Electronic Supporting Information

Cobalt(II/III), Nickel(II) and Copper(II) Coordination Clusters employing a monoanionic Schiff base ligand: Synthetic, topological and computational mechanistic aspects

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Table S1. Crystal data and structure refinement for **1-5**.

Compound	**1**·5MeCN	**2**·5MeCN	**3**·MeCN	**4**	**5**
Empirical formula	$C_{48}H_{51}N_{11}O_6Co$	$C_{48}H_{51}N_{11}O_6Ni$	$C_{40}H_{39}N_7O_6Cu$	$C_{78}H_{78}Cl_2Co_4N_{12}O_{22}$	$C_{152}H_{152}Co_8N_{24}O_{41}$
Formula weight	936.94	936.70	777.32	1842.14	3442.41
Temperature/K	173.0	173.0	173.0	150	173
Crystal system	triclinic	triclinic	triclinic	monoclinic	tetragonal
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$I4_1/a$
a/Å	12.5772(15)	12.5820(5)	10.5901(9)	23.5066(6)	15.0627(5)
b/Å	13.5174(19)	13.4972(7)	12.6454(10)	12.3910(3)	15.0627(5)
c/Å	13.8758(14)	13.9527(5)	14.7745(12)	29.062(2)	33.6307(16)
α/°	88.395(10)	88.824(4)	72.448(7)	90	90
β/°	88.618(9)	88.632(3)	82.861(7)	109.306(8)	90
γ/°	89.946(10)	89.748(4)	88.524(7)	90	90
Volume/Å^3	2357.4(5)	2368.29(18)	1871.7(3)	7988.8(7)	7630.3(6)
Z	2	2	2	4	2
ρ_{calc}g/cm^3	1.3198	1.314	1.379	1.532	1.498
μ/mm^{-1}	0.425	0.470	0.641	0.966	0.936
F(000)	983.1	984.0	810.0	3792.0	3552.0
Crystal size/mm^3	0.32 × 0.18 × 0.12	0.34 × 0.14 × 0.08	0.34 × 0.2 × 0.14	0.14 × 0.04 × 0.01	0.2 × 0.18 × 0.12
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.78 to 58.74	5.22 to 58.472	5.12 to 58.6	6.162 to 54.97	5.928 to 58.212
Index ranges	-10 ≤ h ≤ 16, -18 ≤ k ≤ 18, -19 ≤ l ≤ 17	-16 ≤ h ≤ 16, -17 ≤ k ≤ 18, -18 ≤ l ≤ 18	-14 ≤ h ≤ 13, -16 ≤ k ≤ 15, -20 ≤ l ≤ 18	-30 ≤ h ≤ 30, -16 ≤ k ≤ 15, -37 ≤ l ≤ 37	-11 ≤ h ≤ 18, -20 ≤ k ≤ 8, -23 ≤ l ≤ 43
Reflections collected	15006	21257	16550	90215	9400
Independent reflections	10479 [R_{int} = 0.0295, R_{sigma} = 0.0618]	10852 [R_{int} = 0.0283, R_{sigma} = 0.0424]	8586 [R_{int} = 0.0320, R_{sigma} = 0.0519]	18111 [R_{int} = 0.0793, R_{sigma} = 0.0695]	4381 [R_{int} = 0.0247, R_{sigma} = 0.0330]
Data/restraints/parameters	10479/0/605	10852/0/606	8586/0/494	18111/48/992	4381/0/258
Goodness-of-fit on F^2	1.025	1.031	1.039	1.028	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0526, wR_2 = 0.1218	R_1 = 0.0426, wR_2 = 0.1003	R_1 = 0.0381, wR_2 = 0.0847	R_1 = 0.0690, wR_2 = 0.1874	R_1 = 0.0543, wR_2 = 0.1595
Final R indexes [all data]	R_1 = 0.0723, wR_2 = 0.1355	R_1 = 0.0567, wR_2 = 0.1090	R_1 = 0.0503, wR_2 = 0.0917	R_1 = 0.0995, wR_2 = 0.2090	R_1 = 0.0737, wR_2 = 0.1801
Largest diff. peak/hole / e Å^{-3}	1.64/-0.55	0.44/-0.32	0.38/-0.38	1.79/-1.70	1.39/-0.45

Table S2. Crystal data and structure refinement for **6-9**.

Compound	**6**	**7**·2MeCN	**8**·2MeOH	**9**·6MeOH

Empirical formula	$C_{76}H_{76}Co_4N_{12}O_{24}$	$C_{42}H_{39}CoN_8O_8$	$C_{60}H_{66}ClN_9Ni_2O_{16}$	$C_{84}H_{102}Cl_2Cu_4N_{12}O_{28}$
Formula weight	1777.20	842.74	1322.08	2052.83
Temperature/K	173	100	100	173.0
Crystal system	tetragonal	triclinic	monoclinic	monoclinic
Space group	$I4_1/a$	$P\bar{1}$	I2/c	$P2_1/c$
a/Å	15.0145(4)	12.6956(4)	27.0155(19)	23.7809(3)
b/Å	15.0145(4)	14.4449(4)	13.5650(9)	19.3947(3)
c/Å	33.6543(11)	22.4981(7)	36.028(3)	21.4148(2)
α/°	90	77.797(2)	90	90
β/°	90	79.842(2)	97.0327(8)	97.9199(12)
γ/°	90	72.698(3)	90	90
Volume/Å^3	7586.9(5)	3821.6(2)	13103.5(16)	9782.8(2)
Z	4	4	8	4
ρ_{calc}g/cm^3	1.556	1.465	1.340	1.394
μ/mm^{-1}	0.948	0.516	0.687	0.992
F(000)	3664.0	1752.0	5520.0	4256.0
Crystal size/mm^3	0.2 × 0.14 × 0.1	0.07 × 0.05 × 0.01	0.29 × 0.08 × 0.03	0.26 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.072 to 58.874	4.374 to 54.968	5.158 to 54.944	4.898 to 52.746
Index ranges	-19 ≤ h ≤ 12, -7 ≤ k ≤ 19, -42 ≤ l ≤ 46	-16 ≤ h ≤ 16, -18 ≤ k ≤ 18, -29 ≤ l ≤ 28	-35 ≤ h ≤ 34, -17 ≤ k ≤ 17, -46 ≤ l ≤ 46	-17 ≤ h ≤ 31, -26 ≤ k ≤ 26, -28 ≤ l ≤ 28
Reflections collected	9913	50559	148453	45640
Independent reflections	4352 [R_{int} = 0.0248, R_{sigma} = 0.0408]	17317 [R_{int} = 0.0843, R_{sigma} = 0.1315]	14748 [R_{int} = 0.0721, R_{sigma} = 0.0460]	19849 [R_{int} = 0.0295, R_{sigma} = 0.0451]
Data/restraints/parameters	4352/0/266	17317/0/1036	14748/68/767	19849/146/1156
Goodness-of-fit on F^2	1.061	1.023	1.040	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0515, wR_2 = 0.1477	R_1 = 0.0746, wR_2 = 0.1315	R_1 = 0.0709, wR_2 = 0.2040	R_1 = 0.0545, wR_2 = 0.1529
Final R indexes [all data]	R_1 = 0.0770, wR_2 = 0.1631	R_1 = 0.1450, wR_2 = 0.1562	R_1 = 0.0912, wR_2 = 0.2176	R_1 = 0.0779, wR_2 = 0.1682
Largest diff. peak/hole / e Å^{-3}	0.74/-0.74	1.09/-1.62	1.80/-0.69	0.85/-0.76

Table S3. Selected bond lengths (Å) for **2**.

Ni - O2	2.0105(12)
Ni - O3	2.2125(13)
Ni - O5	2.0101(13)
Ni - O6	2.2045(13)
Ni - N1	2.0333(14)
Ni - N4	2.0335(15)

Table S4. Hydrogen bonds for **5**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [˚]
O5-H5A···O2[1]	0.85	1.96	2.761(4)	157

[1] 5/4-Y, 1/4+X, 5/4-Z

Table S5. Hydrogen bonds for **6**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [˚]
O5-H5A···O2[1]	0.84	2.04	2.707(7)	137
O6-H6···O3[2]	0.84	1.90	2.736(14)	153

[1]-1/4+Y, 5/4-X, 1/4-Z; [2]3/2-X, 3/2-Y, 1/2-Z

Table S6. Selected bond lengths (Å) and angles (°) for **8**.

Ni1−O5	1.984(3)
Ni1−O6	2.098(3)
Ni1−O8	2.056(2)
Ni1−O10	2.102(2)
Ni1−N4	2.086(3)
Ni1−N7	2.076(3)
Ni2−O2	1.993(2)
Ni2−O3	2.143(2)
Ni2−O4	2.295(3)
Ni2−O5	1.986(2)
Ni2−O8	2.117(2)
Ni2−N1	2.020(3)
Ni1−O5−Ni2	102.72(10)
Ni1−O8−Ni2	95.99(9)

Table S7. Hydrogen bonds for **8**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [˚]
O10-H10···O2	0.85(3)	1.93(3)	2.677(4)	146(3)
O11-H11···O12[1]	0.84	2.12	2.805(10)	139
O12-H12···O18	0.84	2.06	2.708(8)	134

[1]1-X, 2-Y, 1-Z

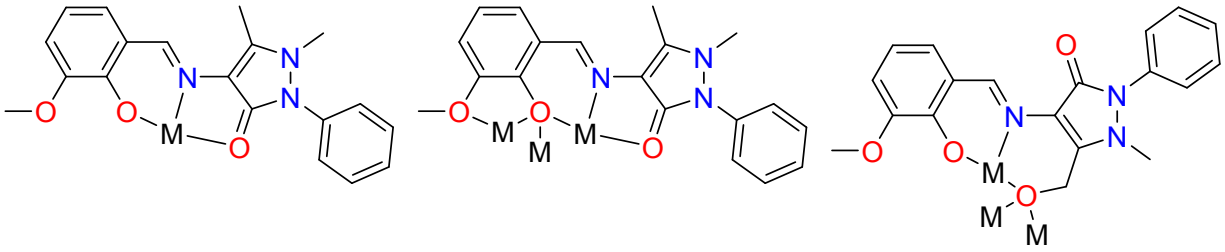
Table S8. Selected bond lengths (Å) and angles (°) for **9**.

