	-1.78288
H	1.58027	5.20731	-0.47072
H	0.48253	-1.69463	-5.00388
H	1.35264	2.37951	-1.86553
H	0.75058	-2.30679	1.99230
C	-5.35170	-1.19415	-0.81995
C	-6.73151	-1.34619	-0.81740
C	-7.53523	-0.27595	-0.41138
C	-6.92121	0.90828	0.00763
C	-5.53575	0.99918	-0.01712
H	-4.68865	-2.01635	-1.09108
H	-7.16227	-2.30239	-1.12263
H	-8.62487	-0.37064	-0.40313
H	-7.50386	1.76048	0.36440
H	-5.01877	1.88780	0.34418
H	-1.64913	-2.05212	-4.32630
H	-3.87746	-1.13123	-3.04958
H	-3.07455	-1.61301	4.11148
H	-4.72748	-0.99410	2.01483
H	-1.90700	4.58389	-1.22895
H	-4.04028	2.87469	-1.32683
H	0.54685	2.39408	1.80355
H	2.30955	-0.91789	0.91797
C	3.63671	-0.90298	1.45197
C	4.02319	0.50285	1.34399
H	3.48575	-1.39610	2.42049
C	4.26926	-1.57516	0.31873
C	3.78674	1.60044	2.18903
C	4.72006	0.70594	0.10690
C	4.28670	-2.92738	-0.06254
C	4.85675	-0.59265	-0.54326
C	4.24686	2.86855	1.81487
H	3.25183	1.46474	3.13501
C	5.15843	1.98470	-0.26455
C	4.87075	-3.29045	-1.28092
H	3.83457	-3.68877	0.58281
C	5.42414	-0.96733	-1.76950
C	4.92595	3.06497	0.59570
H	4.07765	3.72263	2.48007
H	5.68792	2.13584	-1.21210
C	5.42910	-2.31863	-2.13647
H	4.88801	-4.34447	-1.57987
H	5.86160	-0.21225	-2.43255
H	5.27237	4.06710	0.32185
H	5.87312	-2.62481	-3.08962
B	-3.19349	0.05243	-0.34659
N	-4.76398	-0.02459	-0.45955

Transition states for HAA by the $L_4Co^{III}O$ oxidant

$L_4Co^{III}O$ + CHD (*S*=0, closed-shell)

```
97
chd_ts_u0_closed.out      Energy: -2473983.3410898
C           0.55002       -1.09129       -1.38904
N           0.19439       -1.94118       -2.39781
C           1.21008       -2.87547       -2.57984
C           2.24154       -2.53309       -1.72440
N           1.84641       -1.38291       -1.05642
B           2.43115       -0.59288        0.14286
N           2.10685        0.92036       -0.05705
C           0.80383        1.26953       -0.26583
N           0.75560        2.62343       -0.38913
C           2.04270        3.13747       -0.24899
C           2.89276        2.06657       -0.04219
N           1.61981       -1.11637        1.37385
C           0.32034       -0.70578        1.47460
N          -0.17386       -1.20639        2.64170
C           0.75278       -2.10667        3.16587
C           1.87585       -2.05888        2.35875
Co         -0.50919       -0.10696       -0.16514
O          -2.03617       -0.80712        0.19067
C          -1.10973       -1.91258       -3.17568
C          -0.83513       -2.24928       -4.65122
C          -2.04461       -2.93875       -2.52196
C          -1.68388       -0.49160       -3.12539
C          -0.47475        3.47590       -0.62455
C          -0.64908        4.40798        0.58570
C          -0.27969        4.24994       -1.93865
C          -1.70712        2.58146       -0.75165
C          -1.43680       -0.76260        3.38341
C          -1.92551        0.58669        2.83647
C          -2.49788       -1.85342        3.20534
C          -1.06344       -0.55244        4.86363
H          -1.75539       -2.05237       -5.22220
H          -0.03506       -1.61252       -5.06307
H          -1.61745       -3.95327       -2.58280
H          -3.01237       -2.94688       -3.04797
H          -2.21036       -2.67945       -1.46527
H          -0.96249        0.24308       -3.51655
H          -1.98024       -0.20398       -2.11037
H          -2.58917       -0.45728       -3.75053
H           0.18651        5.11423        0.70146
H          -0.74903        3.82014        1.51283
H          -1.56720        5.00086        0.45004
H           0.57020        4.94690       -1.90131
H          -1.18446        4.84478       -2.13913
H          -1.93047        2.03399        0.17479
H          -2.57845        3.22057       -0.96110
H          -1.61417        1.87578       -1.58965
H          -2.70193        0.96451        3.51873
H          -1.10565        1.32421        2.80377
H          -3.41823       -1.55330        3.73020
H          -2.71590       -1.96856        2.13349
H          -0.22739        0.15961        4.96259
H          -0.80810       -1.48116        5.39026
H          -1.93799       -0.12633        5.37841
```

```
H          -0.57912       -3.30341       -4.81602
H          -2.16339       -2.81642        3.62543
H          -0.12976        3.55158       -2.77817
C           4.76811       -0.78957       -0.82191
C           6.15341       -0.83820       -0.74602
C           6.78901       -0.78399        0.52572
C           5.95634       -0.63560        1.66779
C           4.57697       -0.59391        1.51137
H           4.26985       -0.76627       -1.79169
H           3.93149       -0.41794        2.37183
H          -2.36394        0.48203        1.83943
H          -3.12784       -0.81216       -0.42231
C          -4.38425       -0.78813       -0.84742
C          -5.12957       -1.53989        0.24442
C          -4.57449        0.64430       -0.90353
H          -4.33880       -1.30558       -1.81438
C          -5.38808       -0.70622        1.46586
H          -4.59487       -2.46917        0.51570
H          -6.11356       -1.89644       -0.14361
C          -4.98273        1.34550        0.20303
H          -4.28096        1.18231       -1.81200
C          -5.32418        0.64912        1.42770
H          -5.68655       -1.21962        2.38653
H          -5.04286        2.43819        0.17554
H          -5.55104        1.23673        2.32368
N           3.98652       -0.72213        0.29130
C           2.43360        4.50030       -0.29862
N           2.80077        5.60393       -0.32774
C           4.29455        2.15547        0.14731
N           5.44411        2.24668        0.30483
C           3.43887       -3.25919       -1.50467
N           4.42168       -3.85090       -1.30722
C           1.20128       -4.03297       -3.40102
N           1.25971       -5.01724       -4.01842
C           3.02831       -2.88060        2.44357
N           3.97348       -3.55833        2.49111
C           0.56712       -3.01138        4.24362
N           0.46538       -3.80379        5.08949
C           8.20505       -0.83919        0.64571
N           9.36414       -0.88414        0.74330
C           6.50908       -0.50899        2.98215
N           6.95291       -0.40767        4.05086
C           6.91313       -0.92514       -1.95606
N           7.52575       -0.99909       -2.94033
```

$L_4Co^{III}O$ + CHD (*S*=0, open-shell)

```
97
chd_ts_u0_open.out        Energy: -2473988.7504598
C           0.50235       -1.06960       -1.39843
N           0.16984       -1.93634       -2.39362
C           1.15217       -2.91652       -2.49935
C           2.15397       -2.58644       -1.60391
N           1.77321       -1.39634       -0.99462
B           2.37290       -0.56296        0.17302
N           2.08130        0.94610       -0.07184
C           0.77322        1.32075       -0.22895
N           0.75411        2.66996       -0.39197
```

C	2.05640	3.15983	-0.33497
C	2.89202	2.07632	-0.13617
N	1.62375	-1.03572	1.45470
C	0.32747	-0.61406	1.58709
N	-0.15119	-1.15245	2.73893
C	0.78179	-2.05129	3.24837
C	1.89504	-1.99169	2.42737
Co	-0.53092	-0.07121	-0.11607
O	-1.84659	-1.22421	0.13809
C	-1.06775	-1.85145	-3.26568
C	-0.65634	-2.05767	-4.73389
C	-2.04819	-2.92753	-2.77987
C	-1.66706	-0.44615	-3.14019
C	-0.47617	3.52773	-0.58395
C	-0.57957	4.49283	0.60807
C	-0.34832	4.26743	-1.92565
C	-1.71787	2.63577	-0.62278
C	-1.46182	-0.78504	3.41824
C	-2.01844	0.50050	2.79366
C	-2.43847	-1.95219	3.22691
C	-1.16849	-0.50739	4.90376
H	-1.53971	-1.88273	-5.36743
H	0.12583	-1.33872	-5.02844
H	-1.63112	-3.93878	-2.91614
H	-2.98197	-2.86632	-3.36126
H	-2.26749	-2.76515	-1.71367
H	-0.93200	0.32936	-3.40757
H	-2.04166	-0.25760	-2.12912
H	-2.52217	-0.36906	-3.82892
H	0.26953	5.19084	0.66062
H	-0.63642	3.93092	1.55476
H	-1.49678	5.09369	0.50492
H	0.50384	4.96248	-1.94789
H	-1.26095	4.85998	-2.09527
H	-1.88564	2.10559	0.32718
H	-2.59995	3.27266	-0.78739
H	-1.67801	1.91695	-1.45547
H	-2.88683	0.82051	3.38862
H	-1.26963	1.30932	2.80675
H	-3.39899	-1.70344	3.70427
H	-2.60028	-2.11073	2.14954
H	-0.39896	0.27470	5.01328
H	-0.85185	-1.40030	5.45994
H	-2.09468	-0.14646	5.37701
H	-0.30568	-3.07607	-4.94801
H	-2.05894	-2.87920	3.68750
H	-0.24183	3.54779	-2.75379
C	4.69684	-0.85957	-0.83134
C	6.08791	-0.95140	-0.78288
C	6.74061	-0.84813	0.46735
C	5.95063	-0.61348	1.61632
C	4.56342	-0.53969	1.48322
H	4.17535	-0.88037	-1.78929
H	3.93740	-0.30722	2.34557
H	-2.36454	0.32527	1.76863
H	-3.11078	-0.93128	-0.45108
C	-4.26764	-0.79315	-0.78970
C	-5.07068	-1.56855	0.25575
C	-4.49360	0.66043	-0.81039

H -4.30448 -1.25995 -1.78552
C -5.34941 -0.77387 1.50145
H -4.55298 -2.51187 0.50757
H -6.04767 -1.88745 -0.17372
C -4.94541 1.31491 0.29492
H -4.20623 1.22574 -1.70418
C -5.29900 0.57840 1.50197
H -5.65372 -1.31680 2.40347
H -5.04171 2.40600 0.29370
H -5.54483 1.14142 2.40892
N 3.95411 -0.70638 0.28808
C 2.47001 4.51178 -0.45068
N 2.85046 5.60809 -0.53543
C 4.30391 2.13522 -0.03354
N 5.46423 2.18350 0.04782
C 3.31480 -3.34067 -1.29997
N 4.27421 -3.94196 -1.02806
C 1.12331 -4.08969 -3.29711
N 1.14205 -5.08141 -3.90529
C 3.06157 -2.79295 2.50378
N 4.02878 -3.44033 2.54260
C 0.61992 -2.93922 4.34360
N 0.52947 -3.70799 5.21226
C 8.16269 -0.94820 0.56210
N 9.31905 -1.03010 0.63885
C 6.54096 -0.43572 2.90821
N 7.01334 -0.29145 3.95916
C 6.81908 -1.14227 -1.99860
N 7.40566 -1.30074 -2.98817

$L_4Co^{III}O$ + CHD (*S*=1)

97
chd_ts_u2_2.out Energy: -2473990.8391188
C 0.51943 -1.03931 -1.44596
N 0.18552 -1.90672 -2.43694
C 1.14944 -2.90707 -2.52029
C 2.14035 -2.59330 -1.60623
N 1.77377 -1.38936 -1.01344
B 2.36674 -0.55711 0.16202
N 2.08657 0.95263 -0.08733
C 0.78043 1.33799 -0.22843
N 0.77132 2.68205 -0.42597
C 2.07989 3.15868 -0.41105
C 2.90788 2.07143 -0.20139
N 1.60764 -1.01688 1.44185
C 0.30973 -0.59378 1.57374
N -0.16985 -1.13427 2.72368
C 0.76304 -2.03105 3.23582
C 1.87726 -1.97134 2.41686
Co -0.53013 -0.05542 -0.11886
O -1.75662 -1.31824 0.02783
C -1.03465 -1.80172 -3.33121
C -0.58422 -1.95953 -4.79392
C -2.02441 -2.89350 -2.90153
C -1.65406 -0.40886 -3.17224
C -0.45404 3.54343 -0.62759
C -0.52747 4.55624 0.52632

C	-0.34592	4.22765	-2.00002
C	-1.70229	2.65976	-0.60518
C	-1.49550	-0.79470	3.38088
C	-2.07695	0.46488	2.72996
C	-2.43579	-1.99137	3.18839
C	-1.23232	-0.48973	4.86632
H	-1.45557	-1.79061	-5.44560
H	0.18693	-1.21420	-5.04965
H	-1.60934	-3.90190	-3.06161
H	-2.94582	-2.80963	-3.49985
H	-2.26336	-2.76077	-1.83518
H	-0.92244	0.38688	-3.38394
H	-2.06195	-0.27276	-2.16520
H	-2.48645	-0.31598	-3.88644
H	0.32605	5.25067	0.53290
H	-0.56738	4.03307	1.49576
H	-1.44349	5.15801	0.41792
H	0.51305	4.91163	-2.06574
H	-1.25549	4.82322	-2.17546
H	-1.85388	2.17438	0.37115
H	-2.58304	3.29561	-0.78085
H	-1.68355	1.90819	-1.41033
H	-2.96688	0.76670	3.30132
H	-1.35302	1.29551	2.74391
H	-3.41671	-1.75794	3.62993
H	-2.55827	-2.17702	2.11052
H	-0.49513	0.32285	4.97598
H	-0.88658	-1.36390	5.43504
H	-2.17767	-0.16101	5.32510
H	-0.20091	-2.96305	-5.02389
H	-2.04675	-2.89788	3.68024
H	-0.26291	3.47479	-2.80091
C	4.70444	-0.91193	-0.80213
C	6.09390	-1.01365	-0.72828
C	6.72833	-0.86537	0.52659
C	5.92209	-0.58325	1.65374
C	4.53795	-0.50537	1.49625
H	4.19861	-0.96184	-1.76682
H	3.89911	-0.24226	2.34048
H	-2.40096	0.26842	1.70164
H	-3.04608	-0.93084	-0.30694
C	-4.22822	-0.76238	-0.61039
C	-5.04012	-1.61199	0.36757
C	-4.47056	0.68375	-0.55555
H	-4.23531	-1.17109	-1.63275
C	-5.40602	-0.88623	1.63273
H	-4.49882	-2.54745	0.60038
H	-5.98412	-1.94973	-0.11767
C	-4.98621	1.27185	0.56005
H	-4.15489	1.30009	-1.40451
C	-5.39143	0.46514	1.70382
H	-5.74641	-1.48146	2.48773
H	-5.09788	2.36013	0.61262
H	-5.70272	0.97392	2.62269
N	3.94581	-0.71007	0.29797
C	2.50356	4.50268	-0.57285
N	2.89133	5.59258	-0.69761
C	4.32214	2.11520	-0.12826
N	5.48434	2.14902	-0.06982

```
C          3.27722       -3.37210       -1.27407
N          4.21602       -3.99491       -0.97932
C          1.11380       -4.07631       -3.32356
N          1.12088       -5.06220       -3.94142
C          3.04551       -2.76920        2.50060
N          4.01349       -3.41483        2.54878
C          0.60264       -2.91184        4.33686
N          0.51375       -3.67290        5.21248
C          8.14820       -0.96919        0.64754
N          9.30274       -1.05373        0.74572
C          6.49357       -0.36498        2.94796
N          6.95069       -0.18835        4.00071
C          6.84147       -1.25647       -1.92472
N          7.44099       -1.45709       -2.89878
```

$L_4Co^{III}O$ + CHD (*S*=2)

```
97
chd_ts_u4.out     Energy: -2473981.7679737
C          0.51022       -1.22864       -1.30077
N          0.12475       -2.32619       -2.00011
C          1.10120       -3.31002       -1.90520
C          2.14168       -2.77035       -1.16882
N          1.79191       -1.45324       -0.87623
B          2.41026       -0.46823        0.16306
N          2.05739        1.02967       -0.16520
C          0.77850        1.51196       -0.03315
N          0.80112        2.82741       -0.34480
C          2.08187        3.19216       -0.73945
C          2.87329        2.06392       -0.63586
N          1.80237       -0.93668        1.52912
C          0.44600       -0.82095        1.69175
N          0.13400       -1.40765        2.87683
C          1.27660       -1.96540        3.43853
C          2.32587       -1.68949        2.57810
Co        -0.58671       -0.00471        0.02099
O         -2.31550       -0.18248        0.24190
C         -1.22047       -2.44445       -2.69901
C         -1.08275       -3.33410       -3.94305
C         -2.20993       -3.03764       -1.68623
C         -1.64811       -1.03938       -3.14703
C         -0.37518        3.78277       -0.26003
C          0.02343        4.95144        0.65760
C         -0.71361        4.24821       -1.68445
C         -1.57640        3.06130        0.34939
C         -1.29090       -1.44145        3.42370
C         -1.82297        0.00048        3.41864
C         -2.10962       -2.36243        2.50822
C         -1.31347       -1.97738        4.85801
H         -2.00973       -3.24455       -4.52978
H         -0.24458       -3.00951       -4.58160
H         -1.85418       -4.01102       -1.30924
H         -3.18276       -3.19978       -2.17745
H         -2.34996       -2.34206       -0.84358
H         -0.87772       -0.57490       -3.78309
H         -1.85509       -0.38227       -2.29404
H         -2.57547       -1.12746       -3.73351
H          0.85093        5.55298        0.25489
```

H	0.30543	4.58032	1.65644
H	-0.84262	5.62203	0.77003
H	0.11376	4.80205	-2.15455
H	-1.58504	4.92070	-1.64498
H	-1.34433	2.63817	1.33851
H	-2.38726	3.79549	0.47151
H	-1.94774	2.25372	-0.29365
H	-2.82688	0.00629	3.87248
H	-1.16930	0.65872	4.01456
H	-3.13890	-2.42868	2.89664
H	-2.15797	-1.95269	1.48916
H	-0.68466	-1.38244	5.53956
H	-1.02566	-3.03694	4.91912
H	-2.35066	-1.90457	5.21963
H	-0.96220	-4.39773	-3.69880
H	-1.67926	-3.37762	2.49091
H	-0.97009	3.38443	-2.31957
C	4.71809	-0.96375	-0.87273
C	6.11376	-0.97217	-0.86769
C	6.80100	-0.46413	0.25822
C	6.03760	0.05567	1.32921
C	4.64582	0.01198	1.25324
H	4.17000	-1.27275	-1.76216
H	4.03225	0.43126	2.05328
H	-1.91989	0.39058	2.39642
H	-3.30913	0.43856	-0.62875
C	-4.19726	0.86785	-1.31559
C	-5.03875	-0.34876	-1.69929
C	-4.88685	1.83380	-0.44092
H	-3.69179	1.33138	-2.17772
C	-5.91247	-0.82255	-0.56958
H	-4.39196	-1.16495	-2.05876
H	-5.69684	-0.09897	-2.56344
C	-5.86971	1.41856	0.40664
H	-4.53485	2.87056	-0.40849
C	-6.30697	0.02823	0.40812
H	-6.27956	-1.85527	-0.58958
H	-6.33193	2.12043	1.10921
H	-6.98444	-0.31107	1.19949
N	4.00609	-0.52190	0.18632
C	2.51596	4.46220	-1.20172
N	2.91061	5.48219	-1.59816
C	4.24655	2.03569	-0.98588
N	5.37056	2.04902	-1.28838
C	3.29831	-3.45166	-0.71432
N	4.24469	-3.99736	-0.31107
C	1.06886	-4.64720	-2.38196
N	1.11037	-5.76093	-2.71472
C	3.65392	-2.16039	2.72893
N	4.74248	-2.55459	2.85437
C	1.43888	-2.71194	4.63674
N	1.68182	-3.33475	5.58851
C	8.22886	-0.44769	0.30088
N	9.39005	-0.43282	0.33509
C	6.65994	0.62297	2.48657
N	7.15927	1.08129	3.42945
C	6.81428	-1.47018	-2.01217
N	7.37660	-1.87749	-2.94296

