Electronic Supporting Information

Polynuclear Ampyrone based 3*d* Coordination Clusters

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Table S1. Crystal data and structure refinement for HL^1 and compounds **1-4**.

Compound	**HL^1**	**1**	**2**	**3**	**4**
Empirical formula	$C_{18}H_{17}N_3O_2$	$C_{42}H_{41}N_9NiO_4$	$C_{42}H_{41}CoN_9O_4$	$C_{23}H_{27}CuN_3O_5$	$C_{64}H_{64}ClCu_2N_7O_{13}$
Formula weight	307.34	794.55	794.77	489.01	1301.75
Temperature/K	173	173.0	173	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	orthorhombic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	P-1	$P2_12_12$
a/Å	7.4861(3)	13.9150(2)	13.8963(3)	6.8165(3)	13.4231(4)
b/Å	7.4773(3)	13.7467(2)	13.7996(3)	12.1809(6)	30.1689(9)
c/Å	27.3003(10)	20.8267(4)	20.7755(5)	13.8681(5)	14.2158(4)
α/°	90	90	90	97.444(3)	90
β/°	95.532(4)	107.3925(19)	107.426(2)	98.421(3)	90
γ/°	90	90	90	102.838(4)	90
Volume/Å^3	1521.04(11)	3801.68(12)	3801.13(15)	1094.80(8)	5756.8(3)
Z	4	4	4	2	4
ρ_{calc}g/cm^3	1.342	1.388	1.389	1.483	1.502
μ/mm^1	0.725	1.193	0.508	1.038	0.860
F(000)	648.0	1664.0	1660.0	510.0	2704.0
Crystal size/mm^3	0.21 × 0.14 × 0.08	0.2 × 0.14 × 0.1	0.16 × 0.14 × 0.08	0.06 × 0.03 × 0.02	0.11 × 0.04 × 0.02
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71075)
2Θ range for data collection/°	12.01 to 141.988	8.898 to 142.27	6.656 to 52.744	4.202 to 55.088	4.386 to 50.05
Index ranges	-8 ≤ h ≤ 9, -6 ≤ k ≤ 9, -29 ≤ l ≤ 33	-8 ≤ h ≤ 16, -16 ≤ k ≤ 15, -25 ≤ l ≤ 22	-17 ≤ h ≤ 17, -15 ≤ k ≤ 17, -25 ≤ l ≤ 25	-8 ≤ h ≤ 8, -15 ≤ k ≤ 15, -17 ≤ l ≤ 17	-15 ≤ h ≤ 15, -35 ≤ k ≤ 35, -11 ≤ l ≤ 16
Reflections collected	4473	11316	17739	9202	56032
Independent reflections	2808 [R_{int} = 0.0221, R_{sigma} = 0.0338]	7041 [R_{int} = 0.0193, R_{sigma} = 0.0322]	7768 [R_{int} = 0.0235, R_{sigma} = 0.0363]	9202 [R_{int} = ?, R_{sigma} = 0.0373]	10159 [R_{int} = 0.0745, R_{sigma} = 0.0532]
Data/restraints/parameters	2808/0/209	7041/0/512	7768/0/512	9202/0/298	10159/38/795
Goodness-of-fit on F^2	1.052	1.024	1.027	1.048	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0410, wR_2 = 0.1040	R_1 = 0.0377, wR_2 = 0.0985	R_1 = 0.0383, wR_2 = 0.0869	R_1 = 0.0561, wR_2 = 0.1331	R_1 = 0.0642, wR_2 = 0.1494
Final R indexes [all data]	R_1 = 0.0482, wR_2 = 0.1111	R_1 = 0.0458, wR_2 = 0.1060	R_1 = 0.0536, wR_2 = 0.0953	R_1 = 0.0760, wR_2 = 0.1424	R_1 = 0.0809, wR_2 = 0.1589
Largest diff. peak/hole / e Å^{-3}	0.23/-0.18	0.34/-0.29	0.33/-0.34	0.72/-0.67	1.39/-0.62

Table S2. Crystal data and structure refinement for compounds **5-9**.

Compound	**5**	**6**	**7**	**8**	**9**

Empirical formula	$C_{45}H_{44}ClN_7Ni_2O_{14}$	$C_{86}H_{108}Cl_2N_{12}Ni_4O_{25}$	$C_{86}H_{90}Cl_2N_{14}Ni_4O_{21}$	$C_{205}H_{227}Cl_3N_{37}Ni_{10}O_{51}$	$C_{78}H_{73}Cu_4N_{15}O_{14}$
Formula weight	1059.74	2015.58	1961.45	4718.67	1698.67
Temperature/K	173	173	173	173	100(2)
Crystal system	triclinic	monoclinic	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/c$	P-1	$P2_1/c$	C2/c
a/Å	13.6630(8)	15.2703(7)	14.8923(4)	20.7411(10)	21.9366(3)
b/Å	14.4902(8)	28.8077(12)	17.0968(7)	35.8785(14)	18.2644(3)
c/Å	15.6628(8)	22.7473(9)	17.3958(6)	18.2934(8)	18.6976(3)
α/°	70.842(5)	90	87.743(3)	90	90
β/°	67.379(5)	107.926(5)	85.594(2)	109.654(5)	103.4839(15)
γ/°	68.614(5)	90	79.606(3)	90	90
Volume/$Å^3$	2600.8(3)	9520.9(7)	4342.1(3)	12820.1(10)	7284.83(19)
Z	2	4	2	2	4
$\rho_{calc}g/cm^3$	1.353	1.406	1.500	1.222	1.549
μ/mm^1	0.842	2.059	2.216	1.666	1.231
F(000)	1096.0	4216.0	2036.0	4910.0	3496.0
Crystal size/mm^3	0.16 × 0.12 × 0.07	0.24 × 0.18 × 0.12	0.2 × 0.14 × 0.1	0.15 × 0.12 × 0.1	0.13 × 0.12 × 0.07
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	MoKα (λ = 0.71075)
2Θ range for data collection/°	6.582 to 58.486	8.858 to 142.198	9.206 to 142.514	9.268 to 133.2	4.46 to 54.966
Index ranges	-17 ≤ h ≤ 18, -16 ≤ k ≤ 19, -21 ≤ l ≤ 20	-17 ≤ h ≤ 18, -34 ≤ k ≤ 34, -23 ≤ l ≤ 26	-14 ≤ h ≤ 18, -20 ≤ k ≤ 20, -21 ≤ l ≤ 19	-19 ≤ h ≤ 25, -43 ≤ k ≤ 37, -22 ≤ l ≤ 15	-28 ≤ h ≤ 28, -23 ≤ k ≤ 23, -21 ≤ l ≤ 24
Reflections collected	16964	32761	27717	43617	24167
Independent reflections	11603 [R_{int} = 0.0449, R_{sigma} = 0.1063]	17467 [R_{int} = 0.0335, R_{sigma} = 0.0513]	15772 [R_{int} = 0.0489, R_{sigma} = 0.0634]	22143 [R_{int} = 0.0749, R_{sigma} = 0.1218]	8316 [R_{int} = 0.0166, R_{sigma} = 0.0184]
Data/restraints/parameters	11603/3/631	17467/145/1174	15772/0/1163	22143/62/1401	8316/24/517
Goodness-of-fit on F^2	0.978	1.085	1.053	1.016	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0677, wR_2 = 0.1560	R_1 = 0.0754, wR_2 = 0.2190	R_1 = 0.0529, wR_2 = 0.1308	R_1 = 0.0902, wR_2 = 0.2336	R_1 = 0.0280, wR_2 = 0.0739
Final R indexes [all data]	R_1 = 0.1176, wR_2 = 0.1810	R_1 = 0.0941, wR_2 = 0.2432	R_1 = 0.0639, wR_2 = 0.1419	R_1 = 0.1445, wR_2 = 0.2680	R_1 = 0.0320, wR_2 = 0.0760
Largest diff. peak/hole / e $Å^{-3}$	1.18/-0.68	1.29/-0.88	0.68/-0.78	1.34/-0.98	0.50/-0.56

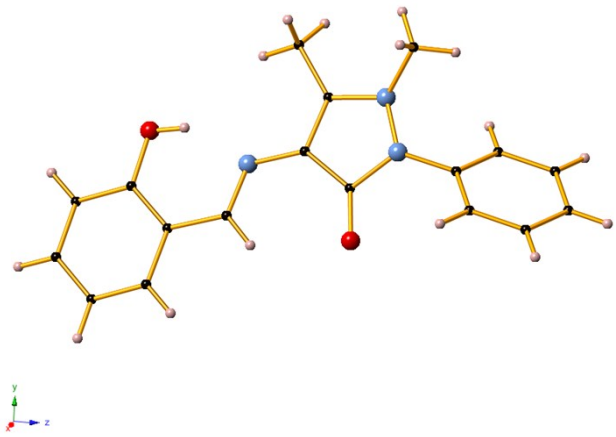

Figure S1. The crystal structure of the ligand HL. Colour code C (black), H (pink), O (red), N (blue).