Cu1−O14	1.917(2)
Cu1−O3	2.031(2)
Cu1−O2	1.966(2)
Cu1−O11	2.6711(2)
Cu1−O9	2.318(2)
Cu1−N1	1.988(3)
Cu2−O14	1.961(2)
Cu2−O13	2.455(2)
Cu2−O5	1.903(2)
Cu2−O11	2.056(2)
Cu2−O10	2.424(2)
Cu2−N4	1.976(3)
Cu3−O13	1.959(2)
Cu3−O2	2.045(2)
Cu3−O1	2.412(2)
Cu3−O8	1.900(2)
Cu3−N7	1.978(3)
Cu4−O13	1.912(2)
Cu4−O12	2.032(2)
Cu4−O2	2.659(2)
Cu4−O6	2.319(2)
Cu4−O11	1.960(2)
Cu4−N10	1.986(3)
Cu4−O13−Cu3	115.28(10)
Cu2−O13−Cu4	93.11(8)
Cu2−O13−Cu3	92.68(8)
Cu2−O14−Cu3	92.58(8)
Cu1−O14−Cu2	115.78(10)
Cu1−O14−Cu3	92.71(8)
Cu4−O2−Cu3	87.04(8)
Cu1−O2−Cu3	105.23(10)
Cu1−O2−Cu4	98.52(8)
Cu1−O11−Cu4	98.28(8)
Cu1−O11−Cu2	87.05(7)
Cu4−O11−Cu2	105.27(10)
Cu1….Cu2	3.286(6)
Cu1….Cu3	3.187(6)
Cu1….Cu4	3.533(7)
Cu2….C3	3.212(6)
Cu2….C4	3.193(6)
Cu3….Cu4	3.270(6)

Table S9. Hydrogen bonds for **9**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [˚]
O17-H17A···O7AA	0.84	1.89	2.590(12)	140
O15-H15A···O5AA[1]	0.84	1.96	2.736(14)	153
O107-H107···O17[2]	0.84	2.06	2.836(6)	153
O139-H139···O15[3]	0.84	2.15	2.919(9)	152

[1]1-X, -Y, 1-Z; [2]X, 1/2-Y, -1/2+Z; [3]X, 1/2-Y, 1/2+Z



Mode A

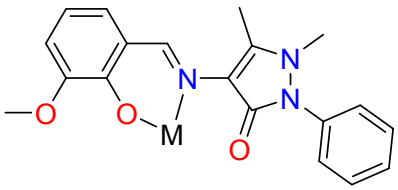
(Compounds **1**, **2**, **7**, **8**)

Mode D

(Compounds **4**, **9**)

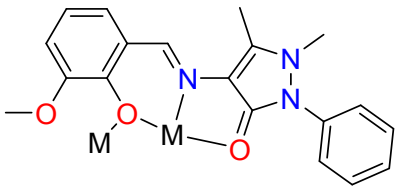
Mode G

(Compound **5**)



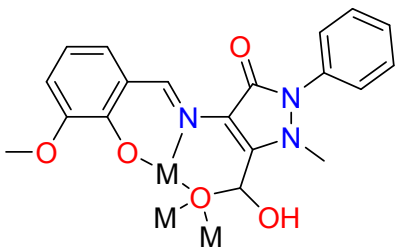
Mode B

(Compound **3**)



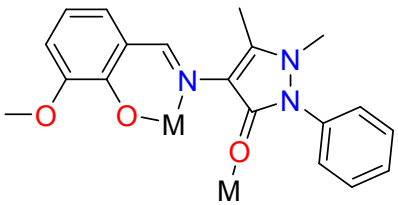
Mode E

(Compound **8**)



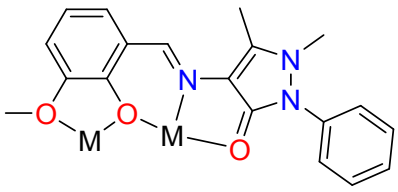
Mode H

(Compound **6**)



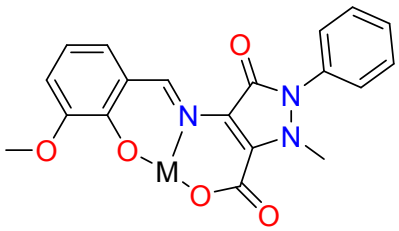
Mode C

(Compounds **4**, **9**)



Mode F

(Compound **8**)



Mode I

(Compound **7**)

Scheme S1. The coordination modes of the ligands HL^1 (modes A-F), H_2L^2 (mode G), H_3L^3 (mode H) and H_2L^4 (mode I).

Table S10. Selected bond lengths (Å) and angles (°) for **4**, **5**, **6**.

4		**5**		**6**	
Co1−O2	1.920(3)	Co1−O2	1.9884(19)	Co1−O2	1.981(2)
Co1−O4	2.303(2)	Co1−O4^{1}	2.1592(18)	Co1−O4^{1}	2.1719(19)
Co1−O5	2.042(2)	Co1−O4	2.0279(18)	Co1−O4	2.030(2)
Co1−O11	2.336(2)	Co1−O4^{2}	2.1617(17)	Co1−O4^{2}	2.182(2)
Co1−O13	2.025(2)	Co1−O5	2.107(2)	Co1−O6	2.106(2)
Co2−O3	2.086(3)	Co1^{3}−O4	2.1615(17)	Co1^{3}−O4	2.1719(19)
Co2−O5	2.090(2)	Co1^{1}−O4	2.1592(17)	Co1^{2}−O4	2.182(2)
Co2−O6	2.098(2)	Co1−O4−Co1^{2}	100.30(8)	Co1−O4−Co1^{3}	100.04(8)
Co2−O13	2.079(3)	Co1−O4−Co1^{3}	99.82(7)	Co1^{3}−O4−Co1^{2}	95.42(7)
Co2−O14	2.064(2)	Co1^{3}−O4−Co1^{2}	95.81(7)	Co1−O4−Co1^{2}	100.00(9)
Co3−O8	1.941(3)	Co1….Co1^{1}	3.216(3)	Co1….Co1^{1}	3.221(2)
Co3−O10	2.412(3)	Co1….Co1^{2}	3.207(3)	Co1….Co1^{2}	3.228(2)
Co3−O11	2.059(2)	Symmetry Operators:		Symmetry Operators:	
Co3−O13	2.145(3)	^{1}1-X,3/2-Y,+Z		^{1}5/4-Y,1/4+X,1/4-Z	
Co3−O14	2.091(3)	^{2}-1/4+Y,5/4-X,5/4-Z		^{2}1-X,3/2-Y,+Z	
Co4−O5	2.196(2)	^{3}5/4-Y,1/4+X,5/4-Z		^{3}-1/4+Y,5/4-X,1/4-Z	
Co4−O9	2.053(3)				
Co4−O11	2.028(2)				
Co4−O12	2.072(3)				
Co4−O14	2.032(2)				
Co1−O13−Co2	94.97(10)				
Co1−O13−Co2	104.92(11)				
Co2−O13−Co3	98.96(10)				
Co1−O5−Co2	94.13(10)				
Co1−O5−Co4	104.42(10)				
Co2−O5−Co4	95.30(10)				
Co3−O11−Co1	97.40(10)				
Co4−O11−Co1	100.07(10)				
Co4−O11−Co3	95.18(10)				
Co3−O14−Co2	101.24(10)				
Co4−O14−Co3	94.09(10)				
Co4−O14−Co2	101.34(10)				
Co1….Co2	3.026(8)				
Co1….Co3	3.306(9)				
Co1….Co4	3.350(7)				
Co2….Co3	3.211(8)				
Co2….Co4	3.168(8)				
Co3….Co4	3.018(8)				

Synthesis of $[Co^{III}_2Co^{II}_2(MeO)_4(L^5)_2Cl_2]$. 0.2 mmol (0.048 g) of HL^1 and 0.3 mmol (0.072 g) of $CoCl_2 \cdot 6H_2O$ were dissolved in 20 ml MeOH while stirring. To this, 0.54 mmol (75 µL) of Et_3N were added. The resulting solution was stirred for a further 5 minutes, filtrated, then left to evaporate slowly. Large red block crystals were formed within 3 days. Yield: 62% (based on Co).

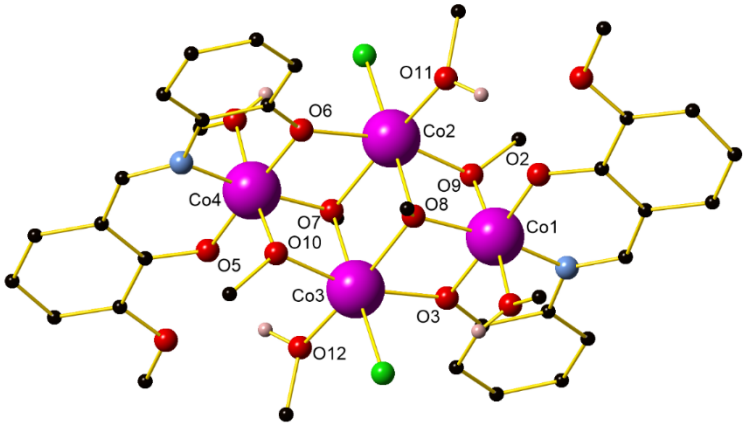


Fig S4. The structure of $[Co^{III}_2Co^{II}_2(MeO)_4(L^5)_2Cl_2]$. Certain H atoms are omitted for clarity. Color code Co (pink), O (red), C (black), N (blue), Cl (green), H (light pink).

Table S11. Crystal data and structure refinement for $[Co^{III}_2Co^{II}_2(MeO)_4(L^5)_2Cl_2]$.

Empirical formula	$C_{36}H_{50}Cl_2Co_4N_2O_{14}$
Formula weight	1041.40
Temperature/K	173
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.7862(5)
b/Å	21.7148(8)
c/Å	16.7640(6)
α/°	90
β/°	101.320(4)
γ/°	90
Volume/Å^3	4207.0(3)
Z	4
ρ_{calc}g/cm^3	1.644
μ/mm^{-1}	1.743
F(000)	2136.0
Crystal size/mm^3	0.24 × 0.18 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.642 to 52.744
Index ranges	$-14 \le h \le 14$, $-27 \le k \le 26$, $-18 \le l \le 20$
Reflections collected	19374
Independent reflections	8574 [R_{int} = 0.0378, R_{sigma} = 0.0495]
Data/restraints/parameters	8574/12/536
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.0850
Final R indexes [all data]	R_1 = 0.0517, wR_2 = 0.0938
Largest diff. peak/hole / e Å^{-3}	0.44/-0.38

Table S12. Cartesian coordinates and energies of the L^n (n = 1-4) ligands, the reactant, intermediate, transition state and product cobalt complexes located on the potential energy surfaces of the transformations undergoing the coordinated ligands.

$[L^1]^-$

O,0,-1.6500877491,4.9253508277,0.9460709273
O,0,-0.2168806217,2.7209625986,0.8261113838
O,0,1.146425912,-1.8982432712,-0.6374354311
N,0,1.5765304158,1.0447856594,-0.7696555294
N,0,3.3566631753,-2.0136693617,-1.3593524589
N,0,4.3977151188,-1.0992718839,-1.5600618395
C,0,-2.4185869037,6.100719346,1.0207031012
H,0,-2.9379369812,6.0729000084,1.9805551341
H,0,-3.1615456175,6.1563867418,0.2131599869
H,0,-1.7929061724,7.0028925642,0.9783117825
C,0,-0.9061015729,4.7396058261,-0.1864426778
C,0,-0.8634712524,5.6225369753,-1.2387816042
H,0,-1.4424731151,6.5411188615,-1.2100730536
C,0,-0.0641454929,5.3509326073,-2.3780415777
H,0,-0.0388062163,6.0601780742,-3.1997780376
C,0,0.6651269228,4.1899876769,-2.4183968088
H,0,1.2826010414,3.9686130778,-3.288704947
C,0,0.6481174324,3.2457835583,-1.3567426843
C,0,-0.1463964846,3.4855465052,-0.1662898762
C,0,1.4613457041,2.0772942493,-1.5471238657
H,0,2.0245547262,2.0885717598,-2.4963065394
C,0,2.4958620401,0.0750493311,-1.1293236865
C,0,3.8146978978,0.1690177062,-1.4760370794
C,0,2.1819830222,-1.34691245,-1.0004283327
C,0,4.6624775589,1.3728275807,-1.6823064689
H,0,5.6426221504,1.2423375964,-1.2128677007
H,0,4.1737128869,2.2420554587,-1.2361689291
H,0,4.8254007623,1.5950098644,-2.7429774864
C,0,5.1825884849,-1.3803558621,-2.7635182724
H,0,5.6217789729,-2.3757814618,-2.6834516501
H,0,5.9932851456,-0.6534052551,-2.8218851925
H,0,4.5682825845,-1.3223245601,-3.6708114855
C,0,3.6718959001,-3.33748707,-0.9963956324
C,0,4.9192335954,-3.6493925093,-0.4458931219
H,0,5.6398391581,-2.8566649986,-0.2743613798
C,0,5.2152159546,-4.9665303634,-0.1088865023
H,0,6.1874733034,-5.2003705045,0.3151652793
C,0,4.2729113834,-5.9744972637,-0.2976689754
H,0,4.5063831585,-7.0000728063,-0.0284835151
C,0,3.0277419013,-5.6546882607,-0.8358383296
H,0,2.2855098872,-6.4327229701,-0.9895550881
C,0,2.7239256758,-4.3465675483,-1.1969827137
H,0,1.7600363069,-4.0940060544,-1.6205491215