$L_4Co^{III}O$ + DHA (*S*=0, closed-shell)

```
109
dha_ts_u0_closed.out      Energy: -2666775.9590959
C          0.72574       -1.08055       -1.32129
N          0.37251       -1.90220       -2.35530
C          1.41482       -2.78930       -2.60154
C          2.45563       -2.44766       -1.75696
N          2.03786       -1.34172       -1.03025
B          2.61653       -0.60350        0.20319
N          2.26206        0.90926        0.09756
C          0.95141        1.23654       -0.08559
N          0.86724        2.59356       -0.14114
C          2.14177        3.13089        0.02567
C          3.01946        2.07294        0.17347
N          1.83689       -1.22497        1.40449
C          0.52094       -0.87636        1.53940
N          0.06054       -1.48564        2.67048
C          1.02731       -2.37986        3.12230
C          2.14056       -2.22561        2.31592
Co        -0.34258       -0.15522       -0.05138
O         -1.93420       -0.75438        0.20292
C         -0.95396       -1.86783       -3.10133
C         -0.74093       -2.28435       -4.56569
C         -1.90902       -2.83179       -2.38672
C         -1.46420       -0.42103       -3.10066
C         -0.38090        3.43346       -0.34620
C         -0.59153        4.28653        0.91498
C         -0.17988        4.28779       -1.60899
C         -1.59592        2.52821       -0.55124
C         -1.23437       -1.17318        3.42499
C         -1.67851        0.25750        3.09356
C         -2.27911       -2.21191        3.00990
C         -0.95090       -1.22775        4.93759
H         -1.67202       -2.06900       -5.11173
H          0.07224       -1.70956       -5.03906
H         -1.49861       -3.85536       -2.38969
H         -2.87688       -2.84489       -2.90929
H         -2.07563       -2.50792       -1.34877
H         -0.69539        0.27170       -3.47833
H         -1.79085       -0.09987       -2.10579
H         -2.34186       -0.36288       -3.75882
H          0.23072        4.99667        1.08862
H         -0.69805        3.64109        1.80226
H         -1.51653        4.87287        0.79896
H          0.64935        5.00354       -1.51445
H         -1.09610        4.87010       -1.79317
H         -1.83463        1.93318        0.34111
H         -2.46832        3.16917       -0.75280
H         -1.47102        1.86767       -1.42151
H         -2.53338        0.50567        3.74012
H         -0.86766        0.97915        3.28924
H         -3.22384       -2.00717        3.53606
H         -2.45678       -2.13476        1.92757
H         -0.08735       -0.59812        5.20917
H         -0.79271       -2.24450        5.31868
H         -1.83613       -0.83039        5.45688
H         -0.54686       -3.35758       -4.68555
```

H	-1.94918	-3.23216	3.26846
H	0.00423	3.64377	-2.48441
C	4.94067	-0.67588	-0.80190
C	6.33038	-0.68812	-0.75389
C	6.98293	-0.69757	0.50657
C	6.17310	-0.65852	1.67021
C	4.78793	-0.64499	1.53907
H	4.42154	-0.60804	-1.75843
H	4.15246	-0.54697	2.41908
H	-2.01549	0.34651	2.05776
N	4.18308	-0.70122	0.32489
C	2.50077	4.50328	0.05572
N	2.84509	5.61386	0.09402
C	4.41858	2.18550	0.36775
N	5.56647	2.28914	0.52979
C	3.68226	-3.13917	-1.59747
N	4.69091	-3.70079	-1.44722
C	1.44165	-3.90893	-3.47413
N	1.54917	-4.86266	-4.13125
C	3.32422	-3.00558	2.33454
N	4.29603	-3.64649	2.32556
C	0.89968	-3.37773	4.12429
N	0.86531	-4.24800	4.89549
C	8.40468	-0.71030	0.59764
N	9.56544	-0.71925	0.67091
C	6.74823	-0.61428	2.98024
N	7.20913	-0.58091	4.04579
C	7.07104	-0.67563	-1.97892
N	7.66732	-0.66896	-2.97564
H	-2.98396	-0.50741	-0.34969
C	-4.26116	-0.13855	-0.69196
C	-4.80148	-1.14666	-1.60947
C	-4.79103	-0.13286	0.67767
H	-4.09166	0.85415	-1.13359
C	-5.22743	-2.39039	-1.07778
C	-4.90415	-0.92315	-2.99849
C	-5.24267	-1.35695	1.23318
C	-4.80812	1.03297	1.47016
C	-5.71229	-3.37911	-1.94046
C	-5.09558	-2.61668	0.41049
C	-5.38554	-1.91913	-3.85017
H	-4.61014	0.05038	-3.40428
C	-5.73660	-1.37622	2.54130
C	-5.28833	0.99682	2.78016
H	-4.44379	1.97346	1.04299
C	-5.78375	-3.15616	-3.32246
H	-6.03894	-4.33969	-1.52650
H	-5.79145	-3.39967	0.75486
H	-4.07549	-3.01632	0.60160
H	-5.45683	-1.73103	-4.92631
H	-6.09402	-2.32080	2.96643
C	-5.76099	-0.20924	3.31772
H	-5.30006	1.90986	3.38418
H	-6.16152	-3.94185	-3.98438
H	-6.14626	-0.24232	4.34181

$L_4Co^{III}O$ + DHA (*S*=0, open-shell)

```
109
dha_ts_u0_open.out        Energy: -2666781.0328174
C          0.58148       -1.26096       -1.33938
N          0.27340       -2.23583       -2.23721
C          1.27782       -3.19841       -2.23644
C          2.27110       -2.74951       -1.38397
N          1.85738       -1.51211       -0.90500
B          2.43195       -0.54613        0.17324
N          2.10696        0.92383       -0.21273
C          0.78836        1.24280       -0.36452
N          0.71782        2.55089       -0.72198
C          2.00646        3.07398       -0.79669
C          2.88154        2.05083       -0.47761
N          1.67907       -0.91515        1.48093
C          0.35961       -0.54399        1.57106
N         -0.09956       -1.01675        2.76337
C          0.86499       -1.83871        3.33609
C          1.98047       -1.78763        2.51972
Co        -0.50235       -0.11897       -0.10353
O         -1.91107       -1.18916       -0.10385
C         -0.93548       -2.25095       -3.16182
C         -0.46721       -2.64618       -4.57390
C         -1.95171       -3.24670       -2.59180
C         -1.52543       -0.83880       -3.23974
C         -0.55250        3.32123       -1.00493
C         -0.65177        4.47609        0.00414
C         -0.50358        3.81703       -2.45900
C         -1.75676        2.39007       -0.83096
C         -1.43878       -0.67915        3.39275
C         -1.96752        0.60933        2.75314
C         -2.37879       -1.86543        3.15027
C         -1.23199       -0.40399        4.89248
H         -1.32007       -2.52939       -5.26015
H          0.34521       -1.98655       -4.92139
H         -1.53825       -4.26848       -2.55776
H         -2.84913       -3.25713       -3.22911
H         -2.24578       -2.92694       -1.58047
H         -0.76106       -0.09921       -3.52937
H         -1.98533       -0.55351       -2.28795
H         -2.31982       -0.84163       -4.00020
H          0.17046        5.19944       -0.10263
H         -0.65196        4.08817        1.03603
H         -1.59478        5.01963       -0.16382
H          0.32112        4.52340       -2.63593
H         -1.44371        4.34191       -2.69033
H         -1.84245        2.01908        0.20234
H         -2.67347        2.96330       -1.03933
H         -1.73719        1.55239       -1.54611
H         -2.85969        0.92859        3.30875
H         -1.21843        1.41591        2.79766
H         -3.37082       -1.64465        3.57165
H         -2.48170       -2.03599        2.06813
H         -0.47054        0.37716        5.05288
H         -0.95538       -1.29875        5.46519
H         -2.18634       -0.04357        5.30633
H         -0.13861       -3.69115       -4.65001
H         -1.99419       -2.77969        3.63208
H         -0.39927        2.96722       -3.15337
C          4.77797       -0.89680       -0.76484
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C          6.17067       -0.93313       -0.68827
C          6.79917       -0.65864        0.54794
C          5.98303       -0.32144        1.65274
C          4.59720       -0.31023        1.49379
H          4.27255       -1.04682       -1.71939
H          3.94818       -0.00517        2.31577
H         -2.27082        0.44912        1.71318
N          4.01337       -0.63439        0.31822
C          2.36965        4.40398       -1.12999
N          2.70422        5.48546       -1.39855
C          4.29346        2.15366       -0.42538
N          5.45407        2.23126       -0.37881
C          3.44891       -3.44060       -1.00476
N          4.42119       -3.99038       -0.67550
C          1.27608       -4.45959       -2.88781
N          1.32049       -5.51979       -3.36490
C          3.17816       -2.53185        2.65993
N          4.16977       -3.13536        2.75172
C          0.73547       -2.66677        4.48141
N          0.68610       -3.39362        5.38851
C          8.22237       -0.69288        0.67007
N          9.37957       -0.72041        0.76928
C          6.54530        0.01498        2.92550
N          6.99497        0.28635        3.96116
C          6.92913       -1.23463       -1.86413
N          7.53814       -1.48246       -2.82126
H         -3.12499       -0.63107        0.07663
C         -4.31844       -0.22608        0.03494
C         -4.76537       -0.86024       -1.23025
C         -5.00424       -0.72398        1.25115
H         -4.23562        0.87013       -0.01698
C         -5.11950       -2.22962       -1.19557
C         -4.81250       -0.16252       -2.44944
C         -5.34672       -2.09544        1.30737
C         -5.31328        0.11016        2.34002
C         -5.53303       -2.86287       -2.37238
C         -4.99369       -2.96390        0.12091
C         -5.21821       -0.80637       -3.62159
H         -4.52793        0.89502       -2.47334
C         -5.96822       -2.60420        2.45312
C         -5.93028       -0.40740        3.48235
H         -5.06890        1.17607        2.28366
C         -5.58150       -2.15953       -3.58371
H         -5.81319       -3.92168       -2.34426
H         -5.58683       -3.89277        0.11752
H         -3.93224       -3.27176        0.23012
H         -5.25515       -0.25291       -4.56548
H         -6.23283       -3.66658        2.49531
C         -6.25294       -1.77017        3.54288
H         -6.16439        0.25200        4.32429
H         -5.90492       -2.66811       -4.49764
H         -6.73644       -2.18215        4.43445
```

$L_4Co^{III}O$ + DHA (*S*=1)

```
109
dha_ts_u2.out     Energy: -2666783.2393980
C          0.55726       -1.17731       -1.36233
```

N	0.24121	-2.11867	-2.29088
C	1.22864	-3.09774	-2.31312
C	2.22159	-2.69311	-1.43835
N	1.82652	-1.46308	-0.92419
B	2.41583	-0.54770	0.18824
N	2.10615	0.93734	-0.14933
C	0.79213	1.26712	-0.30802
N	0.72746	2.59000	-0.60027
C	2.01734	3.11474	-0.62860
C	2.88603	2.07555	-0.34411
N	1.66695	-0.94803	1.49268
C	0.36015	-0.54524	1.61227
N	-0.09580	-1.03696	2.79491
C	0.85578	-1.89326	3.33854
C	1.96237	-1.84996	2.50889
Co	-0.50993	-0.09757	-0.10111
O	-1.83245	-1.26183	0.05966
C	-0.96824	-2.08505	-3.20721
C	-0.50675	-2.39588	-4.64194
C	-1.98320	-3.11014	-2.68915
C	-1.55425	-0.67024	-3.19708
C	-0.54456	3.36314	-0.85760
C	-0.65903	4.47572	0.19593
C	-0.49391	3.91759	-2.28983
C	-1.73716	2.40939	-0.72266
C	-1.41189	-0.67070	3.45648
C	-1.95587	0.60179	2.80048
C	-2.37729	-1.84706	3.27263
C	-1.14662	-0.36149	4.94045
H	-1.36863	-2.26505	-5.31446
H	0.28819	-1.70175	-4.96151
H	-1.57810	-4.13467	-2.73340
H	-2.89287	-3.07173	-3.30746
H	-2.25112	-2.86049	-1.65190
H	-0.78912	0.08535	-3.43691
H	-2.01297	-0.44213	-2.22886
H	-2.34762	-0.62171	-3.95574
H	0.15344	5.21348	0.11641
H	-0.65258	4.04823	1.21193
H	-1.60950	5.01250	0.04963
H	0.33005	4.63272	-2.43314
H	-1.43460	4.44905	-2.50312
H	-1.82743	2.00909	0.29992
H	-2.66298	2.96975	-0.92445
H	-1.69440	1.59534	-1.46467
H	-2.83719	0.93075	3.36832
H	-1.20822	1.41107	2.80807
H	-3.35844	-1.58759	3.69847
H	-2.50142	-2.04807	2.19826
H	-0.38110	0.42444	5.05087
H	-0.84165	-1.24263	5.52072
H	-2.08380	0.00618	5.38614
H	-0.15454	-3.42798	-4.77174
H	-2.00815	-2.75284	3.78156
H	-0.38364	3.09758	-3.01831
C	4.74999	-0.89059	-0.78131
C	6.14260	-0.94702	-0.71820
C	6.78460	-0.72798	0.52243
C	5.98189	-0.42270	1.64589

```
C          4.59486       -0.38748        1.49920
H          4.23529       -0.99987       -1.73656
H          3.95694       -0.10329        2.33715
H         -2.28233        0.40571        1.77338
N          3.99742       -0.66005        0.31765
C          2.38214        4.45842       -0.89843
N          2.71371        5.55210       -1.11653
C          4.29778        2.16663       -0.26946
N          5.45846        2.22979       -0.20602
C          3.38659       -3.41306       -1.07354
N          4.34894       -3.98685       -0.75617
C          1.21053       -4.33090       -3.01540
N          1.23677       -5.36857       -3.54093
C          3.14704       -2.61941        2.62124
N          4.12916       -3.24101        2.69234
C          0.71754       -2.73528        4.47259
N          0.65136       -3.46960        5.37261
C          8.20809       -0.78614        0.63156
N          9.36552       -0.83333        0.72020
C          6.55873       -0.14001        2.92528
N          7.02003        0.08813        3.96624
C          6.88706       -1.21497       -1.91115
N          7.48458       -1.43551       -2.88212
H         -3.04869       -0.76259       -0.12450
C         -4.24764       -0.36770       -0.28578
C         -4.74791       -1.17053       -1.42911
C         -4.91137       -0.66906        1.00675
H         -4.15278        0.70759       -0.50042
C         -5.11972       -2.51414       -1.18684
C         -4.85940       -0.64660       -2.72855
C         -5.28313       -2.00913        1.26763
C         -5.17628        0.32084        1.96873
C         -5.59444       -3.29924       -2.24290
C         -4.96127       -3.05024        0.21867
C         -5.32633       -1.44093       -3.77958
H         -4.57652        0.39558       -2.91111
C         -5.90877       -2.32810        2.47750
C         -5.79444       -0.00816        3.17838
H         -4.89384        1.35827        1.76042
C         -5.69440       -2.77144       -3.53749
H         -5.88700       -4.33776       -2.05259
H         -5.56042       -3.96315        0.36683
H         -3.89987       -3.34766        0.35047
H         -5.40942       -1.02127       -4.78732
H         -6.20064       -3.36537        2.67553
C         -6.16103       -1.33631        3.43522
H         -5.99622        0.77194        3.91953
H         -6.06494       -3.39743       -4.35557
H         -6.64909       -1.59984        4.37902
```

$L_4Co^{III}O$ + DHA (*S*=2)