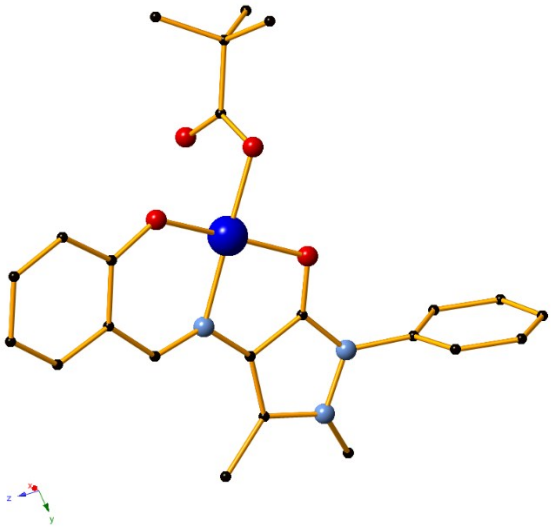

Figure S2. The structure of compound **3**. Lattice solvent molecules and H atoms are omitted for clarity. Colour code Cu (dark blue), O (red), C (black), N (blue).

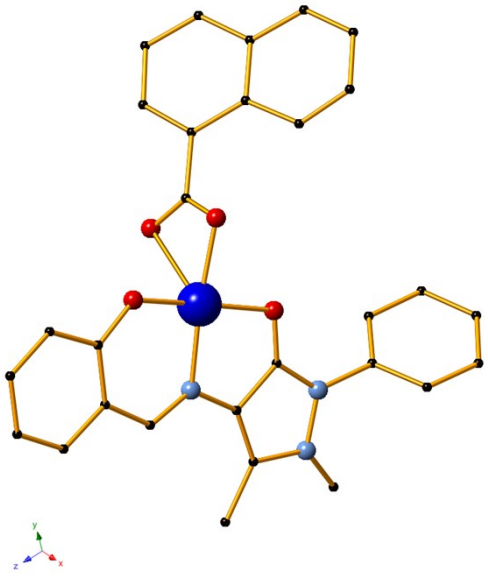

Figure S3. The monomer structure in compound **4**. Lattice solvent and anion molecules as well as H atoms are omitted for clarity. Colour code Cu (dark blue), O (red), C (black), N (blue).

Table S3. Selected bond distances (Å) for compound **1**.

Ni1 – O2	2.0021(13)
Ni1 – O1	2.2037(12)
Ni1 – O3	2.1959(12)

Ni1 – O4	2.0054(13)
Ni1 – N3	2.0384(14)
Ni1 – N6	2.0417(14)

Table S4. Selected bond distances (Å) for compound **2**.

Co1 – O1	2.0055(14)
Co1 – O2	2.2183(14)
Co1 – O3	2.2314(14)
Co1 – O4	2.0022(14)
Co1 – N1	2.0860(15)
Co1 – N4	2.0959(15)

Table S5. Selected bond distances (Å) for compound **3**.

Cu1 – O1	1.896(2)
Cu1 – O2	1.999(2)
Cu1 – O3	1.930(2)
Cu1 – N1	1.967(3)

Table S6. Hydrogen bond values for compound **3**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [°]
O101-H10A···N4	0.85	2.01	2.849(4)	171
O101-H10B···O1^{i}	0.85	2.11	2.912(3)	157

i: -1+x,+y,+z

Table S7. Selected bond distances (Å) for compound **4**.

Cu1 – O1	1.906(6)
Cu1 – O2	2.019(5)
Cu1 – O3	1.972(6)
Cu1 – O4	2.502(8)
Cu1 – N1	1.962(6)

Cu11 – O101	1.911(5)
Cu11 – O102	1.999(5)
Cu11 – O103	1.973(6)
Cu11 – O104	2.473(7)
Cu11 – N101	1.970(7)

Table S8. Hydrogen bond values for compound **4**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [°]
O401-H40A···O303	0.85	2.02	2.806(15)	153
O401-H40B···O101	0.85	2.13	2.885(11)	147
N201-H201···O401	1.00	1.79	2.742(13)	158

Table S9. Selected bond distances (Å) for compound **5**.

Ni1 – Ni2	2.9457(7)
Ni1 – O1	2.112(3)
Ni1 – O2	2.020(3)
Ni1 – O4	2.069(3)
Ni1 – O5	2.035(3)
Ni1 – O9	2.068(3)
Ni1 – N3	2.047(3)
Ni2 – O2	2.100(3)
Ni2 – O3	2.140(3)
Ni2 – O4	1.983(3)
Ni2 – O6	2.025(3)
Ni2 – O10	2.075(3)
Ni2 – N6	2.025(3)

Table S10. Selected bond distances (Å) and angles (°) for **6**.

Ni01 – O00C	1.968(3)	Ni03 – O009	2.103(3)	Ni02–O00A–Ni03	104.52(11)
Ni01 – O00D	2.137(3)	Ni03 – N00E	2.038(3)	Ni02–O00A–Ni04	99.77(12)

Ni01 – O00I	2.217(3)	Ni04 – O00A	2.040(3)	Ni03–O00A–Ni04	101.55(12)
Ni01 – O007	2.033(3)	Ni04 – O00C	2.033(3)	Ni03–O00C–Ni04	100.55(11)
Ni01 – O008	2.048(3)	Ni04 – O00G	1.997(3)	Ni01 – Ni02	3.1734(8)
Ni01 – N00K	2.014(3)	Ni04 – O00I	2.196(3)	Ni01 – Ni03	3.1229(11)
Ni02 – O00A	1.989(3)	Ni04 – O00L	2.126(3)	Ni01 – Ni04	3.1352(9)
Ni02 – O00B	2.100(3)	Ni04 – N00J	2.051(4)	Ni02 – Ni03	3.1781(10)
Ni02 – O00F	2.055(3)	Ni01–O00I–Ni02	95.26(11)	Ni02 – Ni04	3.0821(9)
Ni02 – O00I	2.077(3)	Ni01–O00C–Ni03	101.40(12)	Ni03 – Ni04	3.1528(10)
Ni02 – O007	2.136(3)	Ni01–O007–Ni02	99.09(12)		
Ni02 – N00T	2.036(3)	Ni01–O00I–Ni04	90.55(11)		
Ni03 – O00A	2.029(3)	Ni01–O007–Ni03	91.76(10)		
Ni03 – O00C	2.066(3)	Ni01–O00C–Ni04	103.17(14)		
Ni03 – O00H	1.973(3)	Ni02–O007–Ni03	91.19(9)		
Ni03 – O007	2.309(3)	Ni02–O00I–Ni04	92.27(11)		

Table S11. Hydrogen bond values for compound **6**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [°]
O00C-H00C···O01H	1.00	1.86	2.845(6)	169
O00L-H00L···O00D	0.851(16)	2.230(17)	2.991(4)	149(3)
O009-H009···O00G	0.86(3)	1.88(4)	2.647(5)	147(4)
O01H-H01I···O032	0.84	2.12	2.852(16)	145

Table S12. Selected bond distances (Å) and angles (°) for **7**.

Ni01 – O008	2.1113(18)	Ni03 – O00G	2.089(2)	Ni02–O007–Ni03	100.29(8)
Ni01 – O009	2.1566(19)	Ni03 – N00J	2.054(2)	Ni02–O007–Ni04	89.27(7)
Ni01 – O00A	2.0571(19)	Ni04 – O007	2.1177(19)	Ni03–O008–Ni04	99.93(8)
Ni01 – O00E	2.014(2)	Ni04 – O008	2.1448(19)	Ni03–O007–Ni04	98.85(8)
Ni01 – O00I	2.094(2)	Ni04 – O009	2.0548(18)	Ni01 – Ni02	3.2167(6)

Ni01 – N00O	2.053(2)	Ni04 – O00C	2.013(2)	Ni01 – Ni03	2.9575(6)
Ni02 – O007	2.0648(18)	Ni04 – O00F	2.0961(19)	Ni01 – Ni04	3.2278(6)
Ni02 – O009	2.1099(19)	Ni04 – N00L	2.049(2)	Ni02 – Ni03	3.2253(6)
Ni02 – O00A	2.1530(19)	Ni01–O009–Ni02	97.86(8)	Ni02 – Ni04	2.9388(7)
Ni02 – O00B	1.999(2)	Ni01–O00A–Ni03	90.38(7)	Ni03 – Ni04	3.2309(7)
Ni02 – O00H	2.062(2)	Ni01–O00A–Ni02	99.62(8)		
Ni02 – N00K	2.056(2)	Ni01–O009–Ni04	100.05(8)		
Ni03 – O007	2.1361(19)	Ni01–O008–Ni03	89.91(7)		
Ni03 – O008	2.0746(19)	Ni01–O008–Ni04	98.65(7)		
Ni03 – O00A	2.1113(18)	Ni02–O00A–Ni03	98.28(7)		
Ni03 – O00D	1.999(2)	Ni02–O009–Ni04	89.75(7)		

Table S13. Hydrogen bond values for compound **7**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [°]
O00W-H00A···O00X	0.85	2.24	3.059(5)	160
O00W-H00B···N02Z	0.85	2.15	2.993(6)	170

Table S14. Selected bond distances (Å) and angles (°) for **8**.