Sum of electronic and zero-point Energies=,, -1123.274642
Sum of electronic and thermal Energies=,,, -1123.252498
Sum of electronic and thermal Enthalpies=,,,-1123.251554
Sum of electronic and thermal Free Energies=,,-1123.326791

$[L^2]^-$

O,0,-5.6442145713,-1.6866194502,0.6009934598
O,0,-3.0150125539,-1.614216736,0.6891552337
O,0,1.7425688587,-1.7576355229,-0.8717614701
N,0,-0.5817144899,-0.1307368525,0.0256200291
N,0,2.7293608883,1.3019993768,0.4510272209
N,0,2.9846276765,0.0942892211,-0.2071175264
C,0,-7.0494547161,-1.7330510522,0.5639852603
H,0,-7.4363202944,-1.611795978,-0.4571424853
H,0,-7.3385235383,-2.7164273695,0.9396582678
H,0,-7.5016718917,-0.959646994,1.199951441
C,0,-5.0487061923,-0.5352673962,0.1662221594
C,0,-5.7313107692,0.5646394793,-0.2939834802
H,0,-6.8168550277,0.5629143452,-0.3309006964
C,0,-5.0323189678,1.7208277973,-0.7266499978
H,0,-5.5875658434,2.5832565524,-1.0828333419
C,0,-3.6620772925,1.7252682553,-0.6869263704
H,0,-3.112958745,2.606183784,-1.0184050934
C,0,-2.9125130484,0.6079189098,-0.226858061
C,0,-3.5847878937,-0.5900327824,0.2429983144
C,0,-1.4874902589,0.7606453816,-0.2551723936
H,0,-1.1575392515,1.7609454103,-0.5823735154
C,0,0.7333653048,0.279727286,0.0239011231
C,0,1.3356063813,1.4003996281,0.5241220103
C,0,1.8044754043,-0.6159671288,-0.4252998161
C,0,0.7152928299,2.5926381215,1.1611735072
H,0,1.3776569335,2.9630316841,1.9564509474
O,0,0.4787695633,3.597924182,0.1838760287
H,0,-0.2233797476,2.2666809726,1.6302775544
C,0,3.4303219703,2.4405733773,-0.1509180992
H,0,4.5071749356,2.2930733495,-0.0560509596
H,0,3.1638317531,2.5603422617,-1.2078435451
H,0,3.1498254521,3.3418940733,0.393660756
C,0,4.271835349,-0.4714883543,-0.1298536718
C,0,5.1411814082,-0.1191642123,0.9073953052
H,0,4.8076745853,0.577513461,1.6693653144
C,0,6.4141010403,-0.6781669281,0.9601561127
H,0,7.084557627,-0.397299845,1.7671704232
C,0,6.8226549131,-1.5995426592,-0.0010713815
H,0,7.8150119198,-2.0373350411,0.0470548917
C,0,5.9467374638,-1.954479248,-1.0252564497
H,0,6.2554630804,-2.6705233828,-1.7813931993
C,0,4.678281581,-1.3897247037,-1.1035089669
H,0,3.9956987541,-1.6584781524,-1.8998057654
H,0,0.0595394197,4.3398128792,0.635310926

Sum of electronic and zero-point Energies=,, -1198.404925
Sum of electronic and thermal Energies=,,, -1198.381605
Sum of electronic and thermal Enthalpies=,,,-1198.380661
Sum of electronic and thermal Free Energies=,,-1198.458960

$[L^3]^-$

O,0,-5.6928082819,-1.6240360733,0.6135030427
O,0,-3.0643639832,-1.5979880598,0.7176054744
O,0,1.6283037812,-1.954219997,-0.6910568525
N,0,-0.5975742972,-0.1745873107,0.0390207621
N,0,2.7822290298,1.1726247054,0.286479433
N,0,2.9678028309,-0.1086077107,-0.2418433651
C,0,-7.0980583281,-1.6472683312,0.565119759
H,0,-7.4734608035,-1.592669589,-0.4660452928
H,0,-7.4093453743,-2.5956588751,1.0072368449
H,0,-7.5415206331,-0.8220556125,1.1391853847
C,0,-5.0713038818,-0.5165682815,0.1061275434
C,0,-5.7291497453,0.5598803615,-0.4382589274
H,0,-6.8141192459,0.5739161439,-0.4884674731
C,0,-5.004564837,1.670218009,-0.9422690161
H,0,-5.5397078997,2.5143938316,-1.3665288842
C,0,-3.6348048119,1.6544461695,-0.8823149011
H,0,-3.0660037423,2.5013278937,-1.2652751159
C,0,-2.9103174602,0.5619361218,-0.3320480884
C,0,-3.6096323714,-0.5922663126,0.2033363457
C,0,-1.4826817801,0.6962554951,-0.3424831043
H,0,-1.1349536372,1.6614239004,-0.7420126312
C,0,0.7269802824,0.2054320725,0.008439724
C,0,1.3921482575,1.3383543193,0.385074842
C,0,1.7534654372,-0.7775634254,-0.3663411723
C,0,0.9010570748,2.6493384484,0.9281304488
H,0,1.7164087898,3.111235405,1.5058789654
O,0,0.5726853699,3.4783965758,-0.1628283589
O,0,-0.1857360677,2.3991737288,1.7699548375
C,0,3.5034812794,2.1956753279,-0.4816131573
H,0,4.5715394502,1.9757030114,-0.45013085
H,0,3.160951548,2.2294885401,-1.5226377411
H,0,3.3381906031,3.1667878278,-0.0156887473
C,0,4.2304882896,-0.7210719617,-0.1268593628
C,0,5.1444851432,-0.2866244094,0.8385530217
H,0,4.8642799422,0.5123307228,1.516937832
C,0,6.3929335364,-0.8938524075,0.9291781824
H,0,7.0980377409,-0.5486223401,1.6797226018
C,0,6.733290177,-1.9426754909,0.0784257755
H,0,7.7067653779,-2.4170627914,0.1560854158
C,0,5.8132235161,-2.377504256,-0.8736919922
H,0,6.0683508366,-3.1932221896,-1.543988801
C,0,4.5685847683,-1.7682590126,-0.9905849072
H,0,3.8521763936,-2.0996343816,-1.7314363016
H,0,0.5171978473,4.3880712642,0.1552213221
H,0,-0.3484501213,3.1936089442,2.290787485

Sum of electronic and zero-point Energies=,, -1273.548237
Sum of electronic and thermal Energies=,,, -1273.523841
Sum of electronic and thermal Enthalpies=,,,-1273.522897
Sum of electronic and thermal Free Energies=,,-1273.603245

$[L^{3'}]^-$

H,0,0.8006898681,1.542558597,-0.6012683465
O,0,5.6917562816,0.6830313392,-0.1697963819
O,0,3.0931101773,1.0765754857,-0.3886967908
O,0,0.4741188509,2.4045866044,-1.0793539824
O,0,-1.4516491153,3.3523676306,-1.6780708945
O,0,-1.7867375504,-1.7527335332,1.1908650666
N,0,0.5028655841,0.1818450206,0.1486091803
N,0,-3.0894897933,-0.0394172121,0.3011430535
N,0,-2.8893284432,1.1328931791,-0.4328212936
C,0,7.0808429078,0.4801039292,-0.0583321144
H,0,7.4036053306,0.4413586555,0.9906436077
H,0,7.5584299332,1.3303924393,-0.5479715322
H,0,7.3981346389,-0.4460327092,-0.5559151294
C,0,4.8804505392,-0.2652202366,0.3778121214
C,0,5.3209900909,-1.3927126052,1.0236714402
H,0,6.3844364174,-1.585089754,1.1289221474
C,0,4.3997378128,-2.3297286081,1.5680641834
H,0,4.7755868348,-3.2134746039,2.0743283616
C,0,3.0571657024,-2.1036442316,1.4459973808
H,0,2.3414320307,-2.8126278197,1.8591009815
C,0,2.5506536102,-0.9478716043,0.7826609776
C,0,3.454880289,0.0365493296,0.2093529481
C,0,1.1422295764,-0.8118716544,0.7167323635
H,0,0.5552615879,-1.6081786864,1.1847622366
C,0,-0.8614182833,0.2559126732,0.135206834
C,0,-1.8891829307,-0.6587780676,0.6385609568
C,0,-1.5115872591,1.3044093653,-0.4645245939
C,0,-0.8432532023,2.4467429173,-1.1245815558
C,0,-3.7142792332,2.2595118224,0.0164869694
H,0,-4.7672518522,2.0156123692,-0.1278615519
H,0,-3.446634677,3.1124765806,-0.6045377628
H,0,-3.5290564096,2.4869081543,1.0730309899
C,0,-4.3485736997,-0.6747009148,0.2633398714
C,0,-5.1817663294,-0.5206209423,-0.8482178704
H,0,-4.8471127127,0.0789052412,-1.6885216666
C,0,-6.4224335906,-1.1489532493,-0.8678444522
H,0,-7.0687553512,-1.0235045025,-1.7314029507
C,0,-6.8281196211,-1.9441110657,0.2016919757
H,0,-7.7948386491,-2.4376548185,0.1793513285
C,0,-5.9857840723,-2.1017192051,1.3002945054
H,0,-6.2950263892,-2.7175172938,2.1396055845
C,0,-4.7507940543,-1.4632588473,1.3443141317
H,0,-4.095204845,-1.5750191677,2.1989696725

Sum of electronic and zero-point Energies=,, -1272.424426
Sum of electronic and thermal Energies=,,, -1272.401244
Sum of electronic and thermal Enthalpies=,,,-1272.400300
Sum of electronic and thermal Free Energies=,,-1272.478597

$[L^4]^{2-}$

O,0,5.7586214376,-0.3942576784,-1.3291331012
O,0,3.2776372258,0.474138909,-1.3869291845
O,0,0.0066054753,3.3281961311,0.2984798283
O,0,-1.9509236215,3.8344693275,-0.7042445604
O,0,-1.4663263893,-1.8912260513,0.0867130178
N,0,0.5967889485,0.3442074395,-0.1803505472
N,0,-2.9664616619,-0.1160243916,0.0871593499
N,0,-2.8953999354,1.2657181094,-0.0924187156
C,0,7.0856374092,-0.856696852,-1.3112464041
C,0,4.8945148221,-0.9479568595,-0.422086464
C,0,5.2483369877,-1.9139069447,0.4910186853
C,0,4.2889673286,-2.4366596979,1.3921839461
C,0,3.0009049268,-1.9629715591,1.3401561139
C,0,2.5918936521,-0.9622773087,0.420370406
C,0,3.5386256533,-0.40211663,-0.5252158881
C,0,1.2022767865,-0.5851611793,0.4919464109
C,0,-0.772087362,0.4585712876,-0.0108356609
C,0,-1.6907124479,-0.6794583984,0.0809497478
C,0,-1.540200847,1.595546498,-0.0846493198
C,0,-1.1193598954,3.0587620604,-0.1684361148
C,0,-3.7795929634,2.0134025163,0.8031031624
C,0,-4.1512066408,-0.7976136117,-0.2466525675
C,0,-5.0672387417,-0.236164087,-1.1426618468
C,0,-6.2401021746,-0.9184950402,-1.4497110488
C,0,-6.5017337609,-2.1655126344,-0.8868367422
C,0,-5.5790330311,-2.7250574847,-0.0047914601
C,0,-4.4114169275,-2.0465304584,0.3275081199
H,0,7.5745901067,-0.6652095566,-0.3458346055
H,0,7.6173176045,-0.3103949067,-2.0929532011
H,0,7.1483628198,-1.9334667336,-1.522025136
H,0,6.2673103674,-2.2884190937,0.530129101
H,0,4.579102208,-3.2012899572,2.1066646888
H,0,2.2525203769,-2.3591981849,2.026504311
H,0,0.6344036309,-1.1756581105,1.2256247291
H,0,-4.817451079,1.7407254027,0.6035397794
H,0,-3.625573892,3.0667606855,0.5739226842
H,0,-3.5464731826,1.8087761339,1.8559020617
H,0,-4.8450929857,0.7225640771,-1.5996608189
H,0,-6.9473659214,-0.4735688383,-2.1437587147
H,0,-7.4161740076,-2.6966750306,-1.1329158377
H,0,-5.773158895,-3.6960972653,0.4417452216
H,0,-3.693731404,-2.4741740331,1.0162265747