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109
dha_ts_u4.out     Energy: -2666775.3845231
C          0.44316       -1.30565       -1.14159
N          0.05440       -2.42947       -1.79188
C          1.11725       -3.32059       -1.85001
C          2.19356       -2.70549       -1.22949
```

N	1.77116	-1.43454	-0.84183
B	2.39484	-0.37380	0.14460
N	2.16041	1.11666	-0.31432
C	0.90102	1.60957	-0.55586
N	1.02040	2.90971	-0.90187
C	2.35903	3.27883	-0.86305
C	3.07843	2.15848	-0.49463
N	1.68427	-0.67148	1.50178
C	0.40091	-0.22550	1.67820
N	-0.04723	-0.75482	2.84702
C	0.89489	-1.64597	3.34767
C	1.97711	-1.61643	2.48511
Co	-0.55281	0.24173	-0.18482
O	-2.25049	0.34716	0.15740
C	-1.38555	-2.64765	-2.24755
C	-1.47339	-3.81832	-3.23055
C	-2.22095	-2.93431	-0.99217
C	-1.86055	-1.36829	-2.94834
C	-0.11152	3.85341	-1.27400
C	-0.15550	4.97345	-0.22209
C	0.16255	4.39005	-2.68894
C	-1.44222	3.10187	-1.27103
C	-1.40277	-0.41370	3.46221
C	-1.69359	1.06677	3.17523
C	-2.44926	-1.33119	2.81747
C	-1.35690	-0.61763	4.98283
H	-2.50389	-3.84824	-3.61654
H	-0.79742	-3.68940	-4.09136
H	-1.84828	-3.82524	-0.46105
H	-3.26479	-3.11279	-1.29424
H	-2.20947	-2.06741	-0.31517
H	-1.18375	-1.09016	-3.77209
H	-1.94982	-0.52930	-2.24509
H	-2.86539	-1.54391	-3.35886
H	0.76509	5.57629	-0.20519
H	-0.32332	4.55132	0.78215
H	-0.99081	5.65144	-0.45747
H	1.08077	4.99223	-2.74996
H	-0.67490	5.03899	-2.98920
H	-1.70226	2.70791	-0.27939
H	-2.22946	3.81150	-1.56959
H	-1.44973	2.27170	-1.99381
H	-2.66260	1.32281	3.63298
H	-0.91496	1.71061	3.61683
H	-3.43557	-1.12370	3.26252
H	-2.51435	-1.12176	1.74000
H	-0.49489	-0.10439	5.44049
H	-1.34871	-1.67644	5.27487
H	-2.27236	-0.17651	5.40618
H	-1.28057	-4.78915	-2.75278
H	-2.20404	-2.39295	2.98669
H	0.23295	3.55951	-3.41025
C	4.68331	-0.79729	-0.88464
C	6.07181	-0.92890	-0.86702
C	6.76219	-0.76638	0.35591
C	6.01260	-0.43746	1.50904
C	4.62620	-0.31982	1.40674
H	4.13108	-0.87090	-1.82306
H	4.03271	-0.00536	2.26579

H	-1.77601	1.26008	2.09897
N	3.97777	-0.54180	0.24124
C	2.91403	4.55830	-1.12799
N	3.41180	5.59016	-1.32971
C	4.48749	2.16206	-0.34134
N	5.64447	2.21361	-0.22489
C	3.45383	-3.31086	-0.99482
N	4.48208	-3.82028	-0.79778
C	1.17494	-4.62984	-2.39878
N	1.32224	-5.70700	-2.81162
C	3.12352	-2.44682	2.54672
N	4.06605	-3.13059	2.57300
C	0.81427	-2.50256	4.47798
N	0.82813	-3.25317	5.36641
C	8.18320	-0.89957	0.41850
N	9.33893	-1.00665	0.46894
C	6.64372	-0.20783	2.77307
N	7.14940	-0.02317	3.80197
C	6.76261	-1.22189	-2.08562
N	7.31672	-1.46428	-3.07690
H	-3.33530	0.83466	-0.57488
C	-4.46179	1.18072	-0.89475
C	-4.97516	0.11613	-1.79112
C	-5.06999	1.24095	0.45956
H	-4.34585	2.16147	-1.38081
C	-5.42121	-1.09630	-1.21584
C	-4.98628	0.26269	-3.19032
C	-5.50968	0.03714	1.05535
C	-5.11328	2.43621	1.19980
C	-5.85315	-2.13447	-2.05223
C	-5.37226	-1.25778	0.28661
C	-5.41962	-0.77842	-4.01516
H	-4.64266	1.20519	-3.63072
C	-5.99750	0.05949	2.36875
C	-5.59173	2.44603	2.51238
H	-4.75902	3.36372	0.73620
C	-5.84895	-1.98524	-3.44510
H	-6.19873	-3.07407	-1.60642
H	-6.12106	-1.99440	0.62379
H	-4.38653	-1.69396	0.54854
H	-5.42160	-0.65163	-5.10257
H	-6.34277	-0.87329	2.82898
C	-6.03695	1.25311	3.09997
H	-5.62118	3.38287	3.07829
H	-6.18906	-2.80661	-4.08394
H	-6.41679	1.25306	4.12680

$L_4Co^{III}O$ + fluorene (*S*=0, closed-shell)

106
fluorene_ts_u0_closed.out Energy: -2642111.5257160

C	0.67670	-0.81460	-1.58031
N	0.34443	-1.46567	-2.73145
C	1.27662	-2.47334	-2.96353
C	2.24592	-2.37153	-1.98253
N	1.89870	-1.28781	-1.18626
B	2.44374	-0.70691	0.14270
N	2.27639	0.84112	0.11759

C	1.02549	1.34054	-0.11626
N	1.10776	2.69610	-0.05672
C	2.42356	3.06066	0.21893
C	3.15877	1.89537	0.32759
N	1.50453	-1.29585	1.24043
C	0.23661	-0.78417	1.28930
N	-0.39437	-1.35936	2.34936
C	0.41043	-2.38476	2.84130
C	1.59944	-2.35326	2.13492
Co	-0.39979	0.08243	-0.30948
O	-1.96995	-0.59352	-0.19831
C	-0.84479	-1.16832	-3.63050
C	-0.38543	-1.21330	-5.09804
C	-1.91470	-2.22304	-3.32491
C	-1.34884	0.25139	-3.34629
C	-0.02244	3.69063	-0.23600
C	-0.17534	4.47971	1.07497
C	0.32146	4.59518	-1.43090
C	-1.32776	2.95293	-0.52901
C	-1.68603	-0.90042	3.03484
C	-2.05692	0.51668	2.57928
C	-2.78633	-1.90463	2.68252
C	-1.41379	-0.84017	4.55033
H	-1.22168	-0.87419	-5.72846
H	0.46758	-0.53547	-5.26544
H	-1.56294	-3.23671	-3.57684
H	-2.81738	-2.01907	-3.92185
H	-2.17981	-2.19050	-2.25829
H	-0.54086	0.99155	-3.46055
H	-1.79305	0.34090	-2.34746
H	-2.13899	0.49009	-4.07445
H	0.71528	5.07767	1.31844
H	-0.38514	3.79601	1.91376
H	-1.02313	5.17536	0.97520
H	1.22900	5.19400	-1.26525
H	-0.51034	5.29742	-1.59703
H	-1.65304	2.31320	0.30327
H	-2.11620	3.70708	-0.67169
H	-1.27194	2.36627	-1.45685
H	-2.86750	0.87870	3.22929
H	-1.20035	1.20473	2.67959
H	-3.73539	-1.57667	3.13348
H	-2.91614	-1.93884	1.59220
H	-0.55723	-0.18221	4.77197
H	-1.23929	-1.82284	5.00773
H	-2.30530	-0.41728	5.03793
H	-0.11737	-2.22079	-5.44097
H	-2.55722	-2.91362	3.06274
H	0.45474	3.99254	-2.34428
C	4.81984	-1.01414	-0.69255
C	6.19119	-1.21443	-0.54640
C	6.72878	-1.38309	0.75281
C	5.84509	-1.30185	1.85497
C	4.48547	-1.09710	1.62374
H	4.39190	-0.82019	-1.67682
H	3.79993	-0.96430	2.46050
H	-2.42426	0.53160	1.54887
N	3.98155	-1.00319	0.37137
C	2.94014	4.37377	0.36831

N	3.41161	5.42892	0.50151
C	4.54698	1.81888	0.60122
N	5.68714	1.75954	0.82761
C	3.34586	-3.24085	-1.77475
N	4.25273	-3.94462	-1.58075
C	1.22615	-3.49602	-3.94624
N	1.23270	-4.38210	-4.69994
C	2.67567	-3.27096	2.22869
N	3.56698	-4.01795	2.28256
C	0.06582	-3.37030	3.80323
N	-0.16432	-4.22895	4.55363
C	8.12711	-1.59506	0.94785
N	9.26540	-1.76703	1.10688
C	6.31558	-1.40963	3.20265
N	6.69005	-1.49899	4.29823
C	7.02311	-1.23320	-1.71157
N	7.69178	-1.25106	-2.66085
H	-2.99412	-0.63790	-0.80486
C	-4.29721	-0.59973	-1.28056
H	-4.19575	-0.39940	-2.35344
C	-4.84334	-1.86437	-0.76742
C	-4.73104	0.43265	-0.33343
C	-4.80877	-3.16555	-1.29011
C	-5.42930	-1.62966	0.51411
C	-4.51977	1.81764	-0.33607
C	-5.34105	-0.19552	0.79417
C	-5.34089	-4.21922	-0.53449
H	-4.37495	-3.35973	-2.27571
C	-5.94929	-2.68871	1.26444
C	-4.90447	2.56860	0.78209
H	-4.05508	2.30139	-1.20067
C	-5.71443	0.56058	1.90970
C	-5.90046	-3.98624	0.73462
H	-5.32121	-5.23725	-0.93749
H	-6.39143	-2.50912	2.25022
C	-5.49061	1.94562	1.89901
H	-4.74342	3.65184	0.78953
H	-6.17292	0.08098	2.78106
H	-6.30685	-4.82435	1.31003
H	-5.77731	2.54853	2.76675

$L_4Co^{III}O$ + fluorene (*S*=1)

106
fluorene_ts_u2.out Energy: -2642118.3366535

C	0.66769	-0.74976	-1.66203
N	0.35337	-1.44042	-2.78680
C	1.23687	-2.50576	-2.93598
C	2.16112	-2.41346	-1.91008
N	1.83986	-1.27245	-1.18238
B	2.39322	-0.67043	0.14191
N	2.25816	0.87909	0.09428
C	1.00831	1.40646	-0.08894
N	1.13287	2.75859	-0.08884
C	2.47148	3.09790	0.09183
C	3.17926	1.91681	0.20858
N	1.49091	-1.22321	1.28585
C	0.23071	-0.69240	1.38620

N	-0.38572	-1.31667	2.41999
C	0.42130	-2.35246	2.87988
C	1.59631	-2.30826	2.14971
Co	-0.42192	0.13081	-0.28443
O	-1.68218	-1.10614	-0.42547
C	-0.77223	-1.11057	-3.74843
C	-0.19342	-1.06545	-5.17336
C	-1.85293	-2.18865	-3.58766
C	-1.33364	0.27698	-3.41771
C	0.01621	3.76377	-0.25643
C	-0.03682	4.64344	1.00378
C	0.28929	4.57965	-1.53022
C	-1.31415	3.02670	-0.40285
C	-1.73066	-0.94034	3.01646
C	-2.17714	0.40898	2.44835
C	-2.73232	-2.04165	2.65016
C	-1.55575	-0.78934	4.53778
H	-0.99359	-0.75876	-5.86482
H	0.62348	-0.32823	-5.24116
H	-1.49141	-3.18074	-3.90217
H	-2.72382	-1.93405	-4.21239
H	-2.15875	-2.23152	-2.53218
H	-0.54413	1.04522	-3.42042
H	-1.84520	0.28278	-2.44800
H	-2.07500	0.54006	-4.18760
H	0.87712	5.23886	1.14507
H	-0.19922	4.02291	1.90030
H	-0.87810	5.34812	0.91213
H	1.21764	5.16656	-1.46563
H	-0.53938	5.28798	-1.68642
H	-1.56246	2.43790	0.49270
H	-2.11043	3.77730	-0.51788
H	-1.34154	2.39247	-1.30319
H	-3.11153	0.70527	2.94767
H	-1.42195	1.19131	2.62599
H	-3.72776	-1.77101	3.03267
H	-2.79057	-2.13371	1.55601
H	-0.77861	-0.04307	4.77163
H	-1.30690	-1.73353	5.04206
H	-2.50928	-0.43800	4.96185
H	0.17639	-2.03997	-5.52102
H	-2.45311	-3.01372	3.08755
H	0.34940	3.91500	-2.40762
C	4.76448	-1.07253	-0.71181
C	6.13492	-1.28864	-0.56664
C	6.67995	-1.40225	0.73360
C	5.80881	-1.25507	1.83746
C	4.45108	-1.03224	1.60627
H	4.33068	-0.92932	-1.70210
H	3.77246	-0.84956	2.43982
H	-2.39798	0.33760	1.37737
N	3.93914	-0.98719	0.35630
C	3.02691	4.40219	0.14439
N	3.52475	5.45270	0.19147
C	4.57902	1.81714	0.40413
N	5.72968	1.74244	0.56331
C	3.19980	-3.32861	-1.60538
N	4.05557	-4.06885	-1.33058
C	1.18186	-3.54331	-3.90243

N	1.16610	-4.42812	-4.65770
C	2.67694	-3.22288	2.21409
N	3.57397	-3.96456	2.24803
C	0.10052	-3.32579	3.86153
N	-0.12132	-4.16007	4.64145
C	8.07773	-1.62635	0.92717
N	9.21453	-1.80685	1.08479
C	6.28796	-1.31265	3.18512
N	6.66915	-1.36141	4.28090
C	6.95674	-1.37448	-1.73582
N	7.61700	-1.44431	-2.68850
H	-2.89330	-0.81857	-0.73441
C	-4.14137	-0.65289	-1.02779
H	-4.09214	-0.45167	-2.10721
C	-4.75070	-1.91270	-0.54370
C	-4.64751	0.39259	-0.11214
C	-4.65843	-3.21658	-1.04338
C	-5.45234	-1.65900	0.66874
C	-4.45069	1.77569	-0.12297
C	-5.37741	-0.22002	0.94491
C	-5.26820	-4.26122	-0.33352
H	-4.11813	-3.42001	-1.97298
C	-6.05487	-2.70494	1.37352
C	-4.95434	2.54436	0.93669
H	-3.91213	2.24815	-0.94901
C	-5.87419	0.54958	2.00127
C	-5.95704	-4.00875	0.86509
H	-5.20663	-5.28501	-0.71661
H	-6.59345	-2.51288	2.30736
C	-5.65147	1.93548	1.99391
H	-4.80255	3.62874	0.94097
H	-6.42968	0.08199	2.82087
H	-6.42384	-4.83832	1.40598
H	-6.03264	2.54999	2.81588

$L_4Co^{III}O$ + fluorene (*S*=2)

106

fluorene_ts_u4.out	Energy: -2642110.2760622		
C	0.68186	-0.72986	-1.66122
N	0.37884	-1.40165	-2.79417
C	1.28137	-2.45166	-2.94685
C	2.18234	-2.36679	-1.89875
N	1.83003	-1.25030	-1.15511
B	2.41887	-0.67985	0.18811
N	2.23390	0.88972	0.15481
C	1.01141	1.44000	-0.04772
N	1.14208	2.78655	-0.06706
C	2.48236	3.10242	0.13956
C	3.16665	1.90641	0.27745
N	1.46108	-1.23522	1.30154
C	0.21494	-0.70566	1.43405
N	-0.41198	-1.35213	2.44198
C	0.40018	-2.39746	2.87502
C	1.57078	-2.33604	2.13858
Co	-0.47651	0.17523	-0.24726
O	-1.65470	-1.06105	-0.37139

C	-0.75468	-1.09173	-3.75723
C	-0.17861	-1.02953	-5.18227
C	-1.80916	-2.19652	-3.59990
C	-1.34476	0.28266	-3.42732
C	0.05727	3.81920	-0.30424
C	-0.02608	4.72511	0.93507
C	0.41529	4.59667	-1.58169
C	-1.28635	3.12101	-0.50139
C	-1.75940	-1.00372	3.05755
C	-2.24449	0.34078	2.51134
C	-2.74501	-2.12288	2.69819
C	-1.56268	-0.86069	4.57707
H	-0.98641	-0.73483	-5.86987
H	0.62338	-0.27636	-5.24725
H	-1.42304	-3.17873	-3.91440
H	-2.68369	-1.96175	-4.22685
H	-2.12821	-2.26429	-2.54900
H	-0.57090	1.06665	-3.42535
H	-1.87237	0.28700	-2.46590
H	-2.08666	0.53484	-4.19970
H	0.89538	5.30129	1.10234
H	-0.24202	4.12858	1.83641
H	-0.84476	5.44739	0.79144
H	1.35819	5.15467	-1.48755
H	-0.38149	5.32833	-1.78708
H	-1.62330	2.60174	0.40667
H	-2.04505	3.89129	-0.70795
H	-1.28623	2.45031	-1.37422
H	-3.14932	0.63330	3.06381
H	-1.48965	1.13210	2.64507
H	-3.74182	-1.86563	3.08639
H	-2.81638	-2.23113	1.60558
H	-0.80993	-0.08789	4.80274
H	-1.26841	-1.79904	5.06679
H	-2.52088	-0.55033	5.02176
H	0.20835	-1.99485	-5.53501
H	-2.45166	-3.08949	3.13642
H	0.49147	3.91211	-2.44222
C	4.76757	-1.02697	-0.68419
C	6.10860	-1.27030	-0.53696
C	6.68497	-1.48007	0.77232
C	5.77467	-1.30409	1.88289
C	4.44302	-1.05830	1.66883
H	4.35071	-0.80887	-1.66774
H	3.77637	-0.86091	2.50822
H	-2.53720	0.27374	1.45732
N	3.88941	-1.00660	0.39507
C	3.05701	4.39798	0.20180
N	3.57284	5.43887	0.25999
C	4.56282	1.80089	0.50947
N	5.70958	1.79378	0.70174
C	3.20846	-3.29846	-1.59131
N	4.01906	-4.09633	-1.34885
C	1.25522	-3.47061	-3.93396
N	1.26281	-4.34272	-4.70357
C	2.63469	-3.27520	2.16861
N	3.47591	-4.07792	2.19381
C	0.08124	-3.39070	3.83695
N	-0.13956	-4.24151	4.59872

```
C          8.04809       -1.77269        0.95561
N          9.18269       -2.01697        1.10750
C          6.24791       -1.35863        3.23248
N          6.63392       -1.40810        4.32856
C          6.92876       -1.28880       -1.71010
N          7.59541       -1.30795       -2.66296
H         -2.96801       -0.80226       -0.79712
C         -4.16170       -0.68690       -1.06596
H         -4.13924       -0.51314       -2.15257
C         -4.76314       -1.93673       -0.54240
C         -4.65794        0.38568       -0.16833
C         -4.66421       -3.25078       -1.01312
C         -5.46538       -1.64925        0.66098
C         -4.43637        1.76393       -0.20917
C         -5.38888       -0.20033        0.90062
C         -5.27627       -4.27810       -0.27998
H         -4.11905       -3.47487       -1.93498
C         -6.07242       -2.67421        1.38561
C         -4.93337        2.56053        0.83432
H         -3.88518        2.21189       -1.04055
C         -5.88287        0.59483        1.93521
C         -5.96958       -3.99270        0.90677
H         -5.21228       -5.31105       -0.63530
H         -6.61904       -2.46200        2.30973
C         -5.64267        1.98030        1.89703
H         -4.76580        3.64191        0.81965
H         -6.44599        0.15324        2.76329
H         -6.43868       -4.80760        1.46700
H         -6.01962        2.61495        2.70516
```

$L_4Co^{III}O$ + MeCN (*S*=0, open-shell)