Ni01	O008	2.117(4)	Ni04	O00S	2.185(5)	
Ni01	O00A	2.049(4)	Ni04	N00X	2.021(6)	
Ni01	O00D	2.075(4)	Ni05	O00C	2.068(5)	
Ni01	O00G	2.105(4)	Ni05	O00D	2.081(4)	
Ni01	O1	2.057(4)	Ni05	O00G	2.021(4)	
Ni01	N00N	2.089(4)	Ni05	O00J	2.006(5)	
Ni02	O009	2.139(4)	Ni05	O00K	2.238(5)	
Ni02	O00A	2.115(4)	Ni05	N00Y	2.035(5)	
Ni02	O00B	2.141(4)	Ni01	O00A	Ni02	96.41(16)
Ni02	O00C	2.027(4)	Ni01	O00D	Ni05	98.23(15)
Ni02	O00D	1.990(4)	Ni02	O00C	Ni05	96.68(18)
Ni02	N019	2.009(6)	Ni02	O00D	Ni01	99.57(17)
Ni03	O008	2.010(4)	Ni02	O00D	Ni05	97.42(16)
Ni03	O00E	2.089(4)	Ni03	O1	Ni01	98.18(17)
Ni03	O00F	2.207(4)	Ni03	O1	Ni04	100.36(17)
Ni03	O1	2.002(4)	Ni04	O1	Ni01	100.49(18)
Ni03	O00I	2.119(4)	Ni04	O00I	Ni03	95.37(16)

Ni03	N00O	2.036(5)	Ni04	O00G	Ni01	97.06(16)
Ni04	O00G	2.064(4)	Ni05	O00G	Ni01	99.15(16)
Ni04	O1	2.006(4)	Ni05	O00G	Ni04	98.28(19)
Ni04	O00I	2.043(4)	Ni05	O00J	Ni04	96.39(19)
Ni04	O00J	2.138(4)				

Table S15. Selected bond distances (Å) and angles (°) for **9**.

Cu1 – O1	1.9197(12)	O1–Cu1–O5	83.46(5)
Cu1 – O3	1.9696(12)	O5^{i}–Cu1–O5	78.85(4)
Cu1 – O5	2.0012(12)	O5^{i}–Cu1–O1	96.68(5)
Cu1 – O7	2.4865(13)	O5^{i}–Cu1–O3	75.22(4)
Cu1 – O5^{i}	2.5227(12)	O5^{i}–Cu1–N1	107.83(5)
Cu1 – N1	1.9718(15)	O3–Cu1–N1	95.57(6)
Cu2 – O1	2.3579(13)	O1–Cu1–N1	94.57(6)
Cu2 – O3^{i}	2.0341(12)	O3^{i}–Cu2–O5	88.46(5)
Cu2 – O5	1.9451(12)	O3^{i}–Cu2–O1	90.51(4)
Cu2 – O4	1.8781(12)	O4–Cu2–O1	102.44(5)
Cu2 – N4	1.9450(13)	O4–Cu2–O3^{i}	95.19(5)
C27 – O5	1.3857(19)	O4–Cu2–O5	174.96(5)
C27 – O6	1.4042(19)	O4–Cu2–N4	95.83(6)
C28 – O7	1.229(2)	O5–Cu2–O1	74.00(4)
Cu1 – Cu2	3.1319(6)	N4–Cu2–O1	125.79(5)
Cu1 – Cu1^{i}	3.5100(9)	N4–Cu2–O3^{i}	138.26(5)
Cu1 – Cu2^{i}	3.1696(5)	N4–Cu2–O5	83.67(5)
O3–Cu1–O5	87.04(5)		

i: 3/2-x,3/2-y,1-z

Table S16. Hydrogen bond values for compound **9**.

D–H· · ·A	D–H [Å]	H· · ·A [Å]	D· · ·A [Å]	D–H· · ·A [°]
O6-H6···O3	0.84	1.98	2.7510(16)	151

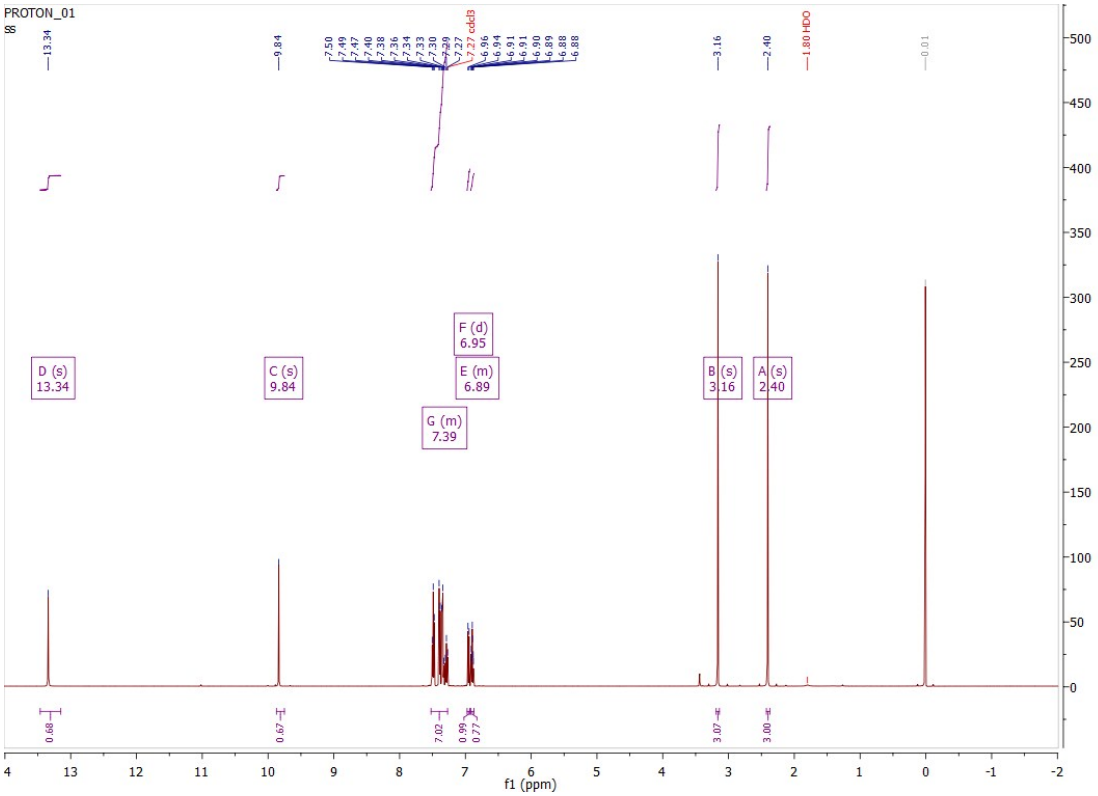

Figure S4. [1]HNMR spectrum of HL[1].

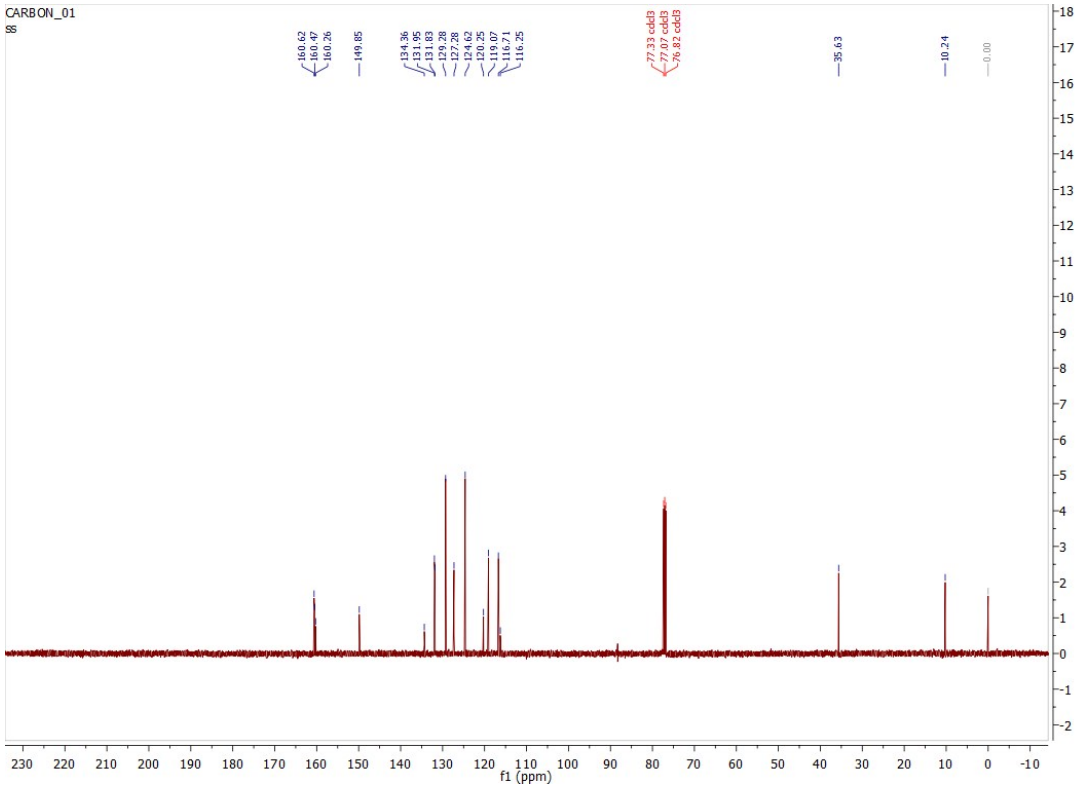

Figure S5. ^{13}CNMR spectrum of HL[1].