Sum of electronic and zero-point Energies=,, -1271.929203
Sum of electronic and thermal Energies=,,, -1271.905822
Sum of electronic and thermal Enthalpies=,,,-1271.904878
Sum of electronic and thermal Free Energies=,,-1271.984505

$[(L^1)_2Co^{II}]$

Co,0,0.4231808125,-0.0063427726,0.0117025045
O,0,3.3223041168,3.4920476696,-0.5775703255

O,0,1.7474440622,1.4218520006,-0.4489874654
O,0,-1.2758770286,-1.4608737415,0.2501194875
O,0,3.1079097553,-3.6295186461,0.8581313947
O,0,1.638262235,-1.4963124628,0.5922178124
O,0,-1.1895252388,1.5444002452,-0.3727052805
N,0,0.4235182232,-0.6785325705,-1.8304431928
N,0,-1.4004618445,-3.7713030805,-2.3242196265
N,0,-1.8831211006,-3.2599490635,-1.1200324095
N,0,0.276094136,0.6605043046,1.8508146323
N,0,-1.8379745118,3.3528218861,0.9641557783
N,0,-1.4477607732,3.8288157545,2.2156111944
C,0,4.1733642371,4.6152124763,-0.6238111112
H,0,3.7564475945,5.4148896182,-1.2497429609
H,0,4.2633471426,4.9743947692,0.4023849247
H,0,5.17015162,4.353950576,-1.0022057361
C,0,3.057630214,2.8639054659,-1.7535870049
C,0,3.5580385108,3.2478141779,-2.9791011698
H,0,4.2155403345,4.1076708676,-3.0545977848
C,0,3.224598822,2.5353985665,-4.1538862716
H,0,3.6299680178,2.8568461107,-5.1079225654
C,0,2.3937112321,1.4491053557,-4.0712227404
H,0,2.1286840398,0.8903109908,-4.966120062
C,0,1.8607200365,1.0206450389,-2.8245628554
C,0,2.1789281323,1.723788298,-1.6171857681
C,0,1.012552338,-0.1266364856,-2.8525284782
H,0,0.8458007105,-0.5554650321,-3.8426682797
C,0,-0.3704917124,-1.8123170364,-1.9454011431
C,0,-0.5065896324,-2.8452281707,-2.8375634032
C,0,-1.214032918,-2.0991846115,-0.8153479525
C,0,0.1452146943,-3.0987650032,-4.1492976685
H,0,0.2122708833,-4.1698144785,-4.3518742127
H,0,-0.3999379834,-2.6262957474,-4.9741700573
H,0,1.1610094849,-2.6964778168,-4.145151609
C,0,-2.4234393005,-4.3462535356,-3.1972324653
H,0,-2.9422758776,-5.1438102124,-2.6651644022
H,0,-3.1442242789,-3.5867769361,-3.5198454965
H,0,-1.9309659669,-4.7797783828,-4.0667749592
C,0,-2.512443418,-4.1141147932,-0.1847475762
C,0,-2.1910912479,-5.4721324979,-0.1359101793
H,0,-1.4423873614,-5.8732759368,-0.811582872
C,0,-2.8269857414,-6.2902406082,0.7928717096
H,0,-2.5809060833,-7.3472574104,0.8277195312
C,0,-3.7579945584,-5.7574294916,1.681933379
H,0,-4.2460612804,-6.3988772111,2.4092665087
C,0,-4.0597199818,-4.397680513,1.633838876
H,0,-4.7853363804,-3.9755381061,2.3225654318
C,0,-3.4501378083,-3.5714992991,0.6952221312
H,0,-3.6884941771,-2.5155604101,0.6419270103
C,0,3.9052082436,-4.7859693656,0.9796474132
H,0,4.0899649622,-5.1394713135,-0.0357849648
H,0,4.865367734,-4.5677986824,1.4649791154
H,0,3.3936502598,-5.5739535164,1.5475480728
C,0,2.7460965192,-3.001068758,2.0081562346
C,0,3.0972628131,-3.4152060994,3.274762597
H,0,3.7071940375,-4.3025341285,3.4092301058
C,0,2.670138513,-2.6982072258,4.4163358356
H,0,2.958040745,-3.0441725088,5.4039068929
C,0,1.8995826865,-1.5761330078,4.2598458293
H,0,1.5657851709,-1.0129138936,5.1286087298
C,0,1.5203192587,-1.1152028744,2.9691944534
C,0,1.9335807511,-1.8240642214,1.7942535684

C,0,0.7274769097,0.0702816862,2.9210510452
H,0,0.476297267,0.4974773685,3.8939353004
C,0,-0.473341445,1.8289067315,1.9032228295
C,0,-1.1952104992,2.1659605498,0.7034341298
C,0,-0.6464814982,2.8567701391,2.7942618828
C,0,-0.1089989729,3.065845328,4.1643792939
H,0,-0.0133101906,4.1305009616,4.3881474655
H,0,-0.7487864839,2.6100735676,4.9284922106
H,0,0.8837284653,2.6171676032,4.2480190172
C,0,-2.5258484633,4.4291410683,3.0014600956
H,0,-2.9642321329,5.253338899,2.4385260914
H,0,-3.3003912434,3.6926525234,3.2427497015
H,0,-2.100472634,4.8311907342,3.9202300466
C,0,-2.3441489919,4.2436029189,-0.010347367
C,0,-3.2123420932,3.7496814872,-0.985455397
H,0,-3.4909169124,2.7023739877,-0.975425137
C,0,-3.7009851628,4.6123329053,-1.9612276155
H,0,-4.3721160697,4.2277888964,-2.7233458821
C,0,-3.3492531915,5.9608741858,-1.9544666773
H,0,-3.7435979678,6.6311257946,-2.7120579866
C,0,-2.4889842527,6.4451183913,-0.9713738987
H,0,-2.2043232042,7.492954305,-0.9622549689
C,0,-1.9729597795,5.5898012686,-0.0026109836
H,0,-1.2785290376,5.9529846461,0.7482993893

Sum of electronic and zero-point Energies=,, -3628.984308
Sum of electronic and thermal Energies=,,, -3628.937420
Sum of electronic and thermal Enthalpies=,,,-3628.936476
Sum of electronic and thermal Free Energies=,,-3629.070176

$[L^{1}Co^{II}]^{+}$

Co,0,-0.5743054401,-1.0783701864,-0.5533925075
O,0,-4.8756311179,-1.8370246948,-0.7919862797
O,0,-2.363471896,-1.1742019446,-0.6338344178
O,0,1.3527761361,-1.1638045196,-0.5523273683
N,0,-0.4864449891,0.7696426194,-0.355659075
N,0,2.926827582,1.8609152301,0.0386355035
N,0,2.992517005,0.5094736965,-0.2574967986
C,0,-6.2321297443,-2.2271762188,-0.8862118269
H,0,-6.7141121905,-1.7931907404,-1.7704580062
H,0,-6.2282534582,-3.3136644674,-0.9753167502
H,0,-6.7958832614,-1.9395814049,0.0093291304
C,0,-4.6150981199,-0.5158641062,-0.6715285723
C,0,-5.5695740418,0.4869657962,-0.6327110492
H,0,-6.6221976677,0.2359739747,-0.7011143944
C,0,-5.1957564874,1.8379009111,-0.5064701572
H,0,-5.9655476795,2.601824096,-0.4789324232
C,0,-3.8688099838,2.1797080848,-0.4192455982
H,0,-3.5670016673,3.2183089809,-0.3200640488
C,0,-2.8685609429,1.1759570743,-0.4545349696
C,0,-3.2297289306,-0.190205554,-0.5841689609
C,0,-1.5050002159,1.5814863334,-0.357274982
H,0,-1.3142920651,2.6509901641,-0.2866002983
C,0,0.8562023652,1.1408303026,-0.2628536782
C,0,1.6230190288,2.2617606888,0.0037742061
C,0,1.732897158,0.0468914574,-0.3962805775
C,0,1.2331913126,3.6768255691,0.2272857979
H,0,1.9767028233,4.2100934719,0.8207982559

H,0,1.1055789203,4.2039416225,-0.7241639048
H,0,0.2873591687,3.7222294735,0.7705872345
C,0,4.0727180643,2.6931874012,-0.2965785256
H,0,4.9730617483,2.265629209,0.1426086057
H,0,4.187861105,2.7757355751,-1.3811680762
H,0,3.9154360342,3.6800961937,0.1333034603
C,0,4.1737813798,-0.2614482123,-0.0663317573
C,0,4.8502997712,-0.2033067783,1.1518137188
H,0,4.4805091372,0.4332835761,1.9498371631
C,0,5.9927262056,-0.9776919493,1.3229596584
H,0,6.5315148127,-0.9356736378,2.2641829387
C,0,6.4322706282,-1.8153859925,0.2988578445
H,0,7.3196953519,-2.4241061112,0.4417058364
C,0,5.7357525078,-1.8745106855,-0.906214757
H,0,6.0780445446,-2.5259032151,-1.7039598278
C,0,4.6050377765,-1.0867008981,-1.1013005925
H,0,4.0620193317,-1.1066401853,-2.0402991733

Sum of electronic and zero-point Energies=,, -2505.623252
Sum of electronic and thermal Energies=,,, -2505.600107
Sum of electronic and thermal Enthalpies=,,,-2505.599163
Sum of electronic and thermal Free Energies=,,-2505.677592