```
89
mecn_percn_u0_open.out    Energy: -2410837.3826015
C          0.85223       -0.87891       -1.59140
N          0.56495       -1.60754       -2.70165
C          1.47270       -2.65716       -2.81168
C          2.38628       -2.51443       -1.78277
N          2.03293       -1.36220       -1.08917
B          2.56083       -0.72509        0.22890
N          2.39723        0.82033        0.15362
C          1.14028        1.31203       -0.06451
N          1.22401        2.66738       -0.06900
C          2.54672        3.04505        0.14877
C          3.28505        1.88465        0.28857
N          1.65121       -1.28241        1.36632
C          0.37926       -0.77853        1.43620
N         -0.24683       -1.41317        2.45919
C          0.57242       -2.42939        2.94094
C          1.76255       -2.36051        2.23767
Co        -0.25603        0.03560       -0.25814
O         -1.60287       -1.17541       -0.38988
C         -0.53922       -1.31807       -3.70297
C          0.06897       -1.34052       -5.11646
C         -1.63280       -2.37951       -3.52049
C         -1.09471        0.08659       -3.44846
C          0.07771        3.63416       -0.26853
C         -0.05622        4.49279        0.99930
```

C	0.36762	4.47819	-1.51999
C	-1.21362	2.84305	-0.48333
C	-1.61294	-1.06055	3.02689
C	-2.03863	0.31092	2.49386
C	-2.59926	-2.15335	2.59368
C	-1.49039	-0.95786	4.55734
H	-0.70949	-1.03723	-5.83362
H	0.90655	-0.62801	-5.19481
H	-1.25996	-3.39098	-3.74913
H	-2.46773	-2.16515	-4.20664
H	-1.99484	-2.35183	-2.48149
H	-0.30155	0.85020	-3.48277
H	-1.60915	0.13893	-2.48352
H	-1.83255	0.31489	-4.23240
H	0.83224	5.11508	1.18283
H	-0.23156	3.85523	1.88118
H	-0.91622	5.17077	0.88331
H	1.26473	5.10494	-1.40858
H	-0.48462	5.15140	-1.70233
H	-1.46751	2.22936	0.39518
H	-2.04253	3.55369	-0.62341
H	-1.16255	2.22788	-1.39513
H	-2.98954	0.58809	2.97202
H	-1.28809	1.08393	2.72416
H	-3.61368	-1.88296	2.92581
H	-2.59782	-2.22856	1.49600
H	-0.71390	-0.22893	4.84238
H	-1.27279	-1.91976	5.04117
H	-2.45464	-0.60773	4.95725
H	0.41714	-2.33623	-5.42300
H	-2.33896	-3.13042	3.03242
H	0.49409	3.82952	-2.40225
C	4.95388	-1.09055	-0.57815
C	6.32605	-1.27252	-0.40428
C	6.84933	-1.35361	0.90734
C	5.95538	-1.20838	1.99308
C	4.59740	-1.02122	1.73371
H	4.53457	-0.97640	-1.57849
H	3.89890	-0.84170	2.55158
H	-2.21838	0.27698	1.41401
N	4.10795	-1.00673	0.47377
C	3.05895	4.36611	0.21837
N	3.51904	5.43268	0.28369
C	4.68195	1.82086	0.51685
N	5.83007	1.77172	0.70184
C	3.44144	-3.39807	-1.44363
N	4.31024	-4.11182	-1.14145
C	1.44536	-3.72952	-3.74081
N	1.45468	-4.64412	-4.45974
C	2.86186	-3.25049	2.33039
N	3.77356	-3.97237	2.38816
C	0.25063	-3.41352	3.91169
N	0.03252	-4.25980	4.67954
C	8.24767	-1.54550	1.12876
N	9.38494	-1.70034	1.30870
C	6.41159	-1.23117	3.34965
N	6.77441	-1.25095	4.45255
C	7.17248	-1.35753	-1.55576
N	7.85321	-1.42643	-2.49399

H	-2.68104	-0.73592	-0.68363
C	-3.84159	-0.17958	-1.04177
H	-4.18586	-0.82210	-1.86461
H	-3.60374	0.84391	-1.36448
C	-4.65243	-0.23714	0.13077
N	-5.25455	-0.29998	1.12899

$L_4Co^{III}O$ + MeCN (*S*=1)

89

mecn_percn_u2.out Energy: -2410840.1719752

C	0.86386	-0.87210	-1.61258
N	0.57575	-1.59835	-2.72210
C	1.47876	-2.65249	-2.82907
C	2.38728	-2.51654	-1.79452
N	2.03680	-1.36255	-1.10177
B	2.56121	-0.72756	0.22001
N	2.40023	0.81818	0.14447
C	1.14388	1.31068	-0.06498
N	1.22618	2.66479	-0.07327
C	2.55086	3.04272	0.13316
C	3.28982	1.88241	0.26994
N	1.64550	-1.27726	1.35641
C	0.37494	-0.76878	1.43060
N	-0.24975	-1.39678	2.45731
C	0.56718	-2.41487	2.93882
C	1.75477	-2.35312	2.23101
Co	-0.26003	0.02944	-0.26031
O	-1.56105	-1.18671	-0.43402
C	-0.52901	-1.30689	-3.72341
C	0.08582	-1.31249	-5.13414
C	-1.61539	-2.37788	-3.55390
C	-1.09974	0.08983	-3.45765
C	0.07654	3.62982	-0.26408
C	-0.04700	4.48989	1.00372
C	0.35345	4.47225	-1.51929
C	-1.21387	2.83384	-0.46503
C	-1.61832	-1.04568	3.01798
C	-2.04155	0.32401	2.47947
C	-2.59822	-2.14260	2.58119
C	-1.50469	-0.93905	4.54864
H	-0.69338	-1.01694	-5.85368
H	0.91325	-0.58738	-5.20417
H	-1.23588	-3.38544	-3.78830
H	-2.44833	-2.16338	-4.24237
H	-1.98355	-2.35925	-2.51675
H	-0.31310	0.86095	-3.47341
H	-1.62688	0.12443	-2.49818
H	-1.82872	0.32095	-4.24903
H	0.84244	5.11339	1.17820
H	-0.21373	3.85369	1.88822
H	-0.90864	5.16682	0.89417
H	1.24927	5.10227	-1.41616
H	-0.50270	5.14210	-1.69554
H	-1.45231	2.21538	0.41447
H	-2.04877	3.54021	-0.58969
H	-1.17446	2.22418	-1.38138

H	-2.99942	0.59830	2.94482
H	-1.29560	1.09876	2.71839
H	-3.61607	-1.87336	2.90245
H	-2.58593	-2.22323	1.48402
H	-0.73133	-0.20798	4.83664
H	-1.28805	-1.89956	5.03561
H	-2.47206	-0.59008	4.94197
H	0.45065	-2.30132	-5.44405
H	-2.33803	-3.11702	3.02576
H	0.47479	3.82251	-2.40145
C	4.95700	-1.10776	-0.57408
C	6.32779	-1.29204	-0.39149
C	6.84438	-1.36246	0.92330
C	5.94527	-1.20587	2.00325
C	4.58917	-1.01785	1.73547
H	4.54382	-1.00023	-1.57761
H	3.88690	-0.83091	2.54848
H	-2.20928	0.29269	1.39745
N	4.10595	-1.01240	0.47276
C	3.06265	4.36430	0.19560
N	3.52232	5.43136	0.25457
C	4.68804	1.81629	0.48956
N	5.83689	1.76399	0.66875
C	3.43535	-3.40650	-1.44983
N	4.29783	-4.12547	-1.14206
C	1.45256	-3.72100	-3.76278
N	1.46237	-4.63173	-4.48655
C	2.85161	-3.24608	2.32381
N	3.76111	-3.97063	2.38210
C	0.24579	-3.39332	3.91538
N	0.02898	-4.23541	4.68814
C	8.24116	-1.55535	1.15329
N	9.37718	-1.71105	1.34029
C	6.39445	-1.21843	3.36231
N	6.75156	-1.22999	4.46718
C	7.17998	-1.38967	-1.53763
N	7.86556	-1.46898	-2.47149
H	-2.63039	-0.77455	-0.64204
C	-3.86377	-0.20705	-0.94691
H	-4.20358	-0.85657	-1.76604
H	-3.62979	0.81675	-1.27171
C	-4.65811	-0.27275	0.23096
N	-5.25347	-0.33947	1.23451

$L_4Co^{III}O$ + MeCN (*S*=2)

89
mecn_percn_u4.out Energy: -2410824.4970146

C	0.85644	-0.85070	-1.58949
N	0.57467	-1.54471	-2.71485
C	1.49352	-2.58532	-2.83565
C	2.38142	-2.46866	-1.77974
N	2.00472	-1.34460	-1.06055
B	2.57653	-0.73966	0.27435
N	2.36545	0.82559	0.20074
C	1.13923	1.34505	-0.03847
N	1.23715	2.69498	-0.08071

C	2.56542	3.04179	0.14685
C	3.27214	1.86344	0.32548
N	1.61425	-1.28146	1.38967
C	0.35930	-0.76870	1.49942
N	-0.26912	-1.40793	2.51112
C	0.55498	-2.43123	2.97247
C	1.73272	-2.36351	2.24839
Co	-0.33163	0.07669	-0.22545
O	-1.54187	-1.16540	-0.38508
C	-0.52950	-1.25403	-3.72193
C	0.09930	-1.21132	-5.12572
C	-1.58741	-2.35796	-3.58918
C	-1.13540	0.12301	-3.43699
C	0.13766	3.70498	-0.36020
C	0.02414	4.64353	0.85182
C	0.50085	4.45063	-1.65481
C	-1.19007	2.97640	-0.55318
C	-1.63687	-1.08433	3.09779
C	-2.13049	0.25258	2.54007
C	-2.58899	-2.22585	2.71532
C	-1.48040	-0.93457	4.62091
H	-0.68124	-0.91968	-5.84521
H	0.90770	-0.46363	-5.17006
H	-1.18118	-3.34803	-3.84884
H	-2.42159	-2.14554	-4.27625
H	-1.97195	-2.39382	-2.55804
H	-0.36780	0.91313	-3.43741
H	-1.68122	0.14252	-2.48622
H	-1.86404	0.35121	-4.22893
H	0.92935	5.24741	1.00818
H	-0.18480	4.06892	1.76878
H	-0.81058	5.34082	0.68021
H	1.43539	5.02318	-1.56520
H	-0.30289	5.16591	-1.88865
H	-1.52868	2.48786	0.37262
H	-1.96190	3.71983	-0.80485
H	-1.15557	2.27983	-1.40498
H	-3.05106	0.53078	3.07356
H	-1.38910	1.05473	2.68389
H	-3.60864	-1.97696	3.04675
H	-2.60309	-2.35592	1.62221
H	-0.74976	-0.14601	4.86376
H	-1.18035	-1.86571	5.12005
H	-2.45598	-0.64406	5.04038
H	0.49207	-2.18282	-5.45393
H	-2.29711	-3.17802	3.18524
H	0.59571	3.74414	-2.49543
C	4.93555	-1.05159	-0.57374
C	6.28113	-1.25817	-0.41168
C	6.85177	-1.43108	0.90500
C	5.92877	-1.26317	2.00590
C	4.59317	-1.05414	1.77838
H	4.52141	-0.86073	-1.56414
H	3.91590	-0.85807	2.60952
H	-2.39559	0.17631	1.48027
N	4.04857	-1.03518	0.49936
C	3.11370	4.34976	0.18703
N	3.61118	5.40022	0.22708
C	4.66465	1.79111	0.58998

```
N          5.80660        1.81249        0.80738
C          3.41910       -3.37655       -1.44148
N          4.24072       -4.15416       -1.17225
C          1.49194       -3.62509       -3.80141
N          1.52163       -4.51435       -4.55042
C          2.81122       -3.28470        2.30783
N          3.66422       -4.07355        2.35753
C          0.24366       -3.41472        3.94713
N          0.03475       -4.25987        4.71832
C          8.22160       -1.68085        1.10370
N          9.36139       -1.88880        1.26875
C          6.39310       -1.28379        3.35960
N          6.77174       -1.30492        4.45909
C          7.11154       -1.27379       -1.57786
N          7.78636       -1.28977       -2.52491
H         -2.66872       -0.82177       -0.63180
C         -3.91620       -0.41355       -0.94631
H         -4.15227       -1.09990       -1.77216
H         -3.77310        0.63328       -1.24968
C         -4.70328       -0.58802        0.22499
N         -5.30108       -0.73469        1.21710
```

$L_4Co^{III}O$ + Ph2CH2 (*S*=0, closed-shell)

```
108
ph2ch2_ts_u0_closed.out   Energy: -2642859.3672730
C          0.66956       -0.84288       -1.70317
N          0.42427       -1.48651       -2.88075
C          1.40824       -2.44997       -3.08331
C          2.32294       -2.32660       -2.05370
N          1.89358       -1.27181       -1.25935
B          2.35638       -0.68083        0.09583
N          2.11316        0.85861        0.07114
C          0.84805        1.29572       -0.20325
N          0.86590        2.65501       -0.15903
C          2.15753        3.08357        0.13800
C          2.94193        1.95449        0.28260
N          1.40209       -1.32296        1.15130
C          0.10942       -0.87626        1.16433
N         -0.52014       -1.49548        2.20204
C          0.32068       -2.48464        2.70796
C          1.52674       -2.38298        2.03824
Co        -0.50565       -0.02142       -0.45825
O         -2.07644       -0.71990       -0.39769
C         -0.71989       -1.22012       -3.84231
C         -0.15980       -1.15803       -5.27437
C         -1.73486       -2.35366       -3.66352
C         -1.34072        0.14491       -3.52697
C         -0.30334        3.59140       -0.38564
C         -0.50114        4.43027        0.88814
C          0.00921        4.45700       -1.61690
C         -1.57233        2.78116       -0.64444
C         -1.85277       -1.10906        2.84849
C         -2.24696        0.31277        2.42946
C         -2.89981       -2.13442        2.40560
C         -1.65725       -1.10229        4.37666
H         -0.97469       -0.85110       -5.94796
```

H	0.64796	-0.41163	-5.34911
H	-1.29976	-3.33147	-3.92584
H	-2.60451	-2.18300	-4.31524
H	-2.08816	-2.38611	-2.62241
H	-0.58567	0.94626	-3.56212
H	-1.84359	0.15331	-2.55272
H	-2.10592	0.35853	-4.28883
H	0.35640	5.08289	1.10731
H	-0.68148	3.77545	1.75626
H	-1.38162	5.07792	0.75414
H	0.89202	5.09734	-1.47171
H	-0.84886	5.11762	-1.81720
H	-1.84981	2.15306	0.21387
H	-2.39906	3.48953	-0.80642
H	-1.49314	2.16494	-1.55170
H	-3.11779	0.61373	3.03103
H	-1.42831	1.02633	2.62229
H	-3.87840	-1.86526	2.83152
H	-2.97488	-2.11117	1.30945
H	-0.82156	-0.44367	4.66570
H	-1.49465	-2.09920	4.80635
H	-2.57717	-0.70634	4.83313
H	0.20970	-2.12451	-5.64103
H	-2.64076	-3.15163	2.74267
H	0.17294	3.82156	-2.50271
C	4.79080	-0.91313	-0.60771
C	6.15492	-1.06142	-0.37443
C	6.62356	-1.16937	0.95974
C	5.67126	-1.07412	2.00517
C	4.32296	-0.93185	1.68920
H	4.42013	-0.75693	-1.62112
H	3.58168	-0.80240	2.47817
H	-2.54005	0.35824	1.37694
N	3.88769	-0.90429	0.40416
C	2.61184	4.42170	0.26453
N	3.03242	5.50082	0.37481
C	4.32620	1.94607	0.58580
N	5.46279	1.94694	0.83651
C	3.44307	-3.15952	-1.80733
N	4.36476	-3.83478	-1.58398
C	1.45180	-3.44819	-4.09111
N	1.53158	-4.30989	-4.86862
C	2.64764	-3.24261	2.15732
N	3.57367	-3.94375	2.23534
C	-0.00205	-3.50273	3.64317
N	-0.20962	-4.38678	4.37044
C	8.01156	-1.33257	1.24143
N	9.14365	-1.46619	1.47081
C	6.06550	-1.10860	3.38081
N	6.37951	-1.13761	4.49855
C	7.05383	-1.08493	-1.48820
N	7.77803	-1.10661	-2.39594
H	-3.06662	-0.79023	-1.05275
C	-4.35687	-0.74941	-1.56611
H	-4.24797	-0.06453	-2.42019
C	-4.93211	-0.07633	-0.38937
C	-4.71017	-2.12338	-1.98045
C	-5.63670	-0.73567	0.64376
C	-4.69423	1.31236	-0.23566

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C          -5.19107       -2.36067       -3.28770
C          -4.51764       -3.24237       -1.13857
C          -6.05931       -0.04216        1.78042
H          -5.86396       -1.80028        0.55261
C          -5.11207        2.00248        0.90008
H          -4.16598        1.84395       -1.03263
C          -5.48685       -3.65337       -3.72810
H          -5.33515       -1.51091       -3.96392
C          -4.81229       -4.53525       -1.57831
H          -4.10085       -3.09725       -0.13899
C          -5.79305        1.32648        1.92361
H          -6.60499       -0.57710        2.56494
H          -4.90491        3.07396        0.99171
C          -5.30067       -4.74891       -2.87470
H          -5.86310       -3.80767       -4.74490
H          -4.64757       -5.38535       -0.90799
H          -6.12057        1.86318        2.81955
H          -5.52706       -5.76289       -3.21957
```

$L_4Co^{III}O$ + Ph2CH2 (*S*=0, open-shell)

```
108
ph2ch2_ts_u0_open.out     Energy: -2642865.0830873
C           0.63710       -0.87184       -1.64450
N           0.36738       -1.59167       -2.76710
C           1.33171       -2.58227       -2.92498
C           2.26166       -2.40958       -1.91622
N           1.85860       -1.29870       -1.18483
B           2.38897       -0.66616        0.13322
N           2.16750        0.87187        0.09563
C           0.89033        1.32265       -0.10293
N           0.93211        2.68141       -0.08417
C           2.24232        3.09943        0.13370
C           3.02002        1.96237        0.24721
N           1.53059       -1.28565        1.27591
C           0.24330       -0.82620        1.38771
N          -0.33419       -1.51119        2.40891
C           0.52661       -2.51713        2.83568
C           1.69590       -2.38950        2.10590
Co         -0.46628       -0.00968       -0.28006
O          -1.81449       -1.19066       -0.35432
C          -0.79157       -1.37276       -3.72309
C          -0.24331       -1.34323       -5.16053
C          -1.79090       -2.51347       -3.49773
C          -1.43222       -0.01252       -3.43438
C          -0.24359        3.61469       -0.25809
C          -0.40353        4.43539        1.03204
C           0.01640        4.50057       -1.48745
C          -1.51096        2.79242       -0.49255
C          -1.68524       -1.20801        3.03526
C          -2.16385        0.16663        2.56032
C          -2.66302       -2.30825        2.60289
C          -1.50935       -1.15229        4.56317
H          -1.07217       -1.08966       -5.83965
H           0.53848       -0.57330       -5.26839
H          -1.35728       -3.49106       -3.76379
H          -2.68623       -2.35598       -4.11878
```

H	-2.09669	-2.52061	-2.44199
H	-0.69729	0.80478	-3.51079
H	-1.89540	0.00338	-2.44363
H	-2.22702	0.15935	-4.17601
H	0.46596	5.07879	1.23330
H	-0.55962	3.76864	1.89585
H	-1.28385	5.08989	0.93439
H	0.89144	5.15491	-1.36072
H	-0.85846	5.14872	-1.65288
H	-1.75080	2.15180	0.37071
H	-2.35419	3.48822	-0.61912
H	-1.44509	2.19384	-1.41437
H	-3.10428	0.40582	3.07865
H	-1.42619	0.95293	2.78784
H	-3.65696	-2.09692	3.02591
H	-2.73582	-2.31095	1.50475
H	-0.73143	-0.42280	4.84303
H	-1.26430	-2.12563	5.00992
H	-2.46247	-0.82493	5.00683
H	0.15882	-2.30963	-5.49331
H	-2.34141	-3.30088	2.95818
H	0.16389	3.87934	-2.38610
C	4.76378	-0.87572	-0.75781
C	6.14667	-1.01838	-0.64353
C	6.71885	-1.16152	0.64215
C	5.86064	-1.11344	1.76473
C	4.48787	-0.96242	1.56413
H	4.30165	-0.71705	-1.73328
H	3.81422	-0.85909	2.41513
H	-2.38089	0.15681	1.48752
N	3.95383	-0.89169	0.32534
C	2.71169	4.43462	0.23068
N	3.13753	5.51378	0.31905
C	4.41808	1.94473	0.47563
N	5.56700	1.93516	0.66277
C	3.37585	-3.23780	-1.63130
N	4.29365	-3.90826	-1.37843
C	1.34794	-3.63551	-3.87602
N	1.40173	-4.53547	-4.61143
C	2.81913	-3.25364	2.13676
N	3.74835	-3.95556	2.14087
C	0.25776	-3.54305	3.77882
N	0.08107	-4.42089	4.52166
C	8.12958	-1.32035	0.80439
N	9.27665	-1.44874	0.93663
C	6.36682	-1.20492	3.10070
N	6.77020	-1.28161	4.18691
C	6.95219	-1.00879	-1.82725
N	7.59943	-1.00255	-2.79134
H	-3.00782	-0.67020	-0.71323
C	-4.14229	-0.29302	-1.05974
H	-3.95343	0.58161	-1.70092
C	-4.80943	0.13263	0.20562
C	-4.67187	-1.43879	-1.86119
C	-5.45000	-0.76286	1.08637
C	-4.75009	1.49283	0.57971
C	-5.20870	-1.21102	-3.14286
C	-4.58839	-2.76825	-1.40051
C	-5.98624	-0.31843	2.29826