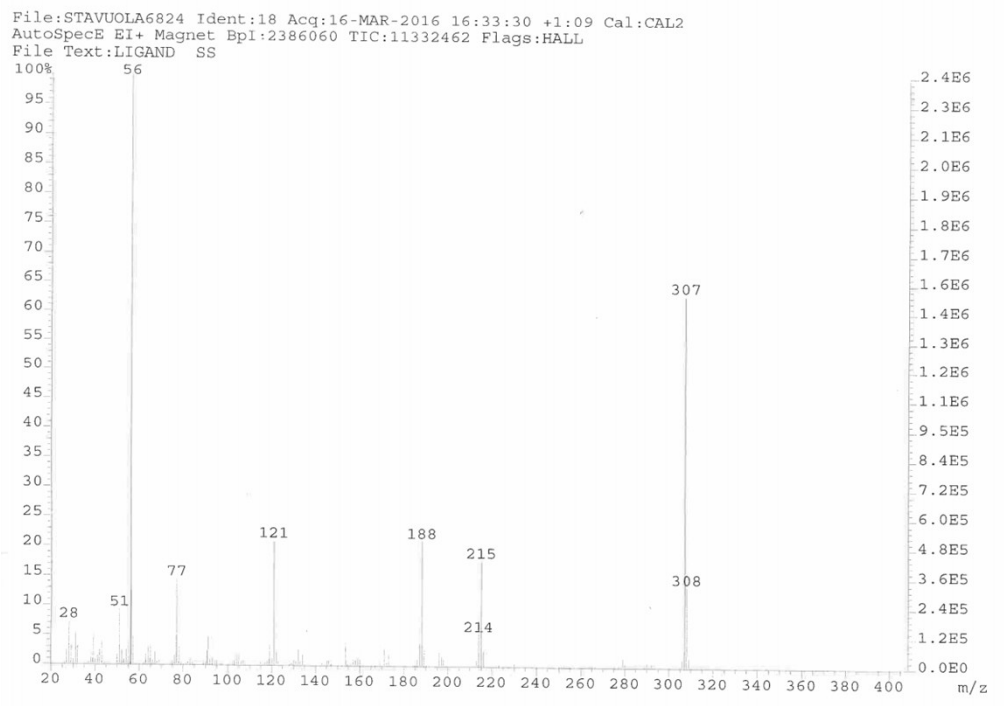

Figure S6. EI spectrum for HL[1].

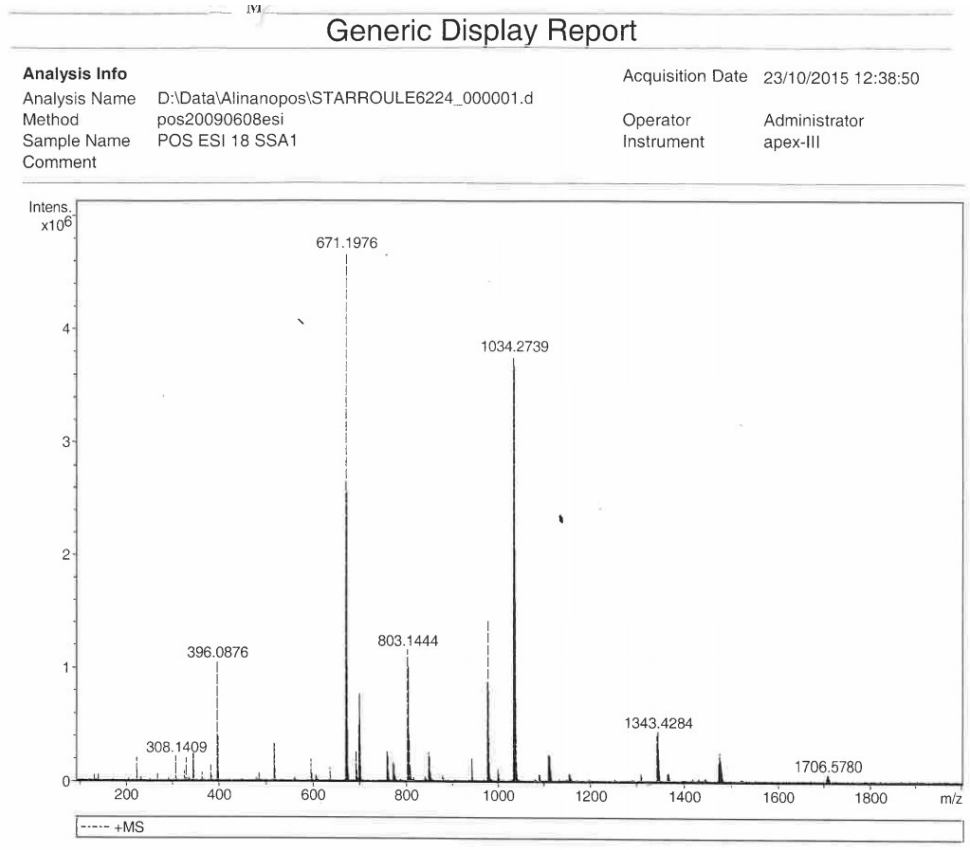

Figure S7. ESI-MS data for compound **1**.

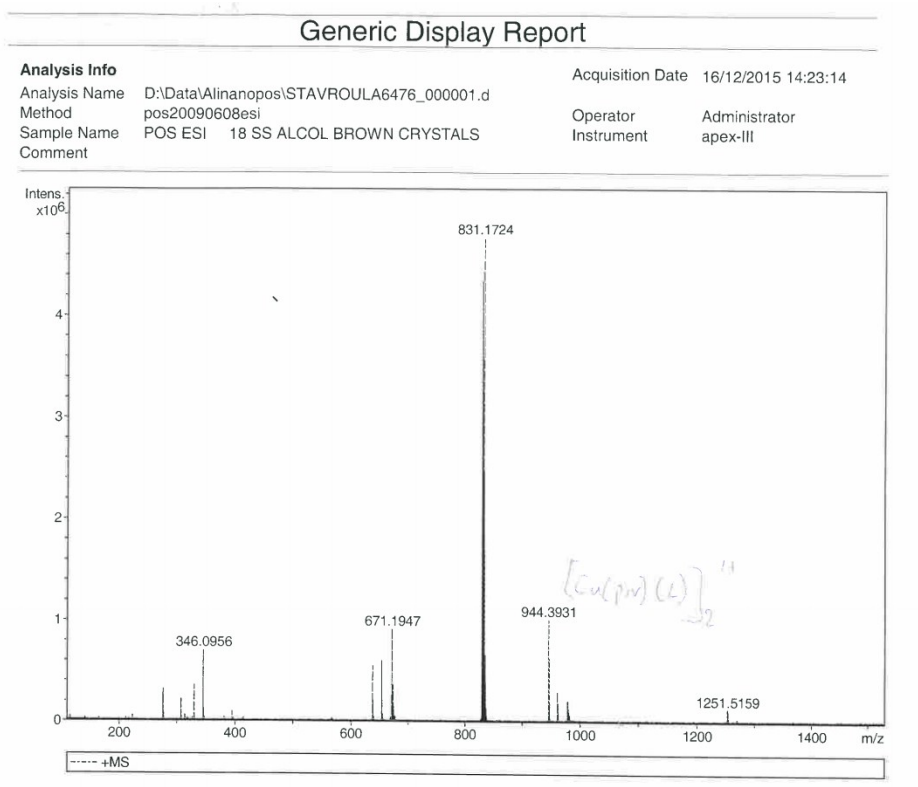

Figure S8. ESI-MS data for compound **3**.