$[L^1Co(\eta^2\text{-}O_2)]^+$

Co,0,-0.9517187549,-1.1059026972,0.652391622
O,0,-5.1496096958,-1.642180373,-0.2538112231
O,0,-2.5968370152,-1.1835408647,0.0157647897
O,0,1.6588079727,-1.336303764,-0.8817862555
N,0,-0.5014087182,0.5186560529,-0.1472628776
N,0,2.8520358307,1.7186786226,0.1988631083
N,0,3.0502613605,0.476386814,-0.389070377
C,0,-6.5315232282,-1.9251136827,-0.4009075316
H,0,-6.859233266,-1.7777889151,-1.4361055542
H,0,-6.6524171892,-2.9730335618,-0.1282206702
H,0,-7.1379042815,-1.3030113781,0.2669626735
C,0,-4.7350314673,-0.3959934748,-0.5424843046
C,0,-5.5428381617,0.6484303557,-0.9662056996
H,0,-6.6093497058,0.4934197087,-1.0828824447
C,0,-5.0021173919,1.9147335978,-1.2498580478
H,0,-5.6623168327,2.7079639181,-1.5834998181
C,0,-3.6531604169,2.1449696938,-1.1147134304
H,0,-3.2277137633,3.1171267098,-1.3421215433
C,0,-2.8041015795,1.1062453223,-0.66734954
C,0,-3.3392080935,-0.1737646151,-0.3715319409
C,0,-1.4028919717,1.3424028335,-0.6128792934
H,0,-1.041531669,2.2789607402,-1.0361670463
C,0,0.8535589502,0.8189155213,-0.1267709156
C,0,1.5227639018,1.9465408809,0.3134148878
C,0,1.8259929979,-0.1685940537,-0.5342181012
C,0,0.9859446382,3.2313313204,0.8258772983
H,0,1.567633366,3.5830129139,1.6810898696
H,0,1.00616892,4.0088823563,0.0547848829
H,0,-0.0482040809,3.1003337871,1.1494482316
C,0,3.8448007628,2.7563520976,-0.0340887686
H,0,4.8312895888,2.3848644871,0.2409440399
H,0,3.8440476827,3.0631616888,-1.0845915684
H,0,3.6053889327,3.6077990893,0.6008945869

C,0,4.2891689993,-0.2022162586,-0.2485472325
C,0,4.9989204522,-0.1492329728,0.95217314
H,0,4.6053989843,0.4176075113,1.790727117
C,0,6.2032671801,-0.8376714139,1.0599043717
H,0,6.7628746447,-0.792631992,1.9891067841
C,0,6.678612337,-1.594713455,-0.0093509301
H,0,7.6146492985,-2.136896247,0.0829312428
C,0,5.951152882,-1.6556022323,-1.1962733312
H,0,6.3180836184,-2.2438399732,-2.0317230429
C,0,4.7589118878,-0.9500604645,-1.3267136043
H,0,4.1914392717,-0.9743084042,-2.2504762174
O,0,-0.5836906086,-0.6986580471,2.3962670949
O,0,0.5220334306,-1.1147171825,1.9007655697

Sum of electronic and zero-point Energies=,, -2655.751665
Sum of electronic and thermal Energies=,,, -2655.725612
Sum of electronic and thermal Enthalpies=,,,-2655.724668
Sum of electronic and thermal Free Energies=,,-2655.809690

$[\{L^1Co(\eta^2\text{-}O_2)\}^+]^{\neq}$

Co,0,-1.5784629955,0.0900423655,1.8069338348
O,0,-5.1232896241,-1.4060818393,-0.2185101823
O,0,-2.7643374786,-0.6960918498,0.662469445
O,0,1.3498394443,0.4696204295,-1.8187164676
N,0,-0.5659959751,0.8692807722,0.435064655
N,0,2.9361891707,0.6155559504,1.2536149619
N,0,2.9486143549,0.5185239217,-0.1330799517
C,0,-6.3988009383,-1.8078834375,-0.6785846051
H,0,-6.3486190576,-2.2160993877,-1.695225838
H,0,-6.7359043,-2.5865341791,0.0059240807
H,0,-7.1129244403,-0.9757104388,-0.659915898
C,0,-4.4889841866,-0.436721562,-0.9150667379
C,0,-4.9868911222,0.1970259901,-2.0392341234
H,0,-5.9645307816,-0.0703068422,-2.4248233664
C,0,-4.2414318291,1.1942458388,-2.7004937035
H,0,-4.6577066234,1.6688363719,-3.5829408088
C,0,-2.9989482625,1.5485533174,-2.2372956425
H,0,-2.4066635896,2.3014628297,-2.7491629464
C,0,-2.4701210884,0.933076249,-1.0753467498
C,0,-3.2093203316,-0.0703584352,-0.3921651927
C,0,-1.1330500983,1.2343337708,-0.6917082209
H,0,-0.5214357772,1.7739816306,-1.4104794596
C,0,0.8288443283,0.9138825393,0.5207541507
C,0,1.6431941736,0.9204334977,1.6306433226
C,0,1.6644289983,0.6350984965,-0.6431727116
C,0,1.3462661276,1.1980809595,3.0323424962
H,0,0.3048979062,0.4026267782,3.4594949741
H,0,2.0655828677,0.7814567672,3.7414078629
H,0,1.0903668194,2.2277315224,3.2595062712
C,0,4.0625079474,1.359530532,1.8207959219
H,0,4.9928251275,0.8945204658,1.4953811145
H,0,4.0418182397,2.4082068871,1.5060405182
H,0,4.012295031,1.2973471502,2.9067361057
C,0,4.0170594453,-0.1360206899,-0.7888357512
C,0,4.71545545,-1.1639744834,-0.151240712
H,0,4.4280128616,-1.4711909396,0.8494747753
C,0,5.7645973221,-1.7908009882,-0.8163781432
H,0,6.3109955162,-2.5863994356,-0.3189222218

C,0,6.1012869097,-1.414475931,-2.1149562896
H,0,6.9159804394,-1.9116836752,-2.6323882237
C,0,5.3879933373,-0.3974659676,-2.7469266299
H,0,5.6462073065,-0.0978192521,-3.7581689473
C,0,4.3520749265,0.2548719018,-2.0864871907
H,0,3.799616971,1.0544183982,-2.5654923171
O,0,-2.5567758601,0.7169935286,2.9883133071
O,0,-0.6977931725,0.8485570622,3.2961883249

Sum of electronic and zero-point Energies=,, -2655.667286
Sum of electronic and thermal Energies=,,, -2655.642341
Sum of electronic and thermal Enthalpies=,,,-2655.641398
Sum of electronic and thermal Free Energies=,,-2655.722510

[L^{2}Co(OH)]

Co,0,0.820155908,1.1265931672,-0.5933828821
O,0,4.5643668196,-0.986253759,-1.5073339926
O,0,2.2358580818,-0.0424211542,-0.7820212294
O,0,-0.9852298515,-1.6089699037,0.4427274968
N,0,0.6657525492,0.7420755404,1.1484245615
N,0,-2.8885096191,1.3445549405,0.5019929012
N,0,-2.7182963019,-0.0617233215,0.3564562245
C,0,5.8052920658,-1.5172748594,-1.9278464001
H,0,5.8617043569,-2.5976540105,-1.7474865509
H,0,5.868664518,-1.3274274102,-2.9995707258
H,0,6.6451331283,-1.0245750356,-1.4228542608
C,0,4.2528064035,-1.0992768126,-0.1959121962
C,0,5.0455292696,-1.6935639389,0.7665624202
H,0,6.0062254754,-2.1152885837,0.4919486918
C,0,4.6229286398,-1.7789371364,2.1118710082
H,0,5.266646035,-2.2641643418,2.8381510831
C,0,3.4125742099,-1.2569391431,2.4881181757
H,0,3.0707685661,-1.3185375685,3.51729984
C,0,2.5936659302,-0.6058920225,1.5306006795
C,0,2.9853573337,-0.5341804277,0.1608050007
C,0,1.3055455307,-0.1270864476,1.8817349274
H,0,0.8234103557,-0.4800895945,2.7938279159
C,0,-0.6465652559,0.7795951806,0.7561619668
C,0,-1.625290375,1.8299556642,0.9647598844
C,0,-1.4173830243,-0.4686118555,0.5326540557
C,0,-1.4456705781,3.0377867578,1.533479603
H,0,-2.2700324748,3.7242863836,1.6956129388
O,0,-0.2160645232,3.4391183379,1.9170451707
C,0,-4.0117032997,1.6393579127,1.392579712
H,0,-4.9019977598,1.1270325726,1.025441183
H,0,-3.8077046602,1.3373937983,2.4281259955
H,0,-4.2113485614,2.7113868754,1.3540944556
C,0,-3.6792276217,-0.7739302876,-0.3960745397
C,0,-4.4831268949,-0.1031461066,-1.323128528
H,0,-4.3597004532,0.965435023,-1.4618194931
C,0,-5.4197327139,-0.8177965391,-2.0626383011
H,0,-6.0409726549,-0.2920908824,-2.7818672385
C,0,-5.5560312442,-2.1939440853,-1.8927381835
H,0,-6.2874663995,-2.7471582327,-2.4738924414
C,0,-4.7495929967,-2.8537264999,-0.9677096165
H,0,-4.8509709225,-3.9253681491,-0.823268313
C,0,-3.8179867555,-2.1525037865,-0.2086493181
H,0,-3.1941815472,-2.6609335971,0.5156082261

O,0,0.083342347,2.5335062271,-1.3626223624
H,0,-0.2842916031,4.3010126489,2.3401540484
H,0,-0.879039612,2.5078150933,-1.4106130433

Sum of electronic and zero-point Energies=,, -2655.966626
Sum of electronic and thermal Energies=,,, -2655.940868
Sum of electronic and thermal Enthalpies=,,,-2655.939924
Sum of electronic and thermal Free Energies=,,-2656.022986

$[L^2Co(OH_2)]$

Co,-0.15882504,1.74620336,-1.89935919
O,-0.54352715,0.18603496,-3.11173522
O,-0.04920616,3.39221529,-0.78995735
O,0.09152831,-1.68053768,1.97325693
O,1.90871538,1.57328544,-2.27219266
N,0.15815884,0.55222682,-0.19009881
N,-0.10070408,-2.85464124,-1.27373576
O,-0.54968791,5.73445370,0.23258617
N,-0.01570362,-3.02578253,0.10196790
C,0.11786059,-0.83890395,-0.32614740
C,0.02109989,-1.51988627,-1.51659163
C,0.08798528,-1.04711295,-2.93154843
C,0.08711541,-1.81780152,0.73291175
C,0.09377940,3.49808522,0.50989444
C,0.42419487,2.42157917,1.36905469
C,0.45928377,1.04966210,0.97783437
C,0.63710585,2.68929251,2.75088300
C,0.46418486,3.93038340,3.26616712
C,0.78695159,-4.68631671,1.65521155
C,-0.15965078,-4.30421471,0.72343099
C,-0.13728302,4.77301749,1.10182930
C,0.13551131,-3.95777717,-2.17927781
C,0.05095399,4.97328306,2.45293312
C,0.67158303,-5.92809373,2.27181023
C,-1.20356271,-5.14050097,0.39743991
C,-0.35882659,-6.77901663,1.91320846
C,-1.29196828,-6.38641126,0.99657680
C,-1.53442310,6.63085050,0.74430716
H,1.04454217,-0.97693351,-3.21529798
H,2.32313873,1.36856243,-1.53181791
H,2.21387179,2.33257456,-2.57298761
H,-0.39277517,-1.71921266,-3.49510886
H,0.73394003,0.42922326,1.64122534
H,0.90452792,1.98331207,3.32376262
H,0.62900989,4.08707515,4.18838261
H,1.50870316,-4.10965851,1.87191870
H,0.77761166,-4.57957107,-1.77668561
H,0.49777769,-3.61407827,-3.02431280
H,-0.70724393,-4.42730900,-2.35145349
H,-0.10363689,5.83363372,2.82796433
H,1.29641679,-6.19002620,2.93657722
H,-1.85839746,-4.86576373,-0.23238459
H,-0.41630495,-7.64131671,2.30906300
H,-2.00546631,-6.97149476,0.76774969
H,-1.90931863,7.15843248,0.00847525
H,-1.12024764,7.22942137,1.39952972
H,-2.24825760,6.11860453,1.17542821

Sum of electronic and zero-point Energies=,, -2656.373695
 Sum of electronic and thermal Energies=,,, -2656.354348
 Sum of electronic and thermal Enthalpies=,,,-2656.353404
 Sum of electronic and thermal Free Energies=,,-2656.420919