H	-5.53237	-1.81977	0.82482
C	-5.28568	1.93957	1.78935
H	-4.27873	2.21011	-0.09850
C	-5.66564	-2.27223	-3.93183
H	-5.26505	-0.18607	-3.52563
C	-5.04493	-3.82990	-2.18651
H	-4.11800	-2.97323	-0.43503
C	-5.90163	1.03223	2.66168
H	-6.47553	-1.03504	2.96615
H	-5.22446	3.00075	2.05209
C	-5.58723	-3.58681	-3.45545
H	-6.08084	-2.07178	-4.92507
H	-4.96313	-4.85589	-1.81294
H	-6.32026	1.37597	3.61286
H	-5.93896	-4.41928	-4.07335

$L_4Co^{III}O$ + Ph2CH2 (*S*=1)

108
ph2ch2_ts_u2.out Energy: -2642867.3710684

C	0.64026	-0.87181	-1.66628
N	0.37063	-1.59521	-2.78560
C	1.33206	-2.58967	-2.93737
C	2.25895	-2.41753	-1.92554
N	1.85749	-1.30213	-1.19968
B	2.38212	-0.66793	0.12070
N	2.16398	0.86988	0.08077
C	0.88684	1.32082	-0.10997
N	0.92965	2.67933	-0.10356
C	2.24220	3.09742	0.09983
C	3.01961	1.96032	0.21545
N	1.51761	-1.28133	1.26077
C	0.22822	-0.82375	1.37322
N	-0.34648	-1.51092	2.39517
C	0.51527	-2.51733	2.81817
C	1.68369	-2.38688	2.08827
Co	-0.47510	-0.01068	-0.28413
O	-1.79854	-1.19752	-0.41439
C	-0.78264	-1.37441	-3.74889
C	-0.21957	-1.33096	-5.18043
C	-1.77864	-2.52190	-3.54349
C	-1.43632	-0.02116	-3.45561
C	-0.24704	3.61088	-0.27828
C	-0.40197	4.43992	1.00697
C	0.00558	4.48853	-1.51489
C	-1.51302	2.78337	-0.50123
C	-1.69964	-1.21747	3.01810
C	-2.17750	0.15953	2.55227
C	-2.67110	-2.31705	2.57024
C	-1.53365	-1.17309	4.54741
H	-1.04329	-1.08173	-5.86736
H	0.55564	-0.55266	-5.27499
H	-1.33708	-3.49630	-3.80782
H	-2.66410	-2.36519	-4.17837
H	-2.10279	-2.53523	-2.49319
H	-0.70619	0.80194	-3.51604
H	-1.90981	-0.02030	-2.46947

H	-2.22240	0.15143	-4.20625
H	0.46881	5.08405	1.20031
H	-0.55483	3.77894	1.87582
H	-1.28231	5.09425	0.90837
H	0.87894	5.14658	-1.39614
H	-0.87207	5.13261	-1.68143
H	-1.74264	2.14636	0.36753
H	-2.36078	3.47424	-0.62451
H	-1.45164	2.18252	-1.42219
H	-3.12387	0.39185	3.06243
H	-1.44394	0.94577	2.79258
H	-3.66899	-2.11222	2.98667
H	-2.73232	-2.31308	1.47138
H	-0.75795	-0.44540	4.83791
H	-1.29130	-2.14962	4.98840
H	-2.48991	-0.84949	4.98707
H	0.19642	-2.29133	-5.51414
H	-2.34866	-3.31109	2.92080
H	0.15153	3.86136	-2.40964
C	4.76463	-0.89677	-0.75049
C	6.14585	-1.04484	-0.62113
C	6.70550	-1.17236	0.67164
C	5.83741	-1.10251	1.78561
C	4.46738	-0.94930	1.57006
H	4.31251	-0.74756	-1.73212
H	3.78540	-0.83288	2.41291
H	-2.38334	0.16162	1.47775
N	3.94498	-0.89515	0.32525
C	2.71248	4.43313	0.18391
N	3.13853	5.51298	0.26191
C	4.41951	1.94151	0.43222
N	5.56997	1.93035	0.60949
C	3.36862	-3.24967	-1.63450
N	4.28255	-3.92352	-1.37658
C	1.34961	-3.64363	-3.88769
N	1.40379	-4.54305	-4.62373
C	2.80858	-3.24879	2.11877
N	3.73894	-3.94918	2.12360
C	0.24870	-3.54623	3.75868
N	0.07551	-4.42721	4.49862
C	8.11359	-1.33778	0.84943
N	9.25844	-1.47189	0.99455
C	6.33067	-1.17532	3.12754
N	6.72345	-1.23658	4.21860
C	6.96256	-1.05566	-1.79708
N	7.61896	-1.06588	-2.75493
H	-2.96377	-0.67941	-0.64988
C	-4.13876	-0.27000	-0.97924
H	-3.92403	0.61337	-1.60006
C	-4.81440	0.13500	0.28142
C	-4.64258	-1.40237	-1.80965
C	-5.47598	-0.76890	1.13973
C	-4.75613	1.49066	0.67683
C	-5.12557	-1.15584	-3.11022
C	-4.58814	-2.73891	-1.36328
C	-6.02771	-0.33876	2.34946
H	-5.56253	-1.82106	0.86150
C	-5.30837	1.92258	1.88385
H	-4.27048	2.21560	0.01717

```
C          -5.56280       -2.20284       -3.92804
H          -5.15751       -0.12616       -3.48281
C          -5.02323       -3.78660       -2.17952
H          -4.15882       -2.96159       -0.38295
C          -5.94149        1.00607        2.73432
H          -6.53172       -1.06215        2.99887
H          -5.24644        2.97970        2.16233
C          -5.51527       -3.52372       -3.46483
H          -5.93787       -1.98660       -4.93385
H          -4.96450       -4.81761       -1.81558
H          -6.37283        1.33823        3.68389
H          -5.85102       -4.34550       -4.10546
```

$L_4Co^{III}O$ + Ph2CH2 (*S*=2)

```
108
ph2ch2_ts_u4.out  Energy: -2642860.4640466
C           0.67079       -0.87210       -1.63720
N           0.40126       -1.58018       -2.75819
C           1.35560       -2.58560       -2.89375
C           2.25470       -2.43511       -1.85237
N           1.84844       -1.32455       -1.12888
B           2.42429       -0.69922        0.19394
N           2.18965        0.86212        0.12314
C           0.95140        1.36396       -0.10210
N           1.03591        2.71449       -0.15519
C           2.36304        3.08068        0.05064
C           3.08602        1.91280        0.22888
N           1.49295       -1.26595        1.32225
C           0.22704       -0.78160        1.45256
N          -0.36856       -1.44647        2.46969
C           0.48181       -2.45923        2.90436
C           1.64697       -2.35718        2.16435
Co         -0.50119        0.05935       -0.25396
O          -1.73453       -1.12947       -0.36606
C          -0.73029       -1.34383       -3.74700
C          -0.12677       -1.26163       -5.16002
C          -1.72239       -2.50397       -3.59944
C          -1.40307       -0.00330       -3.44280
C          -0.08115        3.70494       -0.42515
C          -0.18611        4.65560        0.77865
C           0.24763        4.44230       -1.73359
C          -1.40468        2.95907       -0.58413
C          -1.72333       -1.14297        3.08887
C          -2.22713        0.20495        2.57257
C          -2.68448       -2.27092        2.69026
C          -1.54430       -1.03567        4.61312
H          -0.93349       -1.00765       -5.86500
H           0.64029       -0.47189       -5.21325
H          -1.26672       -3.46920       -3.86984
H          -2.58399       -2.33836       -4.26354
H          -2.09241       -2.55880       -2.56501
H          -0.68083        0.82837       -3.46793
H          -1.91120       -0.01943       -2.47350
H          -2.17054        0.18052       -4.20936
H           0.71394        5.27239        0.91302
H          -0.37086        4.08758        1.70497
```

H	-1.03268	5.34065	0.61584
H	1.17634	5.02759	-1.66667
H	-0.56946	5.14453	-1.96099
H	-1.71019	2.46678	0.35064
H	-2.18973	3.69525	-0.81623
H	-1.38757	2.25584	-1.43103
H	-3.13925	0.47172	3.12586
H	-1.48454	1.00540	2.71853
H	-3.68948	-2.04511	3.07823
H	-2.73834	-2.34184	1.59300
H	-0.79808	-0.26479	4.86550
H	-1.25319	-1.98345	5.08557
H	-2.50928	-0.73893	5.05244
H	0.31161	-2.20933	-5.50048
H	-2.36978	-3.24409	3.09886
H	0.33702	3.72770	-2.56802
C	4.77926	-0.95571	-0.68729
C	6.13054	-1.13981	-0.54730
C	6.72341	-1.31607	0.75939
C	5.81326	-1.17243	1.87503
C	4.47095	-0.98572	1.66797
H	4.34641	-0.76381	-1.66943
H	3.80185	-0.80968	2.51019
H	-2.51159	0.14850	1.51736
N	3.90794	-0.96689	0.39794
C	2.89595	4.39532	0.07198
N	3.37896	5.45319	0.09481
C	4.48155	1.86407	0.48256
N	5.62423	1.90637	0.69374
C	3.32658	-3.30982	-1.53394
N	4.17558	-4.06455	-1.28478
C	1.38259	-3.62394	-3.86065
N	1.44037	-4.50971	-4.61233
C	2.74378	-3.25786	2.19675
N	3.61259	-4.03053	2.22561
C	0.20075	-3.46569	3.86448
N	0.01308	-4.32907	4.62101
C	8.09930	-1.54653	0.93595
N	9.24456	-1.73876	1.08259
C	6.29704	-1.19594	3.22169
N	6.69180	-1.21983	4.31553
C	6.94354	-1.12981	-1.72555
N	7.60460	-1.12554	-2.68249
H	-3.01920	-0.62931	-0.66884
C	-4.16648	-0.32627	-1.01288
H	-3.99150	0.52124	-1.69377
C	-4.82936	0.13764	0.23210
C	-4.61321	-1.54018	-1.75457
C	-5.52411	-0.71931	1.11372
C	-4.71366	1.50442	0.58130
C	-5.10293	-1.40820	-3.06980
C	-4.49367	-2.83500	-1.20735
C	-6.06541	-0.22899	2.30322
H	-5.65197	-1.77440	0.86327
C	-5.25862	1.99429	1.76715
H	-4.18754	2.18445	-0.09582
C	-5.49624	-2.53136	-3.80211
H	-5.17886	-0.41177	-3.51760
C	-4.87691	-3.95835	-1.94319

H	-4.05980	-2.96496	-0.21232
C	-5.93144	1.12616	2.63957
H	-6.60145	-0.90831	2.97337
H	-5.15943	3.05549	2.01551
C	-5.38352	-3.81060	-3.24167
H	-5.88424	-2.40918	-4.81833
H	-4.76822	-4.95621	-1.50696
H	-6.35644	1.50506	3.57419
H	-5.67943	-4.69186	-3.81941

$L_4Co^{III}O$ + 9-Ph-fluorene (*S*=0, closed-shell)

116
phflu_ts_u0_closed.out Energy: -2787063.1930150

C	0.66905	-1.17793	-1.57828
N	0.36812	-2.04537	-2.58926
C	1.38630	-2.98730	-2.69495
C	2.35493	-2.65294	-1.76604
N	1.92407	-1.49517	-1.13599
B	2.40962	-0.71752	0.11132
N	2.21109	0.80476	-0.13223
C	0.98221	1.22103	-0.55010
N	1.02387	2.57402	-0.67408
C	2.27278	3.02689	-0.26020
C	3.02468	1.91454	0.07092
N	1.43680	-1.17205	1.23988
C	0.17342	-0.64861	1.21246
N	-0.45648	-1.06923	2.34692
C	0.32903	-2.04398	2.95690
C	1.51589	-2.11944	2.25080
Co	-0.45426	-0.03309	-0.52725
O	-2.11644	-0.35976	-0.26200
C	-0.94167	-2.06899	-3.36609
C	-0.73362	-2.69272	-4.75375
C	-1.91799	-2.90233	-2.52849
C	-1.42029	-0.62764	-3.56708
C	-0.10170	3.46794	-1.16287
C	-0.68129	4.19926	0.05541
C	0.45773	4.43982	-2.21549
C	-1.16921	2.60609	-1.83140
C	-1.69504	-0.44494	3.00186
C	-1.87669	0.97951	2.46220
C	-2.89571	-1.34018	2.69653
C	-1.43532	-0.33248	4.51601
H	-1.64613	-2.50370	-5.33965
H	0.11259	-2.23075	-5.28813
H	-1.51697	-3.91465	-2.35556
H	-2.86996	-2.99422	-3.06879
H	-2.10229	-2.41136	-1.56090
H	-0.64827	-0.02332	-4.06947
H	-1.71327	-0.14864	-2.62637
H	-2.32232	-0.64125	-4.19543
H	0.06667	4.84673	0.54092
H	-1.06363	3.47491	0.79248
H	-1.52462	4.82790	-0.26961
H	1.17564	5.16257	-1.80547
H	-0.38223	5.01888	-2.62927
H	-1.72530	1.98217	-1.11714
H	-1.91181	3.26943	-2.29305

H	-0.73839	1.98048	-2.62624
H	-2.69035	1.45497	3.03109
H	-0.96128	1.57691	2.61030
H	-3.80733	-0.90224	3.13295
H	-3.03102	-1.41616	1.61090
H	-0.48723	0.19058	4.72437
H	-1.43735	-1.29963	5.03488
H	-2.25350	0.26117	4.95160
H	-0.59718	-3.78111	-4.72170
H	-2.76259	-2.34765	3.12450
H	0.93520	3.88779	-3.04157
C	4.82318	-0.98613	-0.59422
C	6.19366	-1.11811	-0.38164
C	6.68492	-1.17434	0.94575
C	5.75494	-1.04719	2.00490
C	4.39948	-0.91253	1.70843
H	4.42652	-0.89497	-1.60636
H	3.67850	-0.73883	2.50673
H	-2.14657	0.98256	1.40295
N	3.94235	-0.93294	0.43466
C	2.70519	4.37204	-0.12749
N	3.10828	5.45162	0.03130
C	4.36515	1.92821	0.52917
N	5.46734	1.94083	0.90315
C	3.52577	-3.38989	-1.45792
N	4.48691	-3.98744	-1.18509
C	1.46645	-4.13520	-3.52702
N	1.62708	-5.10884	-4.14257
C	2.57250	-3.04767	2.42727
N	3.44908	-3.80530	2.54116
C	-0.03865	-2.91314	4.01751
N	-0.28640	-3.68730	4.84961
C	8.08004	-1.32421	1.20688
N	9.21607	-1.44726	1.41927
C	6.17517	-1.03242	3.37312
N	6.50936	-1.02100	4.48521
C	7.07320	-1.18708	-1.50902
N	7.78173	-1.24616	-2.42721
H	-3.21864	-0.25614	-0.75546
C	-4.55637	-0.04378	-1.06643
C	-4.72398	-0.27516	-2.52716
C	-4.53505	1.43348	-0.92932
C	-5.21386	-0.93821	-0.06971
C	-4.95287	-1.44973	-3.25504
C	-4.65404	0.97114	-3.21555
C	-4.41377	2.24101	0.21093
C	-4.55276	2.03613	-2.21953
C	-4.88727	-2.31045	-0.02110
C	-6.16431	-0.45675	0.85325
C	-5.02804	-1.38960	-4.65418
H	-5.08234	-2.40691	-2.74388
C	-4.71949	1.02465	-4.61228
C	-4.34380	3.63222	0.06198
H	-4.38023	1.79293	1.20635
C	-4.49503	3.42754	-2.36078
C	-5.48312	-3.16517	0.90837
H	-4.12552	-2.70281	-0.69844
C	-6.75593	-1.31024	1.79120
H	-6.45558	0.59645	0.82749

```
C          -4.89314       -0.16567       -5.33181
H          -5.19759       -2.30890       -5.22420
H          -4.65240        1.98422       -5.13560
C          -4.39286        4.22410       -1.21259
H          -4.25447        4.26633        0.94998
H          -4.52221        3.88757       -3.35417
C          -6.41856       -2.66835        1.82587
H          -5.20354       -4.22372        0.92788
H          -7.49199       -0.90971        2.49638
H          -4.94565       -0.14016       -6.42489
H          -4.34460        5.31363       -1.30777
H          -6.87967       -3.33483        2.56181
```

$L_4Co^{III}O$ + 9-Ph-fluorene (*S*=1)