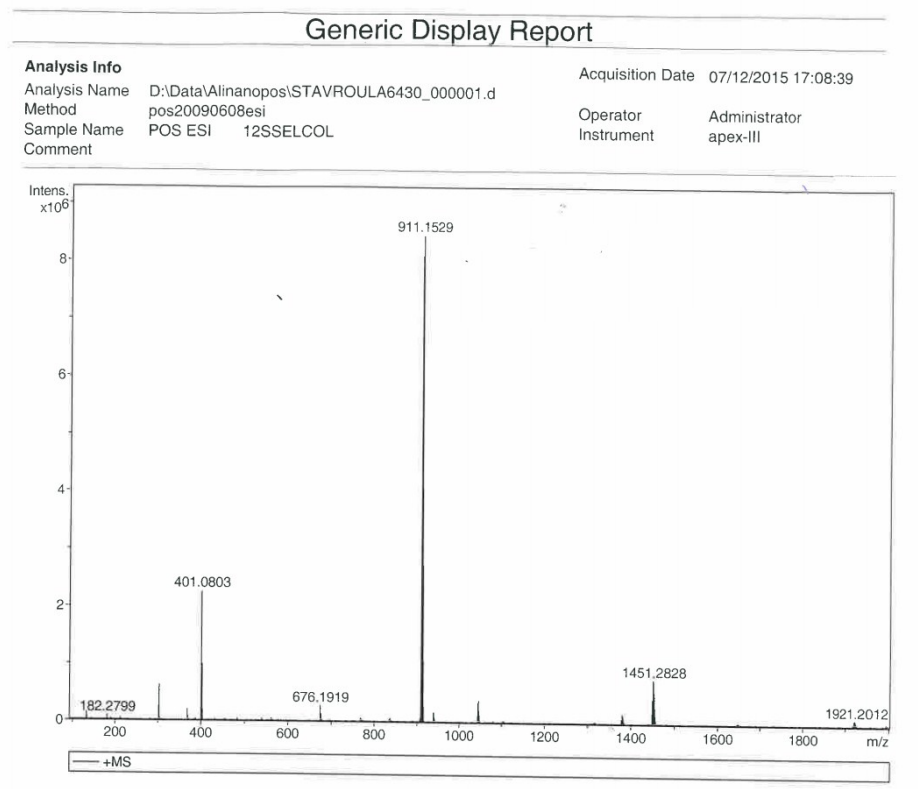

Figure S9. ESI-MS data for compound **4**.

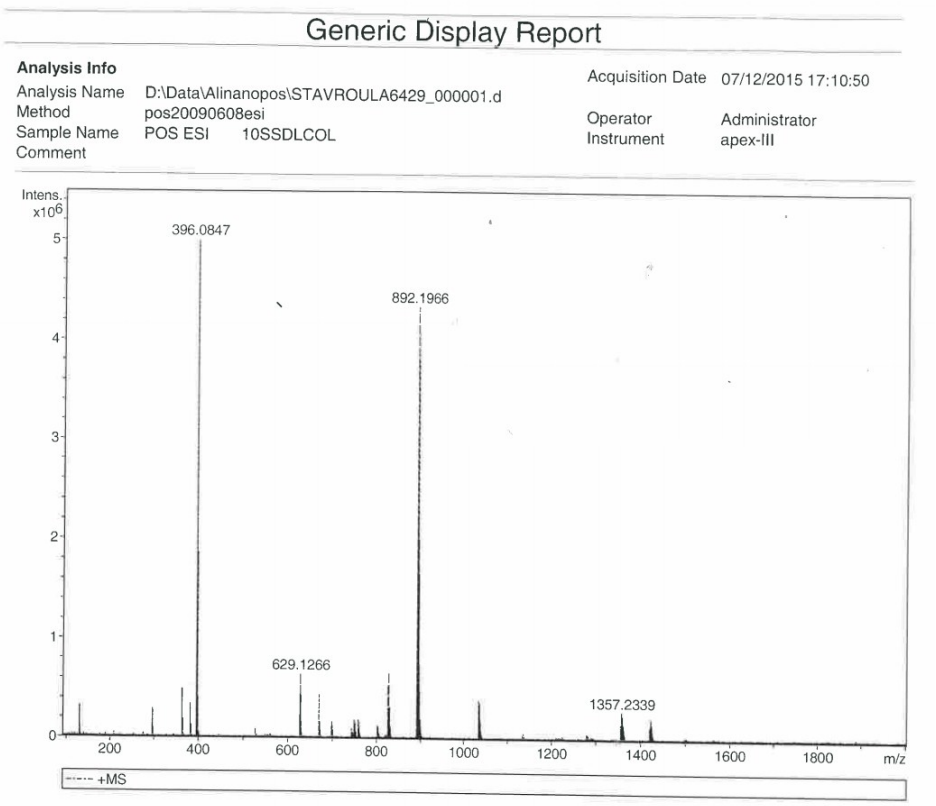

Figure S10. ESI-MS data for compound **5**.

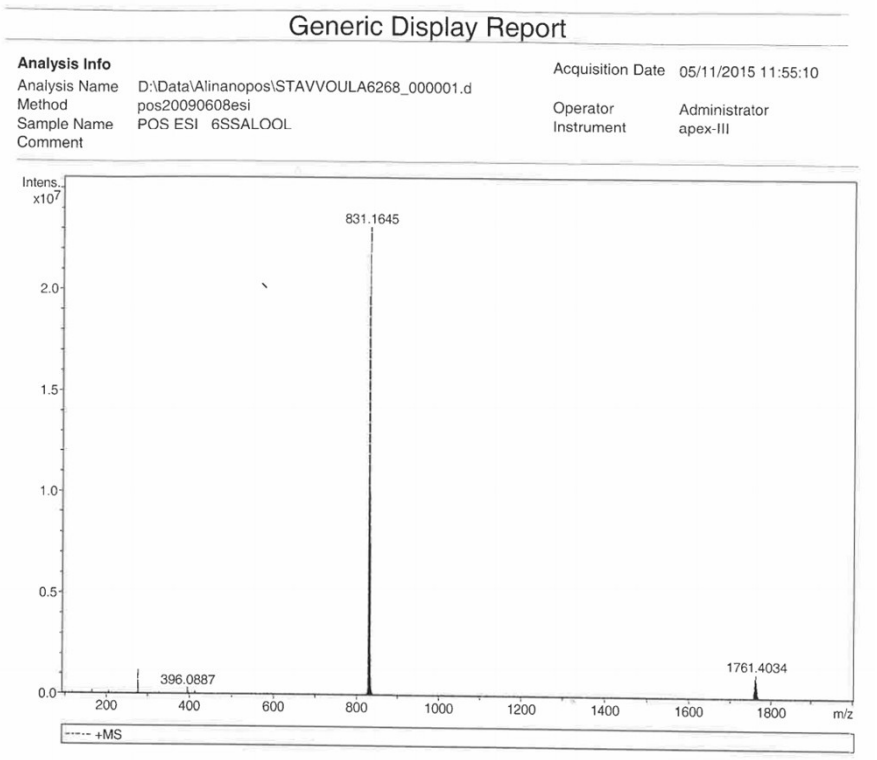

Figure S11. ESI-MS data for compound **6**.

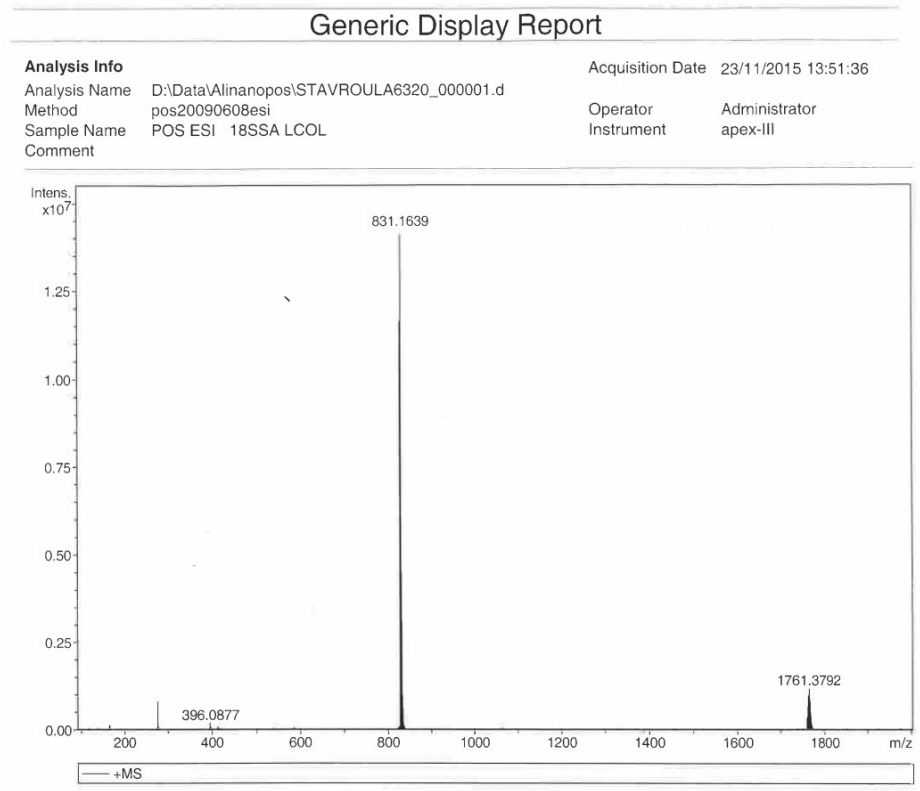

Figure S12. ESI-MS data for compound **7**.