$[L^2Co^{II}]^+$

Co,0,0.7134933986,-1.242375453,-0.0724713653
 O,0,5.0275965203,-1.9402031425,-0.2654898827
 O,0,2.5046533809,-1.3127974163,-0.1416568104
 O,0,-1.2072557192,-1.3626674707,0.0453253259
 N,0,0.5933054178,0.6128484585,-0.0447088139
 N,0,-2.8540161781,1.6783704626,-0.0934456787
 N,0,-2.8809247903,0.3014285363,0.0354878024
 C,0,6.391003682,-2.3117787715,-0.327083528
 H,0,6.9419874985,-1.9649761338,0.5553702663
 H,0,6.4060527632,-3.4014864193,-0.355195665
 H,0,6.8738544504,-1.919886465,-1.2303551125
 C,0,4.7440990037,-0.6187254605,-0.2203919435
 C,0,5.6816385707,0.4006289482,-0.2305246812
 H,0,6.7387487122,0.1639336417,-0.2779586984
 C,0,5.2847692269,1.7499455944,-0.1784820153
 H,0,6.0417517647,2.5270439213,-0.1876806165
 C,0,3.9516154847,2.0730793692,-0.1168359408
 H,0,3.6311011496,3.1099795515,-0.0771074741
 C,0,2.9677341706,1.0526446269,-0.1064157639
 C,0,3.3530655917,-0.3122922549,-0.1561601904
 C,0,1.5979412761,1.4434816506,-0.0438597981
 H,0,1.3701406324,2.5066105575,0.0377613861
 C,0,-0.7555813542,0.9700227757,0.0051820517
 C,0,-1.5576569725,2.0948220018,-0.0793998046
 C,0,-1.6098817228,-0.1488846427,0.0557714899
 C,0,-1.1760085335,3.5355683332,-0.1887538494
 H,0,-2.0559296317,4.1775246259,-0.0774383867
 O,0,-0.2079046945,3.8034541901,0.8008586855
 H,0,-0.7802963308,3.6995103796,-1.2023586395
 C,0,-4.0184788522,2.4358762762,0.342536539
 H,0,-4.9170443285,1.9402453934,-0.0218412842
 H,0,-4.0504101599,2.5103648724,1.4329770441
 H,0,-3.9784459206,3.4271279475,-0.1034642788
 C,0,-4.0623326123,-0.4741776958,-0.1450725375
 C,0,-4.7720742029,-0.3874983384,-1.3422539963
 H,0,-4.4313628571,0.2770078254,-2.1303394265
 C,0,-5.9117628663,-1.1681297555,-1.5036727014
 H,0,-6.4771122028,-1.1058809174,-2.4279633762
 C,0,-6.3156196784,-2.0370399709,-0.4907700125
 H,0,-7.2013990193,-2.6498270396,-0.6262748351
 C,0,-5.5869365637,-2.1228188433,0.6935383965
 H,0,-5.9022759826,-2.7987160439,1.4818723609
 C,0,-4.4573834771,-1.3310044794,0.8784253381
 H,0,-3.8872249375,-1.370925513,1.8006659683
 H,0,0.1254859537,4.6953229374,0.6496350425

Sum of electronic and zero-point Energies=,, -2580.749999
 Sum of electronic and thermal Energies=,,, -2580.725846
 Sum of electronic and thermal Enthalpies=,,,-2580.724902
 Sum of electronic and thermal Free Energies=,,-2580.806149

$[L^2Co(\eta^2\text{-}O_2)]^+$

Co,0,-1.1070023508,-1.450972169,0.4048480663
O,0,-5.3629645711,-1.651710442,-0.3268894982
O,0,-2.7822238762,-1.3378401102,-0.127468092
O,0,1.5788876977,-1.4353516873,-1.1882623762
N,0,-0.6189058706,0.2814101686,-0.1083245203
N,0,2.7319952221,1.5027226224,0.2306001269
N,0,2.9336390824,0.333391938,-0.4844762994
C,0,-6.7628612214,-1.8563434612,-0.4313018411
H,0,-7.140469644,-1.5298116619,-1.4065999463
H,0,-6.9159300281,-2.9297216941,-0.3241831312
H,0,-7.3011931633,-1.3304628032,0.3650871387
C,0,-4.9074603506,-0.3913243466,-0.4234968386
C,0,-5.6851461898,0.7399603111,-0.6224476384
H,0,-6.761598482,0.6475106594,-0.7108217798
C,0,-5.0995779128,2.0144884933,-0.7123146914
H,0,-5.7368955717,2.8771347197,-0.8737438172
C,0,-3.736503529,2.1693041451,-0.604968527
H,0,-3.2779287801,3.1497825238,-0.6830720288
C,0,-2.9163305482,1.0389980713,-0.3867582622
C,0,-3.4968880748,-0.2516232174,-0.2918565661
C,0,-1.5058236065,1.2130698223,-0.358883835
H,0,-1.1170290466,2.20673996,-0.5949137
C,0,0.7409340254,0.5685834348,-0.0988109801
C,0,1.4009300583,1.6576303739,0.4272824524
C,0,1.7204760466,-0.3276169702,-0.6777973116
C,0,0.8157454405,2.8754239306,1.0610016745
H,0,1.5399692788,3.3285147087,1.7478858198
O,0,0.4387635095,3.755465887,0.0195626029
H,0,-0.0470248255,2.5572498127,1.6628153755
C,0,3.647805448,2.6099273123,-0.0220608414
H,0,4.6697666817,2.2849436708,0.1685617304
H,0,3.5518665299,2.9551053127,-1.0554728921
H,0,3.4074410053,3.4214277814,0.6620739196
C,0,4.1998116521,-0.3061039571,-0.4711901304
C,0,4.9902476407,-0.2827396009,0.6794134868
H,0,4.6348674455,0.2243088279,1.5714800979
C,0,6.2242122047,-0.9249987229,0.6694554496
H,0,6.8449258787,-0.9017378165,1.5598692649
C,0,6.6519319039,-1.6085672574,-0.467086204
H,0,7.6118685809,-2.1156159362,-0.4669310579
C,0,5.8451291901,-1.6409814587,-1.6027536432
H,0,6.1743626111,-2.1722829155,-2.4904202191
C,0,4.6205062896,-0.9802334767,-1.6165385723
H,0,3.9910197023,-0.9853713196,-2.4990015903
O,0,-0.5487583074,-1.5434288958,2.1545638057
O,0,0.4631702091,-1.8400843429,1.4275690855
H,0,0.0294042157,4.5304852454,0.4222737544

Sum of electronic and zero-point Energies=,, -2730.878424
Sum of electronic and thermal Energies=,,, -2730.851439
Sum of electronic and thermal Enthalpies=,,,-2730.850494
Sum of electronic and thermal Free Energies=,,-2730.937573

$[\{L^2Co(\eta^2\text{-}O_2)\}^+]^{\neq}$

Co,0,-1.6819951273,1.7211040594,-0.0557714466
O,0,-5.7510512161,0.0223492506,-0.0560689328
O,0,-3.2776592004,0.8352060181,0.0073142716
O,0,1.6978009923,-1.9408207442,-0.1764412

N,0,-0.5484064331,0.2066859536,0.0346821968
N,0,2.8894106897,1.3027837698,-0.2101758439
N,0,3.0456560479,-0.0675280182,-0.3566618289
C,0,-7.1007311935,-0.395541088,-0.079371713
H,0,-7.3589488071,-0.9730934289,0.8168245188
H,0,-7.7000341224,0.5150090236,-0.1051181008
H,0,-7.3204856299,-0.9981326007,-0.9692721771
C,0,-4.802678165,-0.9436003837,-0.0231346692
C,0,-5.0494960669,-2.3026578869,-0.006275305
H,0,-6.0697558853,-2.6699650065,-0.0231826648
C,0,-3.9875820197,-3.2313354123,0.0287702292
H,0,-4.2110635935,-4.2931226156,0.0389622738
C,0,-2.6900125284,-2.7892812322,0.0472468187
H,0,-1.8631232071,-3.4936139781,0.0705316873
C,0,-2.4005592614,-1.3980806787,0.0354267966
C,0,-3.4569909258,-0.4513796666,0.0020700808
C,0,-1.0309705528,-1.0169170154,0.0374061953
H,0,-0.3021824197,-1.8272288469,0.0235182132
C,0,0.8440618468,0.3609340605,-0.0788939622
C,0,1.5468252714,1.5395167658,-0.1131493003
C,0,1.8229542117,-0.7161367126,-0.2115742982
C,0,1.0211882964,2.9365977337,-0.0828452281
H,0,0.8178997306,3.3010194,-1.0969871616
O,0,-0.2010513925,2.9131829836,0.6261187277
H,0,1.73144133,3.6106543201,0.4010421893
C,0,3.7398309699,2.1379770182,-1.0566358671
H,0,4.7820763909,1.868312621,-0.8883325711
H,0,3.4906368577,2.0133781978,-2.115531768
H,0,3.6081414761,3.1795120012,-0.7636702891
C,0,4.3029060139,-0.6658296019,-0.101761031
C,0,5.1740607921,-0.1109822533,0.8383658818
H,0,4.8799928984,0.7776290424,1.3883733371
C,0,6.4069869039,-0.7146084922,1.0661129203
H,0,7.0872533384,-0.2798159516,1.792182335
C,0,6.759991818,-1.875871419,0.3819514189
H,0,7.7201103497,-2.3472258992,0.5682915277
C,0,5.8765901775,-2.4295446765,-0.5429084901
H,0,6.1465693549,-3.3330117749,-1.0813470045
C,0,4.6509428765,-1.8233422382,-0.799244869
H,0,3.9630787131,-2.2380010395,-1.5265527502
O,0,-1.885415613,2.6525532552,-1.3785012486
H,0,-0.2158130368,3.4881315373,1.3962527714

Sum of electronic and zero-point Energies= -2655.780743
Sum of electronic and thermal Energies= -2655.755706
Sum of electronic and thermal Enthalpies= -2655.754761
Sum of electronic and thermal Free Energies= -2655.837273

[L^3Co(OH)]

Co,0,-1.6533132789,1.5587003479,0.2220278545
O,0,-5.7462441136,-0.0791761279,0.5722173055
O,0,-3.2362659583,0.6734213147,0.5115332296
O,0,1.6493140362,-2.0422174585,-0.2889469729
N,0,-0.5851185176,0.0686148499,0.0740981922
N,0,2.830006316,1.1929582172,0.0059512456
N,0,3.0031000814,-0.1594143976,-0.2450376978
C,0,-7.1042937893,-0.4699069921,0.6133293387
H,0,-7.2808774115,-1.2288690128,1.3851973325