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116
phflu_ts_u2.out   Energy: -2787068.3068658
C           0.76717       -1.20364       -1.61544
N           0.54714       -2.13481       -2.58280
C           1.50867       -3.13662       -2.49361
C           2.38906       -2.76746       -1.49493
N           1.96173       -1.53522       -1.01840
B           2.43923       -0.68630        0.19361
N           2.27675        0.82141       -0.13044
C           1.03414        1.22633       -0.50677
N           1.08181        2.56113       -0.73391
C           2.36217        3.02714       -0.45685
C           3.12065        1.93064       -0.08428
N           1.48346       -1.06837        1.35822
C           0.21219       -0.55185        1.33189
N          -0.41818       -1.02174        2.44126
C           0.38218       -1.97194        3.06612
C           1.57517       -2.01824        2.36868
Co         -0.40634       -0.02848       -0.51879
O          -1.85583       -1.03324       -0.50814
C          -0.56304       -2.12894       -3.61898
C           0.04767       -2.43010       -4.99959
C          -1.58149       -3.19113       -3.18966
C          -1.19800       -0.73899       -3.68204
C          -0.10166        3.38327       -1.17569
C          -0.56355        4.23719        0.01325
C           0.29634        4.24229       -2.38592
C          -1.20623        2.41961       -1.60559
C          -1.74625       -0.53858        2.99189
C          -2.16676        0.72422        2.24097
C          -2.77362       -1.65517        2.78598
C          -1.55091       -0.17605        4.47479
H          -0.74112       -2.29835       -5.75629
H           0.86477       -1.72665       -5.22971
H          -1.11948       -4.18852       -3.11139
H          -2.38590       -3.24576       -3.93624
H          -2.01254       -2.90650       -2.21758
H          -0.44578        0.02922       -3.92329
H          -1.70308       -0.48934       -2.74465
H          -1.96222       -0.74170       -4.47325
H           0.21394        4.95116        0.32900
H          -0.82764        3.59659        0.87034
```

H	-1.45894	4.80888	-0.27734
H	1.03554	5.01602	-2.13490
H	-0.60256	4.75697	-2.75968
H	-1.59970	1.82127	-0.76149
H	-2.06707	3.00001	-1.95999
H	-0.88429	1.77202	-2.43379
H	-3.07741	1.11435	2.71930
H	-1.39069	1.50502	2.28649
H	-3.77149	-1.30741	3.09639
H	-2.81774	-1.91159	1.71923
H	-0.75428	0.57684	4.59382
H	-1.32028	-1.04363	5.10832
H	-2.49171	0.25545	4.85054
H	0.42032	-3.45799	-5.10107
H	-2.52923	-2.55535	3.37240
H	0.69699	3.61246	-3.19683
C	4.86608	-1.06811	-0.46481
C	6.23633	-1.17291	-0.22521
C	6.71174	-1.07775	1.10367
C	5.77184	-0.85295	2.13572
C	4.41800	-0.75429	1.81128
H	4.47822	-1.08698	-1.48450
H	3.68433	-0.50999	2.57985
H	-2.39374	0.49745	1.19372
N	3.97828	-0.89910	0.54161
C	2.80544	4.37374	-0.50242
N	3.20042	5.46792	-0.50943
C	4.49089	1.95225	0.27311
N	5.61734	1.96658	0.56654
C	3.47528	-3.53203	-0.99926
N	4.36493	-4.15627	-0.58169
C	1.56501	-4.36173	-3.20822
N	1.65551	-5.39587	-3.73347
C	2.65766	-2.90851	2.57884
N	3.55626	-3.63366	2.72857
C	0.03872	-2.80431	4.16313
N	-0.20032	-3.52789	5.04219
C	8.10817	-1.17420	1.39119
N	9.24378	-1.25027	1.62426
C	6.17733	-0.70271	3.50065
N	6.49895	-0.58200	4.60989
C	7.12929	-1.35932	-1.32867
N	7.84836	-1.51281	-2.22745
H	-3.02246	-0.56210	-0.87663
C	-4.27367	-0.25528	-1.13602
C	-4.45828	-0.59207	-2.58885
C	-4.36088	1.23846	-1.10891
C	-4.96865	-1.10445	-0.11376
C	-4.61428	-1.82485	-3.22824
C	-4.48287	0.60276	-3.35674
C	-4.34851	2.13887	-0.03624
C	-4.43719	1.73975	-2.43750
C	-4.62324	-2.46720	0.01073
C	-5.97885	-0.59863	0.72719
C	-4.73574	-1.86329	-4.62500
H	-4.64110	-2.75452	-2.65638
C	-4.58976	0.56205	-4.75049
C	-4.40683	3.51711	-0.28886
H	-4.30894	1.77970	0.99231

C	-4.49942	3.11495	-2.68767
C	-5.26805	-3.29381	0.93318
H	-3.80933	-2.86820	-0.59724
C	-6.61727	-1.42416	1.65981
H	-6.28459	0.44683	0.63993
C	-4.70563	-0.68271	-5.38434
H	-4.85419	-2.82832	-5.12834
H	-4.60016	1.48709	-5.33595
C	-4.48161	4.00442	-1.60383
H	-4.40050	4.21943	0.55063
H	-4.56492	3.49146	-3.71346
C	-6.26661	-2.77522	1.76743
H	-4.97676	-4.34615	1.01378
H	-7.40160	-1.00802	2.30081
H	-4.79269	-0.73406	-6.47427
H	-4.52892	5.08316	-1.78299
H	-6.76737	-3.41962	2.49710

$L_4Co^{III}O$ + 9-Ph-fluorene (*S*=2)

116
phflu_ts_u4.out Energy: -2787059.8522174

C	0.79479	-1.12971	-1.60225
N	0.58606	-1.98502	-2.63150
C	1.52308	-3.01354	-2.55995
C	2.35678	-2.73026	-1.49420
N	1.93465	-1.52197	-0.96463
B	2.46091	-0.72862	0.28386
N	2.27008	0.80300	-0.03433
C	1.05727	1.24328	-0.42441
N	1.14759	2.55116	-0.74474
C	2.46100	2.96372	-0.54967
C	3.16722	1.85912	-0.09516
N	1.45463	-1.12194	1.41992
C	0.18724	-0.62234	1.42081
N	-0.43973	-1.11268	2.51895
C	0.39482	-2.03300	3.14647
C	1.57971	-2.05743	2.43420
Co	-0.44825	0.01664	-0.46527
O	-1.75517	-1.08683	-0.62494
C	-0.44295	-1.87280	-3.74540
C	0.29550	-1.98487	-5.09176
C	-1.46045	-3.00114	-3.54317
C	-1.11926	-0.50186	-3.69665
C	0.02707	3.38043	-1.32023
C	-0.16641	4.64283	-0.46673
C	0.38498	3.70974	-2.77762
C	-1.25210	2.54854	-1.26590
C	-1.77583	-0.67976	3.09747
C	-2.35682	0.44971	2.25293
C	-2.72403	-1.88521	3.07858
C	-1.51975	-0.14982	4.51940
H	-0.43513	-1.81879	-5.89840
H	1.08010	-1.21501	-5.17211
H	-0.98995	-3.99481	-3.59816
H	-2.22413	-2.94411	-4.33127
H	-1.95499	-2.88892	-2.56657

H	-0.38192	0.31391	-3.76437
H	-1.73105	-0.38271	-2.79791
H	-1.80119	-0.42182	-4.55615
H	0.68769	5.33165	-0.53490
H	-0.33096	4.37775	0.59006
H	-1.05616	5.17964	-0.83137
H	1.30456	4.31051	-2.84980
H	-0.43404	4.29366	-3.22553
H	-1.60698	2.40098	-0.23382
H	-2.05613	3.08344	-1.78926
H	-1.15578	1.59357	-1.82151
H	-3.26660	0.81042	2.75423
H	-1.65932	1.29706	2.15513
H	-3.73026	-1.56150	3.38737
H	-2.79939	-2.29103	2.06009
H	-0.80813	0.69165	4.49918
H	-1.13985	-0.92061	5.20496
H	-2.47417	0.21189	4.93284
H	0.74527	-2.97219	-5.26234
H	-2.40470	-2.68542	3.76240
H	0.51934	2.78633	-3.36428
C	4.86901	-1.16423	-0.37542
C	6.20423	-1.32043	-0.10552
C	6.70007	-1.24962	1.25124
C	5.71653	-0.89279	2.24964
C	4.39479	-0.75082	1.91457
H	4.51199	-1.15342	-1.40532
H	3.66919	-0.42261	2.65887
H	-2.64010	0.08990	1.25755
N	3.92287	-0.97581	0.62590
C	2.97975	4.26184	-0.78871
N	3.43640	5.31332	-0.98508
C	4.54572	1.85520	0.24148
N	5.67625	1.92084	0.50545
C	3.37976	-3.57138	-0.98239
N	4.18812	-4.29948	-0.57148
C	1.59000	-4.18093	-3.36407
N	1.68144	-5.16852	-3.97179
C	2.66617	-2.94773	2.64160
N	3.52195	-3.71478	2.81966
C	0.09566	-2.83581	4.27779
N	-0.10311	-3.52363	5.19445
C	8.05521	-1.45011	1.56881
N	9.18283	-1.61798	1.83401
C	6.10433	-0.65330	3.60653
N	6.42081	-0.46224	4.70932
C	7.10038	-1.52929	-1.20189
N	7.83004	-1.70299	-2.09084
H	-3.07492	-0.54679	-0.87506
C	-4.27297	-0.28318	-1.06595
C	-4.45305	-0.61016	-2.52821
C	-4.38542	1.21336	-1.02298
C	-4.94669	-1.15467	-0.04722
C	-4.58569	-1.84238	-3.17040
C	-4.49440	0.59234	-3.27959
C	-4.40836	2.09600	0.06303
C	-4.46371	1.72313	-2.34665
C	-4.54150	-2.49935	0.09198
C	-6.00563	-0.68486	0.75452

```
C          -4.72083       -1.86985       -4.56726
H          -4.58911       -2.77638       -2.60416
C          -4.61407        0.56255       -4.66997
C          -4.50717        3.47535       -0.17400
H          -4.36828        1.72579        1.08756
C          -4.55674        3.09662       -2.58160
C          -5.18472       -3.35107        0.99123
H          -3.68995       -2.86533       -0.48734
C          -6.64217       -1.53735        1.66212
H          -6.35220        0.34601        0.64950
C          -4.71794       -0.68192       -5.31224
H          -4.82774       -2.83116       -5.07909
H          -4.64683        1.49055       -5.24901
C          -4.57650        3.97266       -1.48357
H          -4.53244        4.16757        0.67282
H          -4.62546        3.48538       -3.60215
C          -6.23647       -2.87223        1.78379
H          -4.85196       -4.38914        1.08824
H          -7.46806       -1.15703        2.27166
H          -4.81560       -0.72392       -6.40144
H          -4.65144        5.05136       -1.65204
H          -6.73678       -3.53698        2.49491
```

$L_4Co^{III}O$ + 9-tBu-fluorene (*S*=0, closed-shell)

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118
tbuflu_ts_u0_closed.out   Energy: -2740758.0259440
C           0.65432       -1.20895       -1.51476
N           0.34314       -2.09068       -2.51051
C           1.36461       -3.02636       -2.62742
C           2.35137       -2.67082       -1.72617
N           1.92427       -1.50912       -1.10175
B           2.43326       -0.71874        0.12558
N           2.20551        0.79704       -0.11611
C           0.95974        1.19691       -0.49919
N           0.98993        2.54998       -0.64182
C           2.24634        3.01673       -0.27098
C           3.01684        1.91423        0.04845
N           1.50123       -1.18413        1.27997
C           0.22715       -0.68191        1.30320
N          -0.34476       -1.13186        2.45789
C           0.48368       -2.09588        3.02833
C           1.64049       -2.13991        2.27461
Co         -0.46768       -0.06976       -0.43820
O          -2.15273       -0.37311       -0.16084
C          -0.96498       -2.10706       -3.28475
C          -0.76355       -2.73682       -4.67085
C          -1.94955       -2.93029       -2.44667
C          -1.41605       -0.65706       -3.48832
C          -0.15404        3.43020       -1.10728
C          -0.73091        4.13452        0.12764
C           0.37047        4.42898       -2.15276
C          -1.20623        2.55335       -1.77699
C          -1.56803       -0.56825        3.17912
C          -1.93308        0.79610        2.58467
C          -2.69592       -1.59199        3.03335
C          -1.18591       -0.33880        4.65500
```

H	-1.67576	-2.54238	-5.25556
H	0.08553	-2.28360	-5.20829
H	-1.54078	-3.93473	-2.24718
H	-2.88846	-3.04687	-3.00303
H	-2.16256	-2.42504	-1.49310
H	-0.61634	-0.06197	-3.95726
H	-1.73021	-0.18407	-2.55128
H	-2.29427	-0.64700	-4.14768
H	0.01852	4.77481	0.62083
H	-1.10559	3.39429	0.85299
H	-1.57809	4.76593	-0.18028
H	1.05724	5.17826	-1.73768
H	-0.49193	4.97575	-2.56438
H	-1.72457	1.89562	-1.06614
H	-1.97914	3.20207	-2.20757
H	-0.76968	1.95973	-2.59276
H	-2.75088	1.22019	3.18733
H	-1.07504	1.48771	2.63469
H	-3.60031	-1.22411	3.54121
H	-2.92024	-1.73869	1.96856
H	-0.28886	0.29672	4.73626
H	-1.02207	-1.26632	5.21910
H	-2.02147	0.18647	5.14245
H	-0.63562	-3.82620	-4.63499
H	-2.42442	-2.55941	3.48576
H	0.87013	3.90190	-2.98199
C	4.83654	-0.97277	-0.63299
C	6.21230	-1.08362	-0.44691
C	6.73349	-1.10824	0.87085
C	5.82297	-0.97405	1.94685
C	4.46093	-0.86069	1.67687
H	4.41838	-0.90482	-1.63813
H	3.75513	-0.68335	2.48801
H	-2.26093	0.71011	1.54459
N	3.97576	-0.91109	0.41309
C	2.67375	4.36560	-0.16090
N	3.07828	5.44693	-0.01850
C	4.37111	1.94797	0.46288
N	5.48440	1.98388	0.80073
C	3.53408	-3.39466	-1.43350
N	4.50523	-3.98253	-1.17545
C	1.43025	-4.18802	-3.44144
N	1.57748	-5.17227	-4.04332
C	2.72119	-3.04892	2.40196
N	3.61267	-3.79369	2.47724
C	0.18258	-2.96974	4.10567
N	-0.01437	-3.74040	4.95457
C	8.13513	-1.23430	1.10484
N	9.27725	-1.33745	1.29531
C	6.26968	-0.93131	3.30620
N	6.62512	-0.89767	4.41127
C	7.06864	-1.16292	-1.59135
N	7.75867	-1.23063	-2.52302
H	-3.20228	-0.24406	-0.70656
C	-4.55991	0.01598	-1.14545
C	-4.66440	-0.22445	-2.61410
C	-4.50750	1.50510	-1.03400
C	-4.84342	-1.40027	-3.36192
C	-4.60733	1.01422	-3.31693

C	-4.34761	2.36028	0.07269
C	-4.53721	2.08984	-2.33535
C	-4.88995	-1.34509	-4.76178
H	-4.94895	-2.36814	-2.87200
C	-4.64306	1.06940	-4.71407
C	-4.30312	3.74748	-0.11658
H	-4.24492	1.96690	1.08217
C	-4.50289	3.47622	-2.51991
C	-4.77353	-0.12115	-5.44043
H	-5.01789	-2.27205	-5.33011
H	-4.58455	2.03209	-5.23255
C	-4.39842	4.31002	-1.39994
H	-4.18929	4.40127	0.75413
H	-4.54802	3.90199	-3.52775
H	-4.80183	-0.09674	-6.53437
H	-4.37052	5.39710	-1.52510
C	-5.41823	-0.85971	-0.18206
C	-6.87526	-0.90593	-0.70512
H	-6.95103	-1.41669	-1.67722
H	-7.51806	-1.44441	0.01373
H	-7.27639	0.11533	-0.82490
C	-4.86191	-2.29792	-0.08909
H	-3.81722	-2.28902	0.25575
H	-5.46082	-2.89027	0.62375
H	-4.88772	-2.82607	-1.05228
C	-5.46587	-0.27960	1.24334
H	-5.95584	-0.99907	1.92101
H	-4.46013	-0.08399	1.63427
H	-6.04382	0.65644	1.28120

$L_4Co^{III}O$ + 9-tBu-fluorene (*S*=1)

118
tbuflu_ts_u2.out Energy: -2740763.0447898

C	0.75309	-1.25005	-1.53890
N	0.52809	-2.19864	-2.48957
C	1.49143	-3.19716	-2.39664
C	2.38540	-2.80716	-1.41865
N	1.96148	-1.56683	-0.96077
B	2.46272	-0.69340	0.21868
N	2.28090	0.80609	-0.12424
C	1.02671	1.19747	-0.47784
N	1.06508	2.53057	-0.72658
C	2.34784	3.00674	-0.48392
C	3.12032	1.91937	-0.11427
N	1.54054	-1.06674	1.40915
C	0.26185	-0.56681	1.40676
N	-0.31916	-1.01384	2.55443
C	0.51719	-1.93237	3.18056
C	1.68367	-1.98377	2.44223
Co	-0.41632	-0.04692	-0.45733
O	-1.92429	-1.01747	-0.37840
C	-0.57645	-2.19382	-3.52671
C	0.03109	-2.52449	-4.90227
C	-1.60825	-3.23800	-3.08567
C	-1.17741	-0.79010	-3.60744
C	-0.12829	3.33961	-1.16130

C	-0.59042	4.19271	0.02790
C	0.24953	4.19944	-2.37764
C	-1.22350	2.36218	-1.58107
C	-1.60613	-0.50497	3.16941
C	-2.08791	0.70817	2.37329
C	-2.62879	-1.64723	3.13623
C	-1.30019	-0.04583	4.60760
H	-0.75283	-2.38281	-5.66228
H	0.86506	-1.84315	-5.13841
H	-1.14512	-4.22991	-2.95767
H	-2.38617	-3.32787	-3.85580
H	-2.06812	-2.92269	-2.13613
H	-0.39982	-0.04381	-3.83654
H	-1.69072	-0.52436	-2.67853
H	-1.92550	-0.77334	-4.41233
H	0.18512	4.91082	0.33936
H	-0.84818	3.55167	0.88662
H	-1.49021	4.75869	-0.25988
H	0.97540	4.98793	-2.13436
H	-0.66032	4.69583	-2.74961
H	-1.61134	1.76663	-0.73176
H	-2.08890	2.93180	-1.93977
H	-0.89539	1.71237	-2.40485
H	-2.98210	1.11294	2.87068
H	-1.32208	1.49996	2.34763
H	-3.58246	-1.30188	3.56350
H	-2.79885	-1.96528	2.09760
H	-0.49928	0.71160	4.61331
H	-1.01623	-0.87030	5.27658
H	-2.21022	0.41168	5.02605
H	0.37954	-3.56206	-4.99075
H	-2.29399	-2.51323	3.72820
H	0.65743	3.57286	-3.18750
C	4.87416	-1.08834	-0.49183
C	6.24971	-1.19178	-0.28368
C	6.75796	-1.06478	1.03035
C	5.84575	-0.79979	2.07754
C	4.48506	-0.70200	1.78362
H	4.46095	-1.13339	-1.50065
H	3.77170	-0.42772	2.56133
H	-2.34521	0.42376	1.34684
N	4.01259	-0.88780	0.53109
C	2.78372	4.35480	-0.55301
N	3.17518	5.45002	-0.57739
C	4.49995	1.95393	0.20378
N	5.63480	1.97991	0.46214
C	3.48179	-3.55814	-0.92502
N	4.38246	-4.16840	-0.51022
C	1.53707	-4.43593	-3.08800
N	1.61859	-5.48018	-3.59442
C	2.78498	-2.85330	2.64233
N	3.69614	-3.56327	2.78847
C	0.23286	-2.72551	4.32250
N	0.04286	-3.41307	5.24160
C	8.15976	-1.16918	1.28757
N	9.29959	-1.25259	1.49629
C	6.28545	-0.61012	3.42685
N	6.63457	-0.45736	4.52377
C	7.11332	-1.41355	-1.40379

N	7.80809	-1.59567	-2.31625
H	-3.06031	-0.61003	-0.83221
C	-4.31431	-0.27686	-1.22409
C	-4.39355	-0.52973	-2.70442
C	-4.36607	1.22642	-1.13358
C	-4.48225	-1.72133	-3.43558
C	-4.42326	0.70086	-3.41263
C	-4.30839	2.10126	-0.03682
C	-4.42786	1.78939	-2.43938
C	-4.54703	-1.68226	-4.83503
H	-4.49369	-2.68817	-2.93454
C	-4.47259	0.74421	-4.80938
C	-4.35717	3.48788	-0.24109
H	-4.21771	1.72900	0.98035
C	-4.48827	3.17174	-2.64372
C	-4.52634	-0.45959	-5.52353
H	-4.60850	-2.62061	-5.39556
H	-4.48486	1.70395	-5.33589
C	-4.45897	4.02553	-1.53293
H	-4.31447	4.15710	0.62401
H	-4.55093	3.58033	-3.65737
H	-4.56698	-0.44676	-6.61727
H	-4.50229	5.11011	-1.67344
C	-5.23694	-1.15894	-0.30955
C	-6.65334	-1.21696	-0.92933
H	-6.66748	-1.75712	-1.88797
H	-7.34250	-1.73309	-0.23794
H	-7.04478	-0.19987	-1.10516
C	-5.38622	-0.57213	1.10485
H	-5.91489	-1.29369	1.75017
H	-4.41206	-0.37088	1.56342
H	-5.97300	0.35895	1.10229
C	-4.67191	-2.58942	-0.16646
H	-4.62948	-3.12587	-1.12471
H	-3.65167	-2.56618	0.24317
H	-5.31591	-3.17972	0.50763

$L_4Co^{III}O$ + 9-tBu-fluorene (*S*=2)