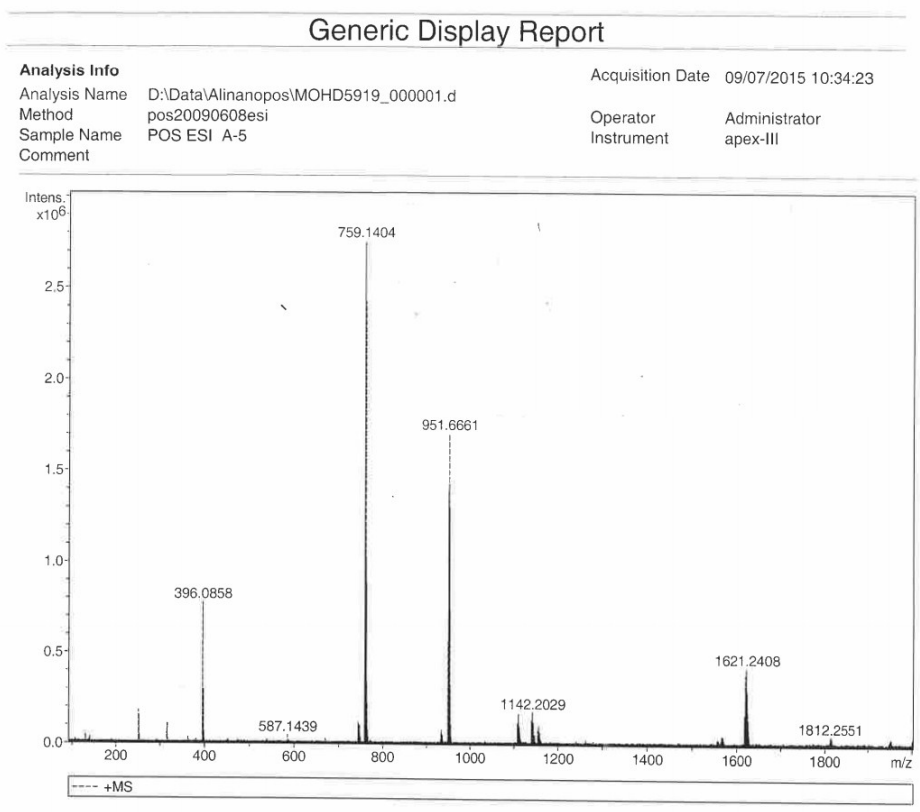

Figure S13. ESI-MS data for compound **8**.

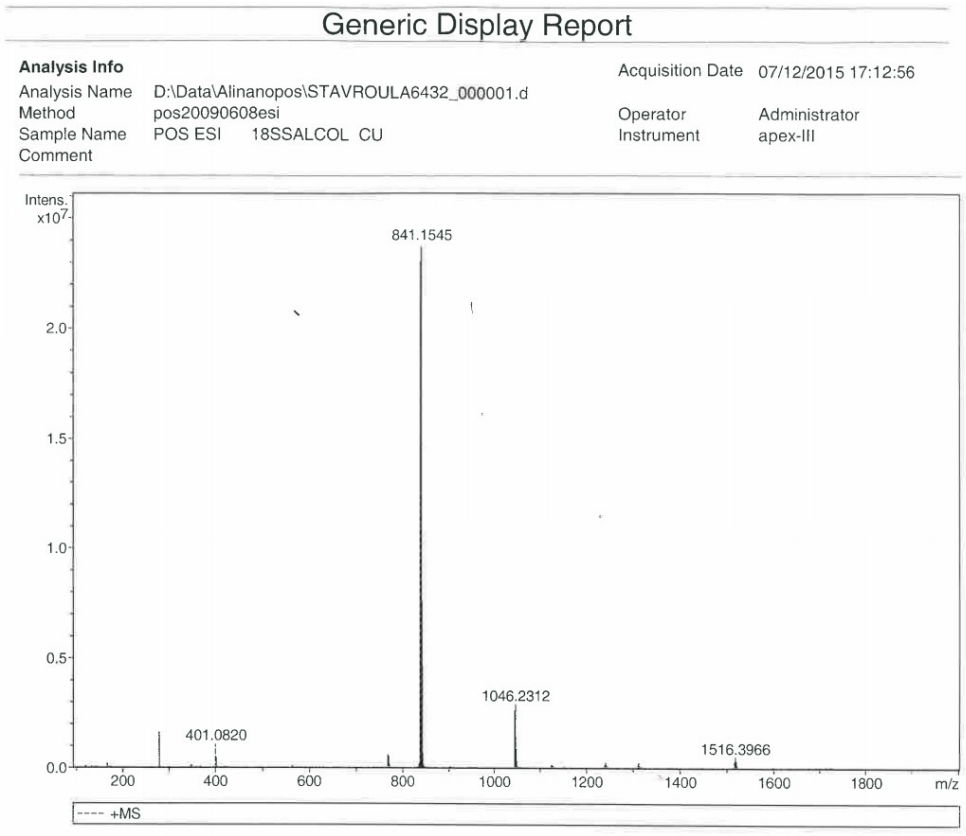

Figure S14. ESI-MS data for compound **9**.

Complete list of ref. 82. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford CT 2010.

Computational Details. All calculations were performed using the Gaussian09, D.01 program suite. The geometries and thermal corrections for all stationary points along the reaction coordinate are computed with the Perdew, Burke and Ernzerhof[1,2] of hybrid density functional denoted as PBE0 (also called PBE1PBE) as implemented in the Gaussian09 program suite. The selection of the PBE0

functional was based on the fact that PBE0 generally gives the best results for various properties of transition metal, lanthanide, actinide, and main group elements compounds.[3-5] For the geometry optimizations we have used the Def2-TZVP basis set.[6] Hereafter the method used in DFT calculations is abbreviated as PBE0/Def2-TZVP. Frequency calculations were also performed at the same level of theory to identify whether the stationary point is a local minimum or a transition state. The transition states were confirmed by IRC calculations and each had only one imaginary frequency. For the open shell systems unrestricted wavefunctions have been used. The computed electronic energies were corrected to constant pressure and 298 K, for zero point energy (ZPE) differences and for the contributions of the translational, rotational and vibrational partition functions. The natural bond orbital (NBO) population analysis was performed using Weinhold's methodology as implemented in the NBO 6.0 software.[7,8] All calculations were performed in vacuum and in solution (acetonitrile solvent) employing the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) being the default self-consistent reaction field (SCRF) methosd.[9]

References

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(9) Tomasi, J.; Mennucci, B.; Cammi, R. Quantum mechanical continuum solvation models. *Chem. Rev.* **2005,** 105 (8), 2999-3093 DOI: 10.1021/cr9904009.