H,0,-7.6712835031,0.4290780607,0.8562823323
H,0,-7.4400205599,-0.8584705884,-0.3558651534
C,0,-4.8342598973,-1.0356864401,0.2819435254
C,0,-5.1186012245,-2.3644567524,0.02798219
H,0,-6.1453566431,-2.7131789796,0.0479185219
C,0,-4.0893297388,-3.2847625723,-0.2615868555
H,0,-4.3445927373,-4.3213543093,-0.4552669598
C,0,-2.7822149292,-2.8692228214,-0.2939508883
H,0,-1.9806325829,-3.5689271677,-0.5120550952
C,0,-2.457955373,-1.5098388242,-0.0458268355
C,0,-3.4817644645,-0.5726735743,0.2475488778
C,0,-1.0877069163,-1.135944468,-0.0675999945
H,0,-0.3566692127,-1.9325218941,-0.2147049081
C,0,0.7992879634,0.2433114903,-0.0211617497
C,0,1.4905095203,1.4238999555,0.0752299842
C,0,1.7784428232,-0.8191581072,-0.2112125503
C,0,0.9339740396,2.8230261358,0.1632725069
H,0,1.0859904748,3.3152525516,-0.8194898778
O,0,-0.3852784541,2.8155039541,0.5085579733
O,0,1.7034924149,3.4982920772,1.1329705909
C,0,3.7467792564,2.111044764,-0.6628120935
H,0,4.7721369298,1.8295527694,-0.4238198813
H,0,3.602867288,2.0897023699,-1.748225634
H,0,3.5520684073,3.1065753222,-0.2675933556
C,0,4.2462077667,-0.781300077,0.02873838
C,0,5.0438518887,-0.3337312449,1.083965747
H,0,4.705686913,0.4907219525,1.7041995032
C,0,6.260324883,-0.9615771165,1.3330686087
H,0,6.8843951574,-0.6104117585,2.1492620375
C,0,6.667262587,-2.0429254748,0.5540886794
H,0,7.6137396211,-2.5345146967,0.7572542893
C,0,5.8557574019,-2.4911976683,-0.4863595456
H,0,6.1681703335,-3.3322486163,-1.097937442
C,0,4.6484215631,-1.8572438701,-0.7627544809
H,0,4.016102669,-2.1889692918,-1.5779666193
O,0,-1.9985569828,1.9204527013,-1.4663134674
H,0,-1.2669424743,2.4759850742,-1.7663289537
H,0,1.4252037773,4.4216230146,1.1097495459

Sum of electronic and zero-point Energies=,, -2731.172636
Sum of electronic and thermal Energies=,,, -2731.146595
Sum of electronic and thermal Enthalpies=,,,-2731.145651
Sum of electronic and thermal Free Energies=,,-2731.229263

$[L^3Co(OH_2)]$

Co,-0.22330000,0.66990000,-2.85600000
O,-1.05830000,-1.17610000,-2.97600000
O,0.22370000,2.59890000,-2.83300000
O,0.13870000,-0.15510000,2.24600000
O,1.71070000,-0.08510000,-3.20800000
N,0.14870000,0.53090000,-0.78700000
N,-0.72930000,-2.80210000,0.19700000
O,0.20870000,5.17190000,-3.23500000
N,-0.44630000,-2.23310000,1.43200000
C,-0.09630000,-0.68110000,-0.13400000
C,-0.47330000,-1.85310000,-0.74600000
C,-0.57430000,-2.22410000,-2.18900000
C,-0.08430000,-0.92310000,1.28800000

C,0.58770000,3.34490000,-1.81700000
C,0.90770000,2.84490000,-0.53100000
C,0.69770000,1.49890000,-0.10600000
C,1.37470000,3.75390000,0.46000000
C,1.45270000,5.08490000,0.21900000
C,0.37070000,-2.94210000,3.58700000
C,-0.65530000,-2.93110000,2.66100000
C,0.62570000,4.75590000,-2.00900000
C,-0.79030000,-4.23810000,0.03300000
C,1.05470000,5.59790000,-1.00500000
C,0.19370000,-3.61810000,4.79000000
C,-1.83930000,-3.58610000,2.91500000
C,-0.98430000,-4.30510000,5.02400000
C,-1.99330000,-4.28010000,4.10400000
C,-0.55330000,6.37790000,-3.23800000
O,0.63170000,-2.68810000,-2.57100000
H,2.20870000,0.05490000,-2.50500000
H,2.06070000,0.32190000,-3.89500000
H,-1.22430000,-2.98110000,-2.25900000
H,0.99170000,1.28290000,0.77000000
H,1.63570000,3.42090000,1.30800000
H,1.78370000,5.66890000,0.89100000
H,1.18770000,-2.49510000,3.40500000
H,-0.17930000,-4.66610000,0.66900000
H,-0.52730000,-4.47310000,-0.88300000
H,-1.70430000,-4.54910000,0.20100000
H,1.07770000,6.53690000,-1.15500000
H,0.87770000,-3.60710000,5.44800000
H,-2.54530000,-3.56210000,2.28100000
H,-1.09030000,-4.79610000,5.83100000
H,-2.80530000,-4.74210000,4.28000000
H,-0.96930000,6.49890000,-4.11700000
H,0.03670000,7.13590000,-3.04700000
H,-1.24930000,6.32490000,-2.55200000
H,0.60870000,-2.88510000,-3.38600000

Sum of electronic and zero-point Energies= -2731.506508
Sum of electronic and thermal Energies= -2731.486227
Sum of electronic and thermal Enthalpies= -2731.485283
Sum of electronic and thermal Free Energies= -2731.554837

$[L^3Co]^+$

Co,0,0.6122969634,-1.2588625348,-0.0548065147
O,0,4.9188693263,-2.0331653723,-0.1421864236
O,0,2.4013254365,-1.3666331407,-0.0983610711
O,0,-1.3025362861,-1.352753063,0.0559055774
N,0,0.5114688916,0.5998798437,-0.075919755
N,0,-2.9447588365,1.6842457101,-0.0756869976
N,0,-2.9662957941,0.3118394451,0.0744544618
C,0,6.2782143128,-2.4238881437,-0.1617260249
H,0,6.8109264746,-2.0687232215,0.7285925961
H,0,6.2790755565,-3.5140027071,-0.1704571805
H,0,6.7894528771,-2.0544263058,-1.0587888526
C,0,4.6530962006,-0.707308229,-0.1281485976
C,0,5.6048989202,0.2987024952,-0.1316926694
H,0,6.6594058881,0.0465677656,-0.1467416026
C,0,5.2264116249,1.6543328394,-0.1150032463
H,0,5.9945705084,2.4204314597,-0.1179575016

C,0,3.8970566964,1.9968784339,-0.0953255597
H,0,3.5901949348,3.0386124406,-0.0831031379
C,0,2.8981239989,0.9904645469,-0.0916884625
C,0,3.2654605736,-0.3801798021,-0.1062198379
C,0,1.5351658194,1.4079586206,-0.0731203073
H,0,1.3294383005,2.4771594842,-0.069987446
C,0,-0.8352447753,0.9797628843,-0.0380605503
C,0,-1.6462236582,2.0983704686,-0.1106893876
C,0,-1.6965372907,-0.1376394406,0.0546051424
C,0,-1.3557320232,3.5748987101,-0.1578396075
H,0,-2.1476572449,4.0778297354,-0.7289376581
O,0,-1.3452380182,4.0161485422,1.1667786343
O,0,-0.1364766894,3.7310591008,-0.8145037194
C,0,-4.0516278949,2.4585506821,0.4724050224
H,0,-4.9864787742,1.9596763992,0.222497582
H,0,-3.9544992892,2.561759609,1.556072513
H,0,-4.0545461598,3.4411724554,0.0041011565
C,0,-4.1526295483,-0.4633440461,-0.0631582593
C,0,-4.9574093409,-0.3050952925,-1.1908596758
H,0,-4.6853692122,0.4137021924,-1.9575961719
C,0,-6.1006727032,-1.0876625909,-1.3130805663
H,0,-6.7389153047,-0.9702375301,-2.1829404191
C,0,-6.4148534222,-2.0286270305,-0.3335307638
H,0,-7.3037174456,-2.6427379593,-0.4393305276
C,0,-5.5917899168,-2.1843325798,0.7797459363
H,0,-5.8369179707,-2.9159273107,1.5429169644
C,0,-4.457343111,-1.3921543107,0.9281433571
H,0,-3.8151622062,-1.4877866129,1.7972207479
H,0,-1.5304555675,4.9628171633,1.1819003233
H,0,-0.0225025206,4.6588619759,-1.0512224992

Sum of electronic and zero-point Energies=,, -2655.896633
Sum of electronic and thermal Energies=,,, -2655.871440
Sum of electronic and thermal Enthalpies=,,,-2655.870496
Sum of electronic and thermal Free Energies=,,-2655.953713

$[L^3Co(\eta^2\text{-}O_2)]^+$

Co,0,-1.1418419211,-1.2501729316,0.6926781307
O,0,-5.3629048098,-1.6295245292,-0.1505235945
O,0,-2.7893700259,-1.2686734313,0.0609084009
O,0,1.4159235936,-1.6375617462,-0.8011662467
N,0,-0.6432263753,0.3526062682,-0.1220297459
N,0,2.7671900321,1.4584162056,-0.0472943871
N,0,2.8864240206,0.1592658336,-0.5172636505
C,0,-6.7579942209,-1.8596781585,-0.2623243694
H,0,-7.1056015184,-1.7021967828,-1.289459768
H,0,-6.9117226777,-2.9016817539,0.016414198
H,0,-7.3231575252,-1.213532156,0.4187278624
C,0,-4.908451428,-0.3990936368,-0.445391313
C,0,-5.6850358297,0.6764129433,-0.8501183879
H,0,-6.7586308554,0.5614580775,-0.9463586687
C,0,-5.1035470334,1.9229093892,-1.1404535085
H,0,-5.7405000325,2.7408294082,-1.4593068741
C,0,-3.7446322605,2.1033660591,-1.0300401944
H,0,-3.2875659607,3.0599551546,-1.2622216883
C,0,-2.9263170297,1.0323331217,-0.6024744716
C,0,-3.5024136716,-0.2292602606,-0.3033562063
C,0,-1.5171500223,1.2152575456,-0.5743207043

H,0,-1.1187696091,2.1387585508,-0.9981869296
C,0,0.7235247779,0.5931249397,-0.1611263698
C,0,1.4536024136,1.7218961291,0.1387219226
C,0,1.6414419688,-0.4547362372,-0.549340185
C,0,0.9252347728,3.0622327077,0.5776315526
O,0,1.8657830937,3.6603901693,1.4097145846
O,0,0.6647688433,3.7836838142,-0.5968278546
H,0,-0.0088487845,2.8819718571,1.1310004614
C,0,3.7485572406,2.4362029594,-0.5109065414
H,0,4.7481081716,2.1074911371,-0.2283158611
H,0,3.6856100877,2.542469598,-1.5977587269
H,0,3.5254166212,3.3808905416,-0.0212811036
C,0,4.1240823561,-0.5298871664,-0.4419727157
C,0,4.9556300157,-0.3711547587,0.6677520086
H,0,4.6563966313,0.283546299,1.4807542476
C,0,6.1581138457,-1.0688196388,0.7196031673
H,0,6.8122068624,-0.9424481227,1.5767754865
C,0,6.5119222568,-1.9375361264,-0.3112115435
H,0,7.4474392199,-2.4861375388,-0.2617852703
C,0,5.663524869,-2.1022840819,-1.4042306777
H,0,5.9355412648,-2.7780526588,-2.2091507263
C,0,4.4702962829,-1.3906189872,-1.4820589083
H,0,3.8087219193,-1.49746884,-2.3344158022
O,0,-0.7483662963,-0.8706296635,2.4359735818
O,0,0.3397825348,-1.3140991519,1.9280931516
H,0,0.1167820547,4.5471774427,-0.3740201948
H,0,1.4351221372,4.3529022064,1.9236444334

Sum of electronic and zero-point Energies=,, -2806.024509
Sum of electronic and thermal Energies=,,, -2805.996278
Sum of electronic and thermal Enthalpies=,,,-2805.995334
Sum of electronic and thermal Free Energies=,,-2806.085517