118
tbuflu_ts_u4.out Energy: -2740755.0001561

C	0.76659	-1.18993	-1.52967
N	0.55239	-2.07055	-2.53751
C	1.48508	-3.10109	-2.44590
C	2.32976	-2.79117	-1.39760
N	1.91609	-1.56749	-0.89895
B	2.48044	-0.73430	0.30100
N	2.27940	0.78322	-0.06564
C	1.05696	1.20836	-0.43999
N	1.13888	2.50350	-0.81129
C	2.45779	2.92117	-0.67227
C	3.17546	1.83491	-0.19355
N	1.51206	-1.09275	1.47788
C	0.24351	-0.59648	1.50499
N	-0.33508	-1.04958	2.64679
C	0.52552	-1.94394	3.27519
C	1.68165	-1.98981	2.51913

Co	-0.46698	-0.00024	-0.40564
O	-1.82668	-1.06797	-0.57759
C	-0.46038	-1.97077	-3.66478
C	0.28816	-2.13699	-5.00053
C	-1.49472	-3.07904	-3.43972
C	-1.09894	-0.58151	-3.66095
C	-0.00058	3.31156	-1.37542
C	-0.15240	4.61471	-0.57627
C	0.29084	3.57040	-2.86142
C	-1.27755	2.49030	-1.21877
C	-1.62976	-0.57232	3.27392
C	-2.21950	0.53341	2.40560
C	-2.59585	-1.76175	3.36995
C	-1.29469	0.01327	4.65795
H	-0.42961	-1.96498	-5.81743
H	1.09779	-1.39458	-5.09049
H	-1.02875	-4.07649	-3.43616
H	-2.23133	-3.05805	-4.25415
H	-2.01125	-2.92022	-2.48135
H	-0.33631	0.20830	-3.75122
H	-1.70404	-0.41737	-2.76577
H	-1.77554	-0.50698	-4.52420
H	0.69760	5.29682	-0.71955
H	-0.26613	4.40217	0.49891
H	-1.05819	5.13576	-0.92392
H	1.20996	4.15989	-3.00210
H	-0.54468	4.13952	-3.29795
H	-1.58485	2.39927	-0.16500
H	-2.10270	2.99792	-1.73503
H	-1.21156	1.50690	-1.73209
H	-3.11098	0.93146	2.91103
H	-1.51075	1.36445	2.26117
H	-3.55531	-1.41494	3.78338
H	-2.78111	-2.19399	2.37498
H	-0.55980	0.82956	4.56788
H	-0.90749	-0.73814	5.36078
H	-2.21794	0.42429	5.09540
H	0.70675	-3.14184	-5.14579
H	-2.21875	-2.55348	4.03360
H	0.39291	2.62087	-3.41160
C	4.86785	-1.19949	-0.41577
C	6.21005	-1.35254	-0.18075
C	6.74743	-1.23191	1.15653
C	5.79665	-0.83025	2.16938
C	4.46598	-0.69388	1.86920
H	4.47974	-1.22616	-1.43395
H	3.76509	-0.33209	2.62163
H	-2.51940	0.13875	1.42760
N	3.95359	-0.96825	0.60577
C	2.97088	4.20602	-0.98388
N	3.42385	5.24564	-1.24215
C	4.56296	1.84244	0.10360
N	5.70074	1.91755	0.33150
C	3.35504	-3.62064	-0.87165
N	4.16518	-4.34025	-0.44945
C	1.53828	-4.29369	-3.21328
N	1.61987	-5.30191	-3.78762
C	2.77959	-2.86777	2.71948
N	3.64312	-3.62569	2.89901

C	0.27431	-2.70376	4.44707
N	0.11410	-3.35507	5.39736
C	8.11069	-1.42803	1.44032
N	9.24507	-1.59237	1.67732
C	6.22609	-0.54137	3.50386
N	6.57604	-0.31062	4.58880
C	7.07077	-1.61111	-1.29473
N	7.77121	-1.82615	-2.19804
H	-3.11872	-0.60011	-0.80347
C	-4.33599	-0.31104	-1.11670
C	-4.37616	-0.48353	-2.61332
C	-4.42988	1.18553	-0.94079
C	-4.41734	-1.63688	-3.40656
C	-4.42436	0.78434	-3.24902
C	-4.43874	1.99382	0.20627
C	-4.47192	1.81708	-2.21469
C	-4.47727	-1.52028	-4.80246
H	-4.40124	-2.63062	-2.96090
C	-4.46566	0.90503	-4.63844
C	-4.52158	3.38899	0.07880
H	-4.38384	1.56670	1.20351
C	-4.56663	3.20352	-2.34336
C	-4.48657	-0.26146	-5.41833
H	-4.51117	-2.42588	-5.41575
H	-4.50107	1.89065	-5.11250
C	-4.59374	3.99329	-1.18274
H	-4.53187	4.00821	0.98075
H	-4.61809	3.66804	-3.33281
H	-4.52262	-0.18786	-6.50956
H	-4.66400	5.08220	-1.26514
C	-5.21260	-1.29374	-0.25939
C	-4.54991	-2.68460	-0.16547
H	-3.57155	-2.62109	0.33541
H	-5.19601	-3.36579	0.41273
H	-4.38233	-3.14742	-1.14785
C	-5.44455	-0.79164	1.17561
H	-5.97432	-1.56951	1.74969
H	-4.50284	-0.58937	1.69844
H	-6.06590	0.11622	1.19975
C	-6.60542	-1.41222	-0.92779
H	-6.56171	-1.92139	-1.90134
H	-7.27805	-1.98950	-0.27058
H	-7.05071	-0.41445	-1.08181

$L_4Co^{III}O$ + THF (*S*=0, open-shell)

96
thf_percn_ts_u0_open.out Energy: -2473389.2914736

C	0.59745	-1.16139	-1.51703
N	0.33255	-2.05131	-2.51362
C	1.35194	-2.99614	-2.57380
C	2.31178	-2.61845	-1.65143
N	1.86668	-1.43721	-1.06896
B	2.38921	-0.59462	0.13018
N	2.04363	0.90306	-0.09780
C	0.72260	1.20397	-0.26916
N	0.62189	2.54865	-0.42660

C	1.89196	3.11426	-0.35535
C	2.78833	2.07962	-0.15055
N	1.61441	-1.12436	1.37300
C	0.29013	-0.77675	1.47355
N	-0.19230	-1.38885	2.58860
C	0.77109	-2.25710	3.09408
C	1.90505	-2.10329	2.31607
Co	-0.52623	-0.20920	-0.22912
O	-1.85600	-1.42335	-0.16893
C	-0.85695	-2.00089	-3.45545
C	-0.35935	-2.22812	-4.89388
C	-1.86003	-3.07375	-3.01098
C	-1.47954	-0.60337	-3.38671
C	-0.67027	3.30435	-0.62697
C	-0.85927	4.26205	0.55967
C	-0.59867	4.04742	-1.97001
C	-1.82662	2.30053	-0.66350
C	-1.54289	-1.13173	3.23283
C	-2.15012	0.14822	2.64787
C	-2.44041	-2.34184	2.94349
C	-1.32581	-0.91115	4.74078
H	-1.20234	-2.05551	-5.58074
H	0.44362	-1.51769	-5.15117
H	-1.42202	-4.08358	-3.07619
H	-2.74278	-3.04408	-3.66999
H	-2.16714	-2.87030	-1.97292
H	-0.74225	0.18147	-3.61895
H	-1.90980	-0.41811	-2.39873
H	-2.29492	-0.54820	-4.12409
H	-0.06624	5.02333	0.61381
H	-0.87931	3.70188	1.50882
H	-1.81946	4.78941	0.44654
H	0.19137	4.81303	-1.98579
H	-1.55816	4.55775	-2.14828
H	-1.93417	1.75035	0.28481
H	-2.77333	2.84331	-0.80428
H	-1.72941	1.60465	-1.51221
H	-3.04826	0.39692	3.23360
H	-1.45051	0.99622	2.72091
H	-3.43534	-2.17085	3.38510
H	-2.53848	-2.45961	1.85277
H	-0.61152	-0.09030	4.91872
H	-0.97624	-1.80935	5.26751
H	-2.29038	-0.63060	5.19134
H	-0.00446	-3.25148	-5.07476
H	-2.03104	-3.26659	3.38211
H	-0.42290	3.33803	-2.79528
C	4.76835	-0.78231	-0.77631
C	6.15965	-0.77830	-0.66687
C	6.74847	-0.62151	0.60939
C	5.89473	-0.44356	1.72231
C	4.51336	-0.46389	1.52838
H	4.29088	-0.84387	-1.75529
H	3.83578	-0.27780	2.36276
H	-2.45757	0.00760	1.60592
N	3.96945	-0.66763	0.30800
C	2.21765	4.49010	-0.46691
N	2.51729	5.61122	-0.55104
C	4.19319	2.21083	-0.02749

N	5.34861	2.31193	0.07363
C	3.49038	-3.32571	-1.30587
N	4.46245	-3.89122	-1.00369
C	1.38873	-4.18323	-3.35066
N	1.45936	-5.18557	-3.93727
C	3.11192	-2.84130	2.40316
N	4.11184	-3.43618	2.45110
C	0.62272	-3.19872	4.14549
N	0.54780	-4.00882	4.97735
C	8.16862	-0.61257	0.76782
N	9.32313	-0.60464	0.89736
C	6.41404	-0.22668	3.03850
N	6.82882	-0.05117	4.10883
C	6.95610	-0.91789	-1.84826
N	7.59632	-1.03383	-2.81011
H	-3.01284	-0.80757	-0.56020
C	-4.08921	-0.28838	-0.84811
O	-4.43403	0.61516	0.16154
C	-5.12549	-1.40108	-0.85076
H	-3.92048	0.24482	-1.79878
C	-5.42788	0.03213	1.02922
C	-5.51219	-1.44512	0.63538
H	-4.72271	-2.35184	-1.23423
H	-5.99205	-1.11732	-1.47753
H	-5.12469	0.19704	2.07622
H	-6.38574	0.55949	0.85706
H	-4.77117	-2.03278	1.20105
H	-6.50896	-1.87435	0.82049

$L_4Co^{III}O$ + THF (*S*=1)

96
thf_percn_ts_u2.out Energy: -2473391.1659134

C	0.50310	-0.95434	-1.48394
N	0.15387	-1.84062	-2.45492
C	1.06966	-2.88876	-2.47488
C	2.05040	-2.58994	-1.54528
N	1.72793	-1.34939	-1.00642
B	2.32629	-0.51220	0.16237
N	2.13453	1.00103	-0.13804
C	0.85467	1.44601	-0.34029
N	0.92562	2.77933	-0.60347
C	2.25725	3.18523	-0.56793
C	3.01777	2.06833	-0.27692
N	1.50546	-0.89923	1.42631
C	0.22300	-0.41487	1.50236
N	-0.32367	-0.92393	2.63958
C	0.54641	-1.85863	3.19242
C	1.69263	-1.85681	2.41703
Co	-0.52232	0.13857	-0.21917
O	-1.87194	-1.04842	-0.18208
C	-1.02341	-1.70820	-3.40336
C	-0.51605	-1.93566	-4.83871
C	-2.08121	-2.74013	-2.98774
C	-1.58758	-0.28501	-3.31847
C	-0.23715	3.69603	-0.90904
C	-0.28327	4.79647	0.16328

C	-0.04332	4.26581	-2.32396
C	-1.53971	2.89515	-0.86354
C	-1.65959	-0.52548	3.24175
C	-2.13449	0.77690	2.59087
C	-2.65284	-1.66507	2.97899
C	-1.45864	-0.26112	4.74448
H	-1.34803	-1.74821	-5.53514
H	0.30089	-1.23616	-5.08141
H	-1.70051	-3.77078	-3.07450
H	-2.95878	-2.65097	-3.64809
H	-2.38042	-2.54332	-1.94663
H	-0.80946	0.47064	-3.51232
H	-2.04264	-0.10197	-2.33863
H	-2.37063	-0.17948	-4.08505
H	0.60960	5.43889	0.14868
H	-0.38513	4.35236	1.16701
H	-1.15699	5.44079	-0.02216
H	0.85945	4.88883	-2.40867
H	-0.90714	4.90041	-2.57676
H	-1.73057	2.48837	0.14166
H	-2.37459	3.57262	-1.10021
H	-1.55086	2.09425	-1.61949
H	-3.06330	1.09349	3.08782
H	-1.38410	1.57705	2.69392
H	-3.63736	-1.38934	3.38761
H	-2.74122	-1.81925	1.89322
H	-0.66901	0.49039	4.91012
H	-1.21620	-1.16654	5.31720
H	-2.40086	0.13509	5.15373
H	-0.17148	-2.96297	-5.01991
H	-2.33024	-2.60072	3.46464
H	0.01783	3.45018	-3.06312
C	4.66752	-1.00140	-0.72559
C	6.04960	-1.15702	-0.61364
C	6.65687	-1.00906	0.65462
C	5.83408	-0.67646	1.75564
C	4.45922	-0.54209	1.55970
H	4.18308	-1.04958	-1.70135
H	3.81040	-0.23458	2.38105
H	-2.37124	0.62290	1.53448
N	3.89089	-0.74215	0.34950
C	2.76273	4.49244	-0.78624
N	3.21851	5.54900	-0.95904
C	4.42856	2.04614	-0.15101
N	5.58817	2.02936	-0.04910
C	3.13789	-3.40911	-1.15111
N	4.03712	-4.06253	-0.80384
C	0.99924	-4.08568	-3.23398
N	0.97624	-5.09530	-3.81193
C	2.81853	-2.70683	2.55148
N	3.75436	-3.39407	2.64160
C	0.30482	-2.72657	4.28889
N	0.15124	-3.48154	5.16083
C	8.06863	-1.16090	0.81450
N	9.21660	-1.28316	0.94458
C	6.38014	-0.46173	3.06124
N	6.81634	-0.28784	4.12330
C	6.81894	-1.44869	-1.78540
N	7.43645	-1.68795	-2.73928

H	-3.02781	-0.44163	-0.23889
C	-4.19134	0.05681	-0.29831
O	-4.81904	-0.16031	0.92445
C	-4.94210	-0.74575	-1.34622
H	-4.03421	1.13518	-0.47183
C	-5.62964	-1.35227	0.85495
C	-5.34739	-1.97399	-0.51773
H	-4.32720	-0.98830	-2.22513
H	-5.83257	-0.18717	-1.69310
H	-5.36900	-2.00911	1.70152
H	-6.68802	-1.04845	0.96218
H	-4.49874	-2.67632	-0.45339
H	-6.21627	-2.51560	-0.92236

$L_4Co^{III}O$ + THF (*S*=2)

96
thf_percn_ts_u4.out Energy: -2473384.7564438

C	0.55451	-1.34924	-1.26922
N	0.27713	-2.39683	-2.08534
C	1.39899	-3.20829	-2.19516
C	2.39946	-2.61470	-1.44167
N	1.87727	-1.42799	-0.92903
B	2.40102	-0.45716	0.19513
N	2.01126	1.04712	-0.06682
C	0.70319	1.43083	-0.18368
N	0.66794	2.76811	-0.38865
C	1.96304	3.26456	-0.40450
C	2.81218	2.18858	-0.20394
N	1.73472	-1.01652	1.49522
C	0.39092	-0.81444	1.67428
N	0.02033	-1.53898	2.76262
C	1.09738	-2.29349	3.21237
C	2.17249	-1.98754	2.39540
Co	-0.59061	-0.10634	-0.06679
O	-2.35292	-0.10197	0.14943
C	-1.10644	-2.60713	-2.69219
C	-1.04984	-3.63848	-3.82278
C	-2.03931	-3.08544	-1.57054
C	-1.57167	-1.25961	-3.26461
C	-0.64946	3.50503	-0.61447
C	-0.41814	5.01128	-0.74805
C	-1.25116	2.95652	-1.91579
C	-1.55513	3.23143	0.59567
C	-1.39697	-1.51069	3.32489
C	-1.86230	-0.04636	3.33726
C	-2.27303	-2.37749	2.41046
C	-1.41796	-2.05186	4.75884
H	-2.03693	-3.65441	-4.30962
H	-0.30476	-3.37316	-4.59006
H	-1.65819	-4.00928	-1.10555
H	-3.03320	-3.29603	-1.99741
H	-2.15908	-2.30617	-0.80295
H	-0.85757	-0.87561	-4.01062
H	-1.70393	-0.50972	-2.47401
H	-2.54880	-1.40018	-3.75239
H	0.19605	5.26847	-1.62392

H	0.02944	5.44749	0.15850
H	-1.40185	5.48440	-0.89061
H	-0.58903	3.16323	-2.77237
H	-2.23156	3.42430	-2.08620
H	-1.06026	3.54351	1.52993
H	-2.48378	3.80922	0.47532
H	-1.83833	2.17190	0.66362
H	-2.86801	-0.00407	3.78503
H	-1.18416	0.57352	3.94676
H	-3.29533	-2.41319	2.82081
H	-2.32549	-1.94008	1.40291
H	-0.69456	-1.53314	5.40902
H	-1.24462	-3.13589	4.80783
H	-2.42326	-1.86929	5.16848
H	-0.85518	-4.65654	-3.45729
H	-1.88578	-3.40848	2.35520
H	-1.41659	1.87193	-1.84758
C	4.74130	-0.59267	-0.82589
C	6.13580	-0.57588	-0.78060
C	6.78123	-0.37821	0.46157
C	5.97864	-0.16641	1.60644
C	4.59037	-0.20810	1.47806
H	4.22004	-0.67916	-1.78039
H	3.94802	-0.00061	2.33515
H	-1.93136	0.36441	2.32159
N	3.99198	-0.46255	0.29207
C	2.42244	4.59840	-0.57642
N	2.89390	5.65359	-0.70572
C	4.22232	2.31347	-0.15807
N	5.37693	2.46074	-0.12781
C	3.67814	-3.17277	-1.19007
N	4.72140	-3.64200	-0.97240
C	1.56612	-4.43684	-2.88864
N	1.79745	-5.44853	-3.41349
C	3.44638	-2.60745	2.43200
N	4.49142	-3.12147	2.44410
C	1.16529	-3.24523	4.26509
N	1.31911	-4.04890	5.09169
C	8.20684	-0.36040	0.55367
N	9.36608	-0.34536	0.62892
C	6.55723	0.09714	2.88898
N	7.02090	0.30900	3.93234
C	6.87676	-0.74966	-1.99263
N	7.47155	-0.89560	-2.97923
H	-3.16232	0.49386	-0.83787
C	-4.07371	0.96575	-1.47727
O	-4.26986	2.28891	-1.07199
C	-5.29287	0.17700	-1.02577
H	-3.79383	0.92842	-2.54342
C	-5.22967	2.33031	0.00378
C	-5.57963	0.86914	0.31628
H	-5.08718	-0.90080	-0.93120
H	-6.13010	0.31367	-1.73619
H	-4.78477	2.86891	0.85856
H	-6.10801	2.90384	-0.34783
H	-4.89503	0.47055	1.08338
H	-6.61617	0.74971	0.66779