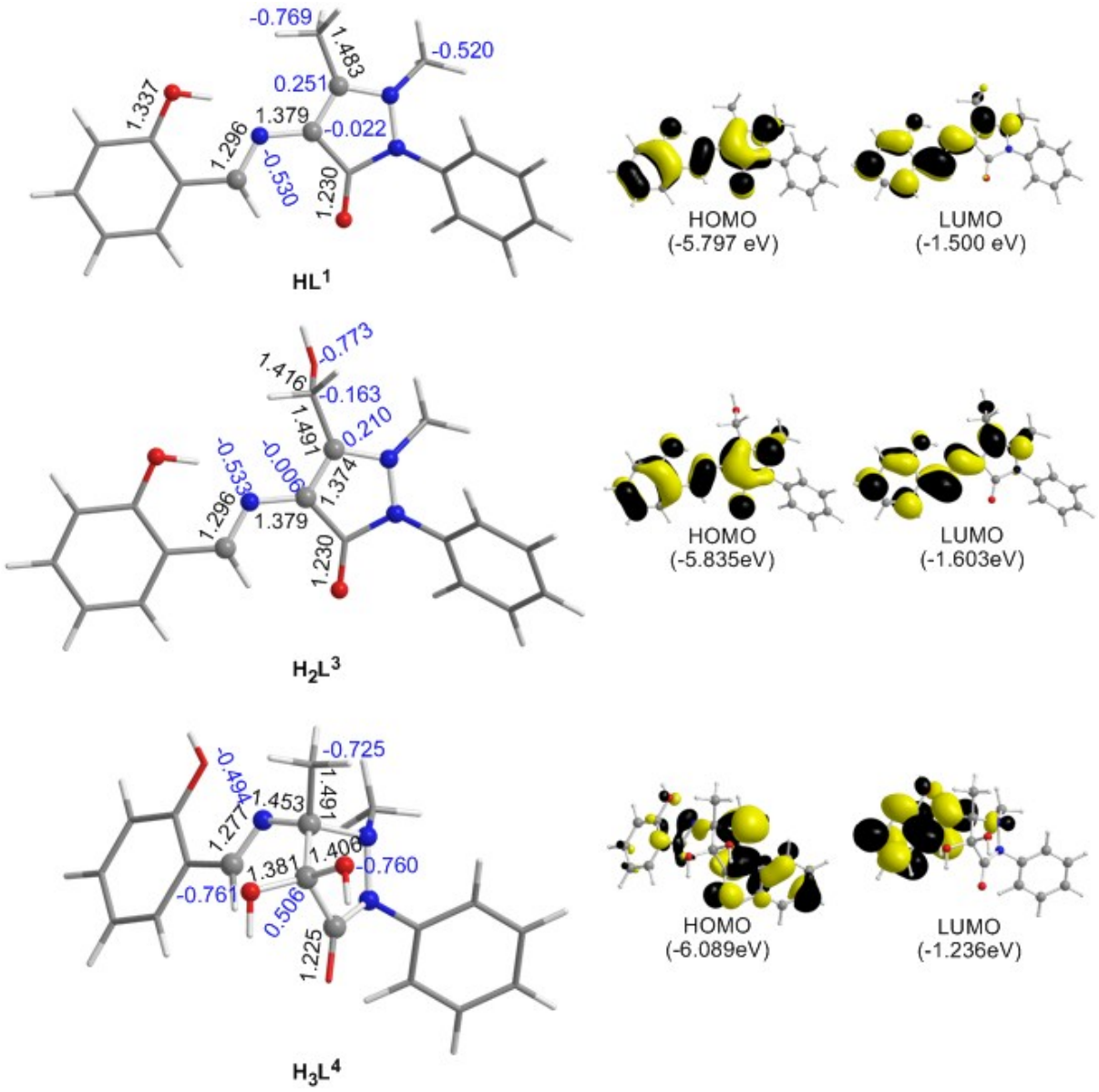

Figure S15. Ground state geometries of the [HL^1], [H_2L^3] and [H_3L^4] species, the natural atomic charges on selected atoms and the frontier molecular orbitals (FMOs) relevant to coordination of the ligands in MeCN solutions calculated by the PBE0/6-31G(d,p)/PCM computational protocol

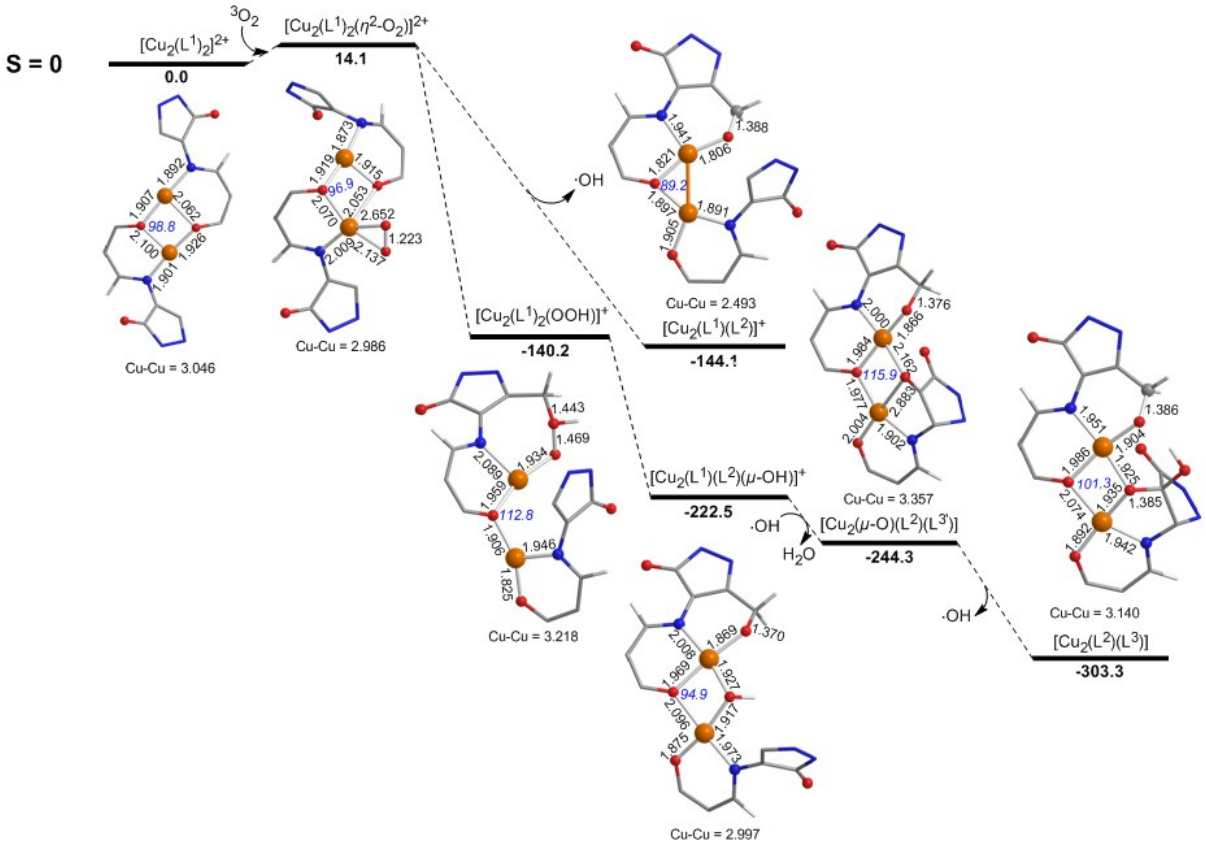

Figure S16. Geometric and energy profile of the reaction trajectory for the $L^1 \rightarrow L^2$ and $L^1 \rightarrow L^3$ ligand transformations in the dinuclear $[Cu_2(L^1)_2]$ complex along the singlet PES calculated by the PBE0/Def2-TZVP(Co) ∪ 6-31G(d,p)(E)/PCM (E = main group element) computational protocol.

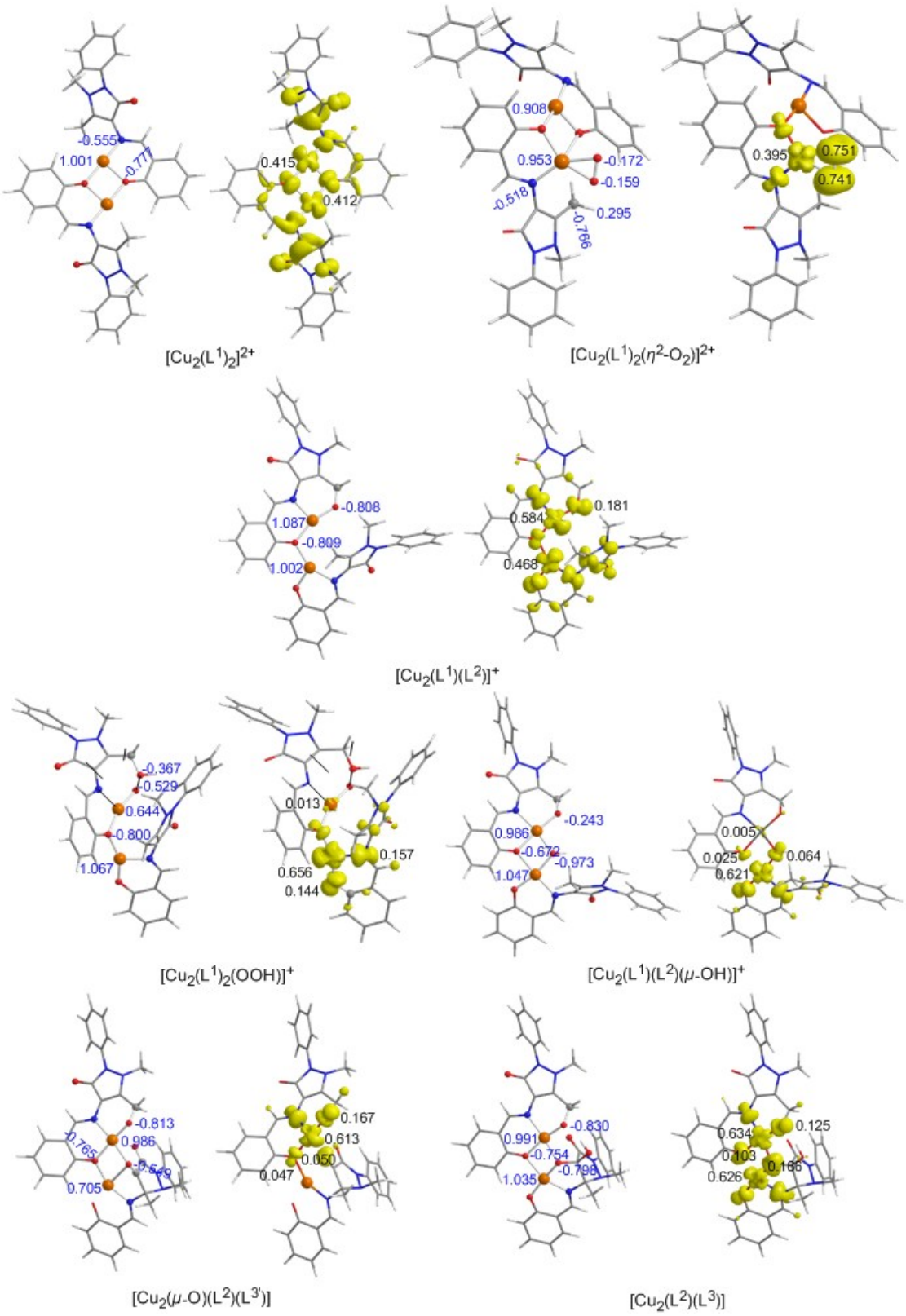

Figure S17. The natural atomic charges along with the 3D plots of the spin density distribution (isosurface = 0.002) of all stationary point located on the triplet PES calculated at the PBE0/Def2-TZVP(Cu)∪6-31G(d,p)(E) level.