$[\{L^3Co(\eta^2\text{-}O_2)\}^+]^{\neq}$

Co,,,,-1.77996200,1.55040500,0.29158800
O,-5.46269400,-0.62113700,1.27284600
O,-3.08875300,0.39940300,0.84410800
O, 1.30175000,-2.08178700,-0.40938500
N,-0.62162100,0.21731900,-0.33878100
N, 2.93555500,0.93829700,-0.05255000
N, 2.91164500,-0.43458500,-0.22593600
C,-6.75227700,-1.15104700,1.51085200
C,-4.68334900,-1.26423300,0.37526500
C,-5.04434800,-2.39170900,-0.33811400
C,-4.15221300,-2.99116400,-1.25258100
C,-2.90052600,-2.46413700,-1.44119100
C,-2.50298900,-1.29802000,-0.73538700
C,-3.39684300,-0.67135600,0.17466100
C,-1.15464600,-0.87100100,-0.86024100
C, 0.77782100,0.31473000,-0.35353500
C, 1.62685100,1.37667100,-0.16780800
C, 1.62008200,-0.89662200,-0.36381300
C, 1.43859100,2.86603400,-0.06910200
O, 2.24306600,3.46968000,0.84078100
C, 3.99368100,1.62004400,-0.81332200
C, 4.02659200,-1.21999300,0.15264000
C, 4.83600500,-0.81908900,1.21732600
C, 5.93220800,-1.59954100,1.57065300

C, 6.20673100,-2.78038400,0.88392700
C, 5.38392500,-3.17661300,-0.16880600
C, 4.29732000,-2.39559600,-0.54871100
O,-2.58401900,2.67596400,-0.63557800
O,-0.78680900,3.04318900,-0.18507800
O, 1.51713200,3.56485200,-1.22977800
H,-6.69985700,-2.17481000,1.90064100
H,-7.21191100,-0.50415000,2.25831100
H,-7.36363900,-1.14331900,0.60037800
H,-6.02751800,-2.82837000,-0.20132100
H,-4.46565100,-3.87784500,-1.79352100
H,-2.19671500,-2.92966800,-2.12503100
H,-0.49145200,-1.54146000,-1.39835400
H, 2.38217700,2.88463600,1.59840800
H, 4.95461800,1.19481400,-0.52526600
H, 3.83794300,1.49796100,-1.88956700
H, 3.98451100,2.67500300,-0.54753200
H, 4.59965600,0.08934000,1.76258700
H, 6.56578600,-1.28644600,2.39485900
H, 7.05936000,-3.38958300,1.16770000
H, 5.59439500,-4.09419300,-0.70978300
H, 3.65931200,-2.68932500,-1.37364600
H, 0.65531400,3.44902700,-1.66086800
H, 0.21051500,3.03707500,0.37040600

Sum of electronic and zero-point Energies=,, -2805.956911
Sum of electronic and thermal Energies=,,, -2805.929865
Sum of electronic and thermal Enthalpies=,,,-2805.928921
Sum of electronic and thermal Free Energies=,,-2806.015337

[L^{4}Co(OH)]

Co,0,1.6146455936,0.1981777022,-1.5409171484
H,0,1.1256616862,2.1264619352,-2.5047320888
O,0,1.8151606066,1.8974797499,-1.8652238501
O,0,5.7058882578,-0.3502308553,-0.0534341492
O,0,3.1846167117,-0.1655233278,-0.7342914419
O,0,0.3360371081,-0.0009153479,-2.8479892713
O,0,-1.6985106392,-0.2614004185,-3.7210110318
O,0,-1.6359698497,0.3409791691,2.0950504349
N,0,0.5711218498,0.0654286079,-0.0473139455
N,0,-3.0108012187,0.2931602015,0.224102814
N,0,-2.8535950863,0.1083771651,-1.1413460801
C,0,7.0689425857,-0.4353755777,0.2901526404
H,0,7.4125243537,0.4712250646,0.8052901714
H,0,7.6110624377,-0.5411115556,-0.649960468
H,0,7.2722120665,-1.3080189917,0.9248503512
C,0,4.8195799299,-0.204641613,0.9512798944
C,0,5.1252867591,-0.1461498934,2.2971818834
H,0,6.1584319612,-0.2116518808,2.6203935486
C,0,4.1131745065,0.0016455259,3.2702084863
H,0,4.3904654068,0.0430582777,4.3183457668
C,0,2.7985028019,0.0869694687,2.89522465
H,0,2.0105186275,0.1937728172,3.6346472376
C,0,2.4481334805,0.0379642712,1.520023059
C,0,3.4570819292,-0.0997331053,0.5301689135
C,0,1.0789833883,0.0777102048,1.1703925432
H,0,0.3471278237,0.1140872984,1.9800625179
C,0,-0.8095495713,0.1550758415,-0.2048630762

C,0,-1.7829349748,0.2881778361,0.8777386885
C,0,-1.5046674969,0.0799766595,-1.385312901
C,0,-0.9583482706,-0.0701169587,-2.7714958924
C,0,-3.7686427885,0.8679120774,-1.9947861802
H,0,-4.794400648,0.5854266872,-1.7579736528
H,0,-3.5328984721,0.6005304111,-3.0230798033
H,0,-3.6399968657,1.944476843,-1.8339180153
C,0,-4.2480025576,0.0002934803,0.8443090032
C,0,-5.0874189285,-0.9794182765,0.3095196388
H,0,-4.7766419963,-1.5293613193,-0.5734913358
C,0,-6.3017088349,-1.2506014323,0.9301037801
H,0,-6.95657912,-2.0090650027,0.5116639708
C,0,-6.667255302,-0.5704044295,2.088868733
H,0,-7.6130536086,-0.7905979807,2.5744172227
C,0,-5.8120577019,0.3888963499,2.62536484
H,0,-6.0884458864,0.9187488547,3.5319715868
C,0,-4.6045767882,0.6882957354,2.0043922868
H,0,-3.9313451461,1.4311302114,2.4144883587

Sum of electronic and zero-point Energies=,, -2729.995279
Sum of electronic and thermal Energies=,,, -2729.970100
Sum of electronic and thermal Enthalpies=,,,-2729.969156
Sum of electronic and thermal Free Energies=,,-2730.050963

[L^1L^4Co]

Co,0,-0.45309759,-0.398273017,0.9792625851
O,0,-1.7398302381,-3.082758506,-2.2472624037
O,0,-1.0238403379,-1.6840556363,-0.22357136
O,0,0.1485666262,1.0368768627,2.2219328137
O,0,3.6847215478,-1.9437568951,1.3699622514
O,0,1.3165360567,-1.0019280059,0.8932963773
O,0,-2.228063445,0.0426929318,1.4524658418
O,0,-4.2615429255,0.9091471794,1.2445747132
O,0,-0.7314689075,2.3507920626,-3.1600325135
N,0,-0.5624201094,-1.5617957121,2.5284118988
N,0,0.5184630367,1.0977114618,4.5337868306
N,0,0.5228708053,0.1318003901,5.5438138297
N,0,-0.3058868045,0.8046410109,-0.5080609806
N,0,-2.9396597856,2.3202928869,-2.4457490687
N,0,-3.6329655491,1.9287633692,-1.3058255807
C,0,-2.1121972553,-3.8219785281,-3.3821121996
H,0,-2.0067155021,-3.1468154555,-4.2324894917
H,0,-3.1543397646,-4.1651743202,-3.3212258562
H,0,-1.4604190796,-4.6937327475,-3.5317151173
C,0,-1.7766093764,-3.7162076868,-1.0530193257
C,0,-2.1676773555,-5.0225578654,-0.8578138847
H,0,-2.4764433563,-5.6261094117,-1.7045828661
C,0,-2.1784425513,-5.5977765507,0.4330775615
H,0,-2.4933252195,-6.628650482,0.556342708
C,0,-1.7930311332,-4.8473307646,1.5087039384
H,0,-1.7950364868,-5.2730049972,2.5093060121
C,0,-1.3777953005,-3.4972224996,1.3480185001
C,0,-1.362883804,-2.8932222535,0.0557118312
C,0,-0.9861439402,-2.7872100887,2.5115196112
H,0,-1.0620570185,-3.3312603555,3.4551047918
C,0,-0.1841216634,-0.8459240708,3.6441946383
C,0,0.0495583363,-1.0529778906,4.9748821069
C,0,0.1470744378,0.5197392865,3.3604528735
C,0,-0.1021016096,-2.2686543387,5.8177840164
H,0,0.5375558172,-2.2181373473,6.7017897344

H,0,0.1946724321,-3.1547049741,5.2507374434
H,0,-1.1379244007,-2.4130311323,6.146822292
C,0,-0.1019876957,0.5906052293,6.785983592
H,0,0.4192084467,1.4811436434,7.1393332057
H,0,0.0067306441,-0.1918241397,7.5373333914
H,0,-1.1643678371,0.819961024,6.6398276161
C,0,1.2180454406,2.3165699904,4.6932945183
C,0,2.324749474,2.3862028899,5.5404233761
H,0,2.6641515592,1.4929958869,6.0551971557
C,0,2.9921294283,3.5974255959,5.687679226
H,0,3.8528342131,3.6552060416,6.3472158306
C,0,2.5750264232,4.721544845,4.9801297836
H,0,3.1047491436,5.6625826157,5.0914732063
C,0,1.4804393104,4.6327900229,4.1233884157
H,0,1.1537665806,5.5039614872,3.5639756914
C,0,0.7871591097,3.4363264242,3.9816055859
H,0,-0.0670218817,3.3581002651,3.3188838781
C,0,4.9516540723,-2.4994831731,1.6039475885
H,0,5.3758776048,-2.9469834374,0.6943892408
H,0,4.8102712605,-3.2813555907,2.3523964316
H,0,5.6612164151,-1.7551980152,1.9928087602
C,0,3.6050472857,-0.9563504689,0.4408623825
C,0,4.6755887745,-0.4320868778,-0.2535955864
H,0,5.6762840837,-0.810902222,-0.0739335695
C,0,4.4938526093,0.5955698883,-1.2034807199
H,0,5.352582886,0.9868019634,-1.7390231258
C,0,3.2350069732,1.080569202,-1.4427648892
H,0,3.0714134116,1.8640296073,-2.1779509212
C,0,2.114005405,0.57063826,-0.7384032687
C,0,2.275048382,-0.4632156423,0.218924591
C,0,0.8346074232,1.0900479279,-1.0779341067
H,0,0.7955604465,1.7785594158,-1.9228685382
C,0,-1.4713811042,1.3185160558,-1.0594956836
C,0,-1.5833873881,2.0195979265,-2.3405016241
C,0,-2.7194160748,1.2735680888,-0.5035236879
C,0,-3.1303844397,0.7039056476,0.8162363254
C,0,-4.92873939,1.2980900331,-1.5724163287
H,0,-5.570373657,2.007974608,-2.0959553995
H,0,-5.3564650033,1.0482475819,-0.6030450741
H,0,-4.8022373006,0.3978293602,-2.1858237504
C,0,-3.4738968447,3.3263952156,-3.2769557005
C,0,-4.3940708159,4.2468939866,-2.7674483409
H,0,-4.6725956009,4.1975498043,-1.719595727
C,0,-4.9206483206,5.2255667907,-3.6031802599
H,0,-5.6381946572,5.9364724555,-3.2035754687
C,0,-4.520880704,5.3069640548,-4.9342957557
H,0,-4.9300569725,6.076533016,-5.5819782773
C,0,-3.5884921771,4.3973326975,-5.4274336877
H,0,-3.266235766,4.4562003789,-6.4630429277
C,0,-3.067483916,3.3995533814,-4.6116388739
H,0,-2.338087846,2.692040349,-4.9853230522

Sum of electronic and zero-point Energies=,, -3777.476445
Sum of electronic and thermal Energies=,,, -3777.430370
Sum of electronic and thermal Enthalpies=,,,-3777.429426
Sum of electronic and thermal Free Energies=,,-3777.558508

List of authors in Ref. 50

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