$L_4Co^{III}O$ + xanthene (*S*=0, open-shell)

```
107
xanthene_ts_u0_closed.out Energy: -2689310.7124113
C           0.82081       -0.98244       -1.52467
N           0.54354       -1.74451       -2.62701
C           1.65480       -2.52888       -2.92244
C           2.64545       -2.19990       -2.01493
N           2.13489       -1.19762       -1.20461
B           2.61768       -0.58463        0.13709
N           2.23456        0.92167        0.17438
C           0.94572        1.24381       -0.11961
N           0.81939        2.59511       -0.01602
C           2.02905        3.12519        0.42562
C           2.92381        2.07477        0.53274
N           1.77306       -1.34297        1.21024
C           0.45223       -1.00209        1.31367
N          -0.07028       -1.73308        2.34139
C           0.86544       -2.68827        2.72992
C           2.02083       -2.45230        2.00568
Co         -0.33105       -0.15020       -0.25514
O          -1.94045       -0.69374       -0.04186
C          -0.80780       -1.82086       -3.32846
C          -0.62781       -2.27264       -4.78526
C          -1.65782       -2.83052       -2.54582
C          -1.42915       -0.41778       -3.34719
C          -0.44634        3.39052       -0.27869
C          -1.09738        3.68016        1.08127
C          -0.09012        4.68072       -1.03515
C          -1.37997        2.56257       -1.16664
C          -1.37925       -1.45457        3.08864
C          -1.74280        0.02705        2.91669
C          -2.45768       -2.39158        2.53743
C          -1.14715       -1.69678        4.59179
H          -1.58937       -2.12684       -5.30042
H           0.13083       -1.67102       -5.31230
H          -1.16818       -3.81849       -2.53184
H          -2.63947       -2.93941       -3.03001
H          -1.81668       -2.48556       -1.51322
H          -0.74767        0.30968       -3.81634
H          -1.70253       -0.06904       -2.34580
H          -2.35646       -0.45512       -3.93868
H          -0.43053        4.27313        1.72844
H          -1.35264        2.74063        1.59758
H          -2.02466        4.25515        0.92929
H           0.46882        5.40164       -0.42489
H          -1.02733        5.17427       -1.33473
H          -1.78816        1.68642       -0.64234
H          -2.23640        3.19136       -1.45439
H          -0.87347        2.23587       -2.08723
H          -2.61578        0.23993        3.55094
H          -0.91113        0.67389        3.24271
H          -3.39967       -2.21853        3.07987
H          -2.61961       -2.18193        1.47131
H          -0.26457       -1.14706        4.95886
H          -1.04910       -2.75782        4.85456
H          -2.02938       -1.31769        5.12967
H          -0.37998       -3.33779       -4.87648
H          -2.16984       -3.44747        2.67539
```

```
H          0.48629        4.45581       -1.94741
C          4.98339       -0.42107       -0.72832
C          6.36797       -0.40647       -0.61339
C          6.96546       -0.62590        0.65698
C          6.10124       -0.81145        1.76706
C          4.72427       -0.80902        1.57170
H          4.50398       -0.20632       -1.68436
H          4.04983       -0.87615        2.42460
H         -2.01701        0.26906        1.88636
N          4.17523       -0.66685        0.33789
C          2.31422        4.46825        0.78411
N          2.60903        5.54033        1.12638
C          4.27754        2.17763        0.93812
N          5.38900        2.26851        1.27175
C          3.91338       -2.82044       -1.88667
N          4.95338       -3.32923       -1.76565
C          1.81573       -3.53409       -3.91265
N          2.05423       -4.38563       -4.66824
C          3.19367       -3.24816        1.97746
N          4.15662       -3.90051        1.92743
C          0.67444       -3.79667        3.59634
N          0.58491       -4.75094        4.25564
C          8.38042       -0.62527        0.81621
N          9.53658       -0.62435        0.94624
C          6.61427       -0.97876        3.09291
N          7.02526       -1.11638        4.17054
C          7.16106       -0.16060       -1.77937
N          7.80077        0.03523       -2.72891
H         -3.03166       -0.49136       -0.58032
C         -4.30116       -0.17246       -0.86889
C         -4.94732       -1.43333       -1.23922
C         -4.66941        0.35684        0.44875
H         -4.18995        0.56765       -1.67357
C         -5.44408       -2.26264       -0.20650
C         -5.04953       -1.90569       -2.56265
C         -5.18427       -0.54019        1.41250
C         -4.43562        1.68635        0.85240
C         -5.98015       -3.52560       -0.47188
C         -5.59096       -3.16137       -2.84125
H         -4.68812       -1.26828       -3.37614
C         -5.45852       -0.13377        2.72163
C         -4.70197        2.10306        2.15659
H         -4.03699        2.39419        0.12020
C         -6.04544       -3.97826       -1.79259
H         -6.34749       -4.12887        0.36298
H         -5.65780       -3.50978       -3.87634
H         -5.86215       -0.86498        3.42741
C         -5.21306        1.19025        3.09427
H         -4.50971        3.14009        2.44780
H         -6.46535       -4.96598       -2.00583
H         -5.42281        1.51177        4.11891
O         -5.42662       -1.85258        1.10289
```

$L_4Co^{III}O$ + xanthene (*S*=0, closed-shell)

```
107
xanthene_ts_u0_open.out    Energy: -2689314.7791244
```

C	0.58520	-1.22992	-1.35803
N	0.27836	-2.19529	-2.26734
C	1.27808	-3.16247	-2.26981
C	2.26945	-2.72494	-1.40927
N	1.85876	-1.48965	-0.92220
B	2.43337	-0.53619	0.16588
N	2.11508	0.93902	-0.20509
C	0.79818	1.26616	-0.35570
N	0.73532	2.57910	-0.69837
C	2.02703	3.09579	-0.76514
C	2.89610	2.06462	-0.45618
N	1.67451	-0.91777	1.46573
C	0.35373	-0.54985	1.55012
N	-0.11251	-1.03726	2.73450
C	0.84921	-1.86448	3.30402
C	1.97043	-1.80139	2.49653
Co	-0.50234	-0.09225	-0.11823
O	-1.94501	-1.10248	-0.16124
C	-0.92203	-2.18877	-3.20265
C	-0.45293	-2.60496	-4.60849
C	-1.96663	-3.15717	-2.63705
C	-1.47125	-0.76053	-3.29467
C	-0.52864	3.36287	-0.97568
C	-0.62008	4.50771	0.04556
C	-0.47152	3.87382	-2.42432
C	-1.74255	2.44200	-0.81521
C	-1.45630	-0.70650	3.35642
C	-1.96001	0.60972	2.75284
C	-2.40521	-1.87370	3.06194
C	-1.27136	-0.48470	4.86768
H	-1.29453	-2.46162	-5.30350
H	0.38512	-1.97550	-4.95116
H	-1.57084	-4.18531	-2.58429
H	-2.85194	-3.16159	-3.29076
H	-2.27334	-2.82218	-1.63436
H	-0.68104	-0.04482	-3.57497
H	-1.93511	-0.45807	-2.34992
H	-2.25178	-0.74388	-4.06887
H	0.20827	5.22540	-0.05140
H	-0.62580	4.10861	1.07315
H	-1.55812	5.06097	-0.11840
H	0.35991	4.57447	-2.59215
H	-1.40623	4.40974	-2.65229
H	-1.83571	2.06073	0.21355
H	-2.65223	3.02702	-1.02166
H	-1.72823	1.61064	-1.53743
H	-2.84298	0.93285	3.32007
H	-1.19447	1.39929	2.81751
H	-3.39362	-1.66399	3.49642
H	-2.51013	-1.99791	1.97335
H	-0.50045	0.27776	5.06797
H	-1.02077	-1.40271	5.41473
H	-2.22715	-0.12218	5.27629
H	-0.16086	-3.66112	-4.67742
H	-2.02678	-2.81042	3.50400
H	-0.37341	3.03036	-3.12733
C	4.78104	-0.89045	-0.76739
C	6.17320	-0.93515	-0.68600
C	6.79852	-0.67390	0.55470

```
C          5.98019       -0.34013        1.65892
C          4.59506       -0.31961        1.49489
H          4.27834       -1.03031       -1.72494
H          3.94450       -0.01703        2.31661
H         -2.26723        0.48421        1.70889
N          4.01392       -0.63211        0.31485
C          2.39933        4.42711       -1.08294
N          2.74235        5.50906       -1.33866
C          4.30850        2.15981       -0.40157
N          5.46948        2.23096       -0.35348
C          3.44180       -3.42479       -1.02941
N          4.40948       -3.98217       -0.69922
C          1.27393       -4.41979       -2.92863
N          1.31779       -5.47797       -3.41023
C          3.16851       -2.54466        2.63824
N          4.16064       -3.14692        2.73277
C          0.71506       -2.70941        4.43646
N          0.66523       -3.45106        5.33146
C          8.22099       -0.71783        0.68200
N          9.37761       -0.75330        0.78539
C          6.53965       -0.01678        2.93626
N          6.98702        0.24391        3.97566
C          6.93428       -1.23222       -1.86129
N          7.54536       -1.47641       -2.81805
H         -3.17465       -0.54758        0.05521
C         -4.37371       -0.18287       -0.00161
C         -4.82107       -0.91512       -1.20755
C         -5.06387       -0.62685        1.22786
H         -4.31827        0.90934       -0.12528
C         -5.26477       -2.24447       -1.04265
C         -4.75870       -0.39740       -2.51208
C         -5.48820       -1.97076        1.29695
C         -5.28215        0.18909        2.35156
C         -5.61867       -3.04039       -2.13577
C         -5.11722       -1.17826       -3.61279
H         -4.41341        0.63194       -2.65323
C         -6.04703       -2.50557        2.46144
C         -5.85066       -0.32740        3.51806
H         -4.99114        1.24287        2.29962
C         -5.54052       -2.50361       -3.42380
H         -5.95866       -4.06419       -1.95728
H         -5.06266       -0.75878       -4.62195
H         -6.35178       -3.55571        2.46808
C         -6.21703       -1.68189        3.57785
H         -6.00622        0.32225        4.38461
H         -5.81796       -3.12052       -4.28407
H         -6.65402       -2.09413        4.49251
O         -5.37553       -2.80054        0.20860
```

$L_4Co^{III}O$ + xanthene (*S*=1)

```
107
xanthene_ts_u2.out        Energy: -2689316.7319590
C          0.55533       -1.17853       -1.35576
N          0.23801       -2.13448       -2.26993
C          1.22619       -3.11265       -2.28132
C          2.22226       -2.69348       -1.41745
```

N	1.82755	-1.45671	-0.91967
B	2.41848	-0.53414	0.18526
N	2.11112	0.94892	-0.15934
C	0.79765	1.27857	-0.31945
N	0.73389	2.60019	-0.61890
C	2.02408	3.12376	-0.65000
C	2.89208	2.08551	-0.36016
N	1.66957	-0.93046	1.49023
C	0.36036	-0.53324	1.60842
N	-0.09418	-1.03212	2.78943
C	0.85957	-1.88748	3.33025
C	1.96710	-1.83558	2.50280
Co	-0.51155	-0.07855	-0.10621
O	-1.87423	-1.18716	0.04498
C	-0.97302	-2.11480	-3.18380
C	-0.52093	-2.47370	-4.61047
C	-1.99664	-3.11434	-2.63334
C	-1.54028	-0.69240	-3.21484
C	-0.53730	3.37315	-0.88015
C	-0.65161	4.48991	0.16898
C	-0.48566	3.92159	-2.31468
C	-1.73090	2.42106	-0.74235
C	-1.41113	-0.67274	3.45199
C	-1.94205	0.61803	2.82053
C	-2.38053	-1.84105	3.23924
C	-1.15414	-0.39682	4.94413
H	-1.38167	-2.34319	-5.28446
H	0.28711	-1.80497	-4.95069
H	-1.59269	-4.14039	-2.63199
H	-2.89814	-3.10101	-3.26407
H	-2.27496	-2.82312	-1.60938
H	-0.76290	0.04619	-3.46816
H	-2.00073	-0.43296	-2.25535
H	-2.32575	-0.65284	-3.98188
H	0.16214	5.22609	0.08788
H	-0.64723	4.06603	1.18654
H	-1.60103	5.02765	0.01938
H	0.33900	4.63531	-2.46090
H	-1.42577	4.45310	-2.53050
H	-1.82234	2.02449	0.28176
H	-2.65566	2.98235	-0.94657
H	-1.68885	1.60423	-1.48150
H	-2.81532	0.94891	3.39917
H	-1.18377	1.41725	2.83941
H	-3.35430	-1.59642	3.68925
H	-2.51901	-2.00637	2.16029
H	-0.37931	0.37635	5.07737
H	-0.86704	-1.29332	5.50951
H	-2.09023	-0.02534	5.38888
H	-0.19099	-3.51598	-4.71345
H	-2.00469	-2.76341	3.71235
H	-0.37606	3.09826	-3.03955
C	4.75193	-0.88300	-0.78339
C	6.14457	-0.93929	-0.72075
C	6.78714	-0.71556	0.51874
C	5.98510	-0.40565	1.64142
C	4.59805	-0.36998	1.49509
H	4.23630	-0.99691	-1.73761
H	3.96036	-0.08239	2.33209

H	-2.27271	0.44425	1.79069
N	4.00011	-0.64713	0.31490
C	2.38989	4.46586	-0.92630
N	2.72214	5.55830	-1.14957
C	4.30383	2.17639	-0.28590
N	5.46454	2.23969	-0.22282
C	3.38993	-3.40735	-1.04944
N	4.35452	-3.97682	-0.73107
C	1.20775	-4.35831	-2.96124
N	1.23620	-5.40625	-3.46586
C	3.15436	-2.60085	2.61587
N	4.13832	-3.21935	2.68871
C	0.72458	-2.73888	4.45775
N	0.66403	-3.48218	5.35077
C	8.21068	-0.77375	0.62737
N	9.36814	-0.82089	0.71554
C	6.56262	-0.11896	2.91959
N	7.02450	0.11239	3.95959
C	6.88861	-1.21184	-1.91291
N	7.48585	-1.43596	-2.88323
H	-3.09600	-0.64638	-0.14710
C	-4.29230	-0.26976	-0.30424
C	-4.79855	-1.08979	-1.42728
C	-4.95994	-0.59459	0.97585
H	-4.22153	0.80667	-0.52103
C	-5.24367	-2.39721	-1.13786
C	-4.82383	-0.66781	-2.76735
C	-5.39681	-1.92211	1.17079
C	-5.14810	0.32059	2.02543
C	-5.65564	-3.27265	-2.14659
C	-5.24355	-1.52739	-3.78485
H	-4.49916	0.35053	-3.00362
C	-5.95518	-2.34088	2.38183
C	-5.71615	-0.07995	3.23669
H	-4.83322	1.35868	1.87965
C	-5.64766	-2.83585	-3.47432
H	-5.98946	-4.27704	-1.87195
H	-5.25315	-1.18189	-4.82303
H	-6.27559	-3.38122	2.48526
C	-6.10734	-1.41623	3.41892
H	-5.85155	0.64647	4.04368
H	-5.97093	-3.51525	-4.26896
H	-6.54608	-1.73666	4.36885
O	-5.30476	-2.84717	0.15899

$L_4Co^{III}O$ + xanthene (*S*=2)

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xanthene_ts_u4.out Energy: -2689310.8834264

C	0.31257	-1.26137	-0.81598
N	-0.14866	-2.38404	-1.41610
C	0.89089	-3.29209	-1.56183
C	2.02851	-2.68746	-1.04723
N	1.65824	-1.41046	-0.63023
B	2.38361	-0.31012	0.23703
N	2.20240	1.14570	-0.33473
C	0.96872	1.63315	-0.68540

N	1.13376	2.89086	-1.14908
C	2.47176	3.25207	-1.04223
C	3.14589	2.16097	-0.52718
N	1.72532	-0.45948	1.63363
C	0.51027	0.13724	1.85883
N	0.04591	-0.35780	3.03705
C	0.88158	-1.37424	3.48414
C	1.92872	-1.45942	2.58493
Co	-0.54404	0.45138	-0.01625
O	-2.18925	0.76235	0.42522
C	-1.61336	-2.52552	-1.81637
C	-1.83617	-3.79189	-2.64507
C	-2.44421	-2.58503	-0.52625
C	-1.96681	-1.29545	-2.66452
C	0.04388	3.79075	-1.71037
C	-0.13268	4.97159	-0.74364
C	0.47726	4.24407	-3.11513
C	-1.26938	3.01329	-1.82630
C	-1.23180	0.11022	3.72261
C	-1.48820	1.56883	3.32111
C	-2.36712	-0.81346	3.26223
C	-1.04470	0.05287	5.24749
H	-2.89204	-3.79832	-2.95682
H	-1.22063	-3.80843	-3.55843
H	-2.12732	-3.43148	0.10483
H	-3.50551	-2.71969	-0.78460
H	-2.35863	-1.64895	0.04521
H	-1.25696	-1.17278	-3.49813
H	-1.97860	-0.37685	-2.06042
H	-2.97510	-1.42245	-3.08037
H	0.78026	5.58063	-0.65350
H	-0.41870	4.60854	0.25714
H	-0.93480	5.62667	-1.11848
H	1.38156	4.86902	-3.10851
H	-0.33185	4.84777	-3.55474
H	-1.66448	2.70069	-0.84969
H	-2.01307	3.67734	-2.29398
H	-1.16203	2.12281	-2.46655
H	-2.38600	1.91493	3.85766
H	-0.63954	2.20993	3.61193
H	-3.30175	-0.52583	3.76822
H	-2.52307	-0.70666	2.17864
H	-0.11715	0.56079	5.56006
H	-1.04998	-0.96973	5.64729
H	-1.89202	0.58045	5.71175
H	-1.66233	-4.71047	-2.06583
H	-2.14815	-1.86545	3.51185
H	0.65093	3.37212	-3.76667
C	4.57485	-0.78506	-0.92975
C	5.95321	-0.97599	-1.01759
C	6.72935	-0.92369	0.16351
C	6.07332	-0.63894	1.38343
C	4.69029	-0.45009	1.38479
H	3.95296	-0.79325	-1.82729
H	4.17384	-0.16233	2.30051
H	-1.68067	1.66381	2.24517
N	3.95888	-0.56316	0.25506
C	3.05818	4.50676	-1.35389
N	3.57877	5.52196	-1.58102

C	4.53543	2.15492	-0.24635
N	5.67695	2.18324	-0.02036
C	3.30025	-3.30320	-0.93327
N	4.33855	-3.82213	-0.84342
C	0.87600	-4.60884	-2.09512
N	0.96282	-5.69305	-2.50660
C	2.96074	-2.42970	2.57131
N	3.80840	-3.22723	2.52542
C	0.70778	-2.24802	4.59031
N	0.62315	-3.02309	5.45353
C	8.14263	-1.12858	0.12174
N	9.29189	-1.29522	0.08745
C	6.79678	-0.52442	2.61314
N	7.37810	-0.43240	3.61417
C	6.54686	-1.22223	-2.29670
N	7.02142	-1.42501	-3.33692
H	-3.42274	0.92816	-0.27743
C	-4.58914	1.07931	-0.55002
C	-4.90602	0.40677	-1.83211
C	-5.25762	0.47685	0.63063
H	-4.67474	2.17753	-0.59645
C	-5.43933	-0.89785	-1.81248
C	-4.64408	0.98877	-3.08585
C	-5.73686	-0.84505	0.54818
C	-5.32646	1.12302	1.87728
C	-5.69808	-1.60296	-2.99405
C	-4.89696	0.29832	-4.27264
H	-4.22523	2.00050	-3.11512
C	-6.25379	-1.50988	1.66585
C	-5.84730	0.47670	2.99950
H	-4.94433	2.14606	1.95786
C	-5.42288	-1.00317	-4.22530
H	-6.11383	-2.61204	-2.92520
H	-4.68277	0.76931	-5.23668
H	-6.61405	-2.53592	1.54962
C	-6.30483	-0.84675	2.89407
H	-5.88902	0.99739	3.96103
H	-5.62148	-1.55195	-5.15096
H	-6.70805	-1.36262	3.77101
O	-5.72044	-1.54452	-0.63523

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