Table S1. Cartesian Coordinates and energies of molecules under study calculated at the PBE0/Def2-TZVP(Cu)∪6-31G(d,p)(E) level in solution.

$[L^1]^-$

```
C,0,-6.2941982769,-1.1472107307,0.1472635974
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 C,0,-4.0262705422,-1.8278727807,-0.189620828
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 H,0,0.3108010066,3.8394861044,-0.8812465655
 H,0,2.767227045,3.4743903935,-0.6544300851
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Sum of electronic and zero-point Energies=          -1008.913518
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 Sum of electronic and thermal Enthalpies=          -1008.892786
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```

HL^1

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 C,0,-4.7994752332,-3.1094690354,0.5786695866
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$[L^2]^{2-}$

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O,0,-4.1206525328,1.4489015621,0.9505220506
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Sum of electronic and thermal Energies= -1083.510042
Sum of electronic and thermal Enthalpies= -1083.509098
Sum of electronic and thermal Free Energies= -1083.580166

H_2L^2

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 C,0,-4.6767190754,-3.3611189411,-0.9507463055
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 Sum of electronic and thermal Energies=            -1084.514916
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$[HL^3]^{2-}$

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 C,0,3.1052383392,-0.3177431897,-0.2151730967
 C,0,3.7064281456,-0.586990845,-1.4610390416
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 C,0,-2.7714159929,-0.9158861875,0.149214481
 C,0,-3.7855494616,-0.5152041796,1.0282228372
 C,0,-4.9387789524,-1.2823041539,1.1563220054
 C,0,-5.1039343034,-2.4460605916,0.4074142737
 C,0,-4.0964922731,-2.8384847306,-0.4720601631
 C,0,-2.9311567807,-2.0891906627,-0.5985041016
 C,0,-0.0012600115,2.8906398635,1.1961718821
 O,0,-1.8187848692,2.5619038288,-0.9376289487
```

O,0,0.2551371614,2.2030649786,-1.8862914907
C,0,-0.8957966405,-0.0011727744,2.2422702511
H,0,6.4648959615,-2.2991899267,-0.5159483549
H,0,5.4778526814,-1.8716542497,1.7025899012
H,0,3.1968343914,-0.2181573168,-2.3524211581
H,0,5.3209799212,-1.4682154687,-2.5876125821
H,0,1.5681326337,0.7105226172,-1.3149512746
H,0,-3.6602653315,0.4062644769,1.586831076
H,0,-5.7180749859,-0.9608425972,1.8420617951
H,0,-6.0057191534,-3.0422554356,0.5105799084
H,0,-4.2101782095,-3.74572055,-1.0592421771
H,0,-2.1436072761,-2.3964980732,-1.2752485859
H,0,-0.9709862123,3.3881269739,1.229539383
H,0,0.6974981628,3.5184394251,0.6332028219
H,0,0.3923591671,2.7630093116,2.2093587518
H,0,-1.7100825553,3.0165482284,-1.783583871
H,0,-0.4792102312,0.6947143637,2.9733251135
H,0,-0.158704766,-0.7897919563,2.0566453525
H,0,-1.8011659391,-0.4409486909,2.6702895481

Sum of electronic and zero-point Energies= -1159.865763
Sum of electronic and thermal Energies= -1159.844017
Sum of electronic and thermal Enthalpies= -1159.843073
Sum of electronic and thermal Free Energies= -1159.916243

H_3L^3

C,0,2.7619668525,-0.8207566117,-4.9833415164
C,0,2.1403530625,-2.03434518,-4.7211678002
C,0,1.3195098307,-2.1943409702,-3.6003480172
C,0,1.1207987932,-1.107736494,-2.7179480645
C,0,1.7628763922,0.1054655466,-3.0160026134
C,0,2.5753279425,0.2639678431,-4.1280289456
O,0,0.7115283617,-3.3705613526,-3.3515830247
C,0,0.2934729269,-1.124248154,-1.5077110526
N,0,-0.3196642219,-2.1496403667,-1.0579342686
C,0,-1.0321113801,-0.9042318531,1.0504638671
C,0,-1.8242044935,0.1945143901,0.3549708707
N,0,-2.7159936964,-0.4229007072,-0.4565092558
N,0,-2.614819578,-1.8582276153,-0.3692482505
C,0,-1.2080353206,-2.100547741,0.0913299451
O,0,-1.6888999983,1.3903899235,0.5819709286
C,0,-3.9343114472,0.1705678754,-0.8676038532
C,0,-5.1525097811,-0.4382969607,-0.5575746188
C,0,-6.3396625245,0.1719319573,-0.9478727635
C,0,-6.3173603109,1.3890857806,-1.626448926
C,0,-5.0974931545,1.994079854,-1.9203936162
C,0,-3.9012795565,1.3853564769,-1.5527920474
C,0,-1.1217073131,-3.443141214,0.795391028
O,0,-1.7207663725,-1.2039524702,2.2395958803
O,0,0.2802147892,-0.5444418005,1.2864322193
C,0,-2.9312006116,-2.4688405081,-1.6595661609
H,0,3.3935281861,-0.7255405007,-5.8616946107
H,0,2.2869640665,-2.8782465876,-5.3914660357
H,0,1.6082786902,0.9430730094,-2.3398860412
H,0,3.0563070766,1.2157431546,-4.32718333
H,0,0.9429327346,-3.9927748815,-4.0525499447
H,0,0.2767619651,-0.1486658107,-1.0086556911
H,0,-5.1573924207,-1.3738206973,-0.0077145589
H,0,-7.2867151179,-0.3032746957,-0.7103872451
H,0,-7.24708282,1.8628765876,-1.9261564908
H,0,-5.0723776366,2.9409822758,-2.4512354611
H,0,-2.9474246585,1.8423381049,-1.7899030036
H,0,-1.8368211618,-3.5004930239,1.6150775922
H,0,-0.10983309,-3.5758428056,1.1885624878
H,0,-1.310237439,-4.2471185675,0.0806352681
H,0,-1.7418743559,-0.3969179235,2.7715212654
H,0,0.2824540442,0.419740924,1.398674128
H,0,-2.6679533826,-3.5254558543,-1.5977386166
H,0,-2.3922646974,-2.0177874142,-2.5000546797
H,0,-4.0058631738,-2.3965969417,-1.8367939759

Sum of electronic and zero-point Energies= -1160.836957
Sum of electronic and thermal Energies= -1160.814534
Sum of electronic and thermal Enthalpies= -1160.813590

Sum of electronic and thermal Free Energies= -1160.888748

$[Cu_2(L^1)_2]^{2+}$ (S =1)

```
Cu,0,-1.3906484923,0.0209433661,0.452909477
 O,0,-0.0071296056,1.3207121222,-0.1443463973
 O,0,-5.1659620604,1.9689872864,-0.779832474
 N,0,-2.7067017461,1.2934872639,0.8482393071
 N,0,-6.1189399376,0.2753130921,0.5099912825
 N,0,-5.6385157547,-0.6048758597,1.4651841763
 C,0,-0.0875822589,2.6306640267,0.0033545666
 C,0,1.0482437088,3.4363376135,-0.1730210721
 C,0,0.9547087095,4.8146140014,-0.1075904223
 C,0,-0.270826132,5.4469829996,0.1532933668
 C,0,-1.3907751929,4.6734967374,0.3580899032
 C,0,-1.3345027071,3.2584761066,0.3121422773
 C,0,-2.5477223636,2.5759310521,0.6266408362
 C,0,-3.9639088236,0.7438136059,0.9412382563
 C,0,-5.092154119,1.1252136789,0.1044127669
 C,0,-4.3691672069,-0.3017531942,1.7715271488
 C,0,-7.258843699,-0.0378036502,-0.2813409865
 C,0,-7.3603212512,-1.2761464602,-0.9170266247
 C,0,-8.4785480663,-1.5460323115,-1.6991639774
 C,0,-9.4668674004,-0.5772615894,-1.8673759555
 C,0,-9.3439383792,0.6626262798,-1.2439719588
 C,0,-8.2429280858,0.9351453605,-0.4371783665
 C,0,-6.5732573675,-1.3369552065,2.2989375127
 C,0,-3.6317404614,-0.9568156083,2.8801663194
 Cu,0,1.3843463121,0.0129812877,-0.4457144425
 O,0,-0.0042344828,-1.2863249175,0.1439298248
 O,0,5.1437983811,-1.9805322961,0.7974430894
 N,0,2.695159841,-1.2708041397,-0.8359359799
 N,0,6.1175474251,-0.2913398117,-0.4829701981
 N,0,5.6488407321,0.5978695416,-1.4356755608
 C,0,0.0568341525,-2.5918509053,-0.0438930505
 C,0,-1.0964465888,-3.3821209342,0.079523727
 C,0,-1.0220441067,-4.7595957896,-0.0177203559
 C,0,0.2011159958,-5.40422744,-0.2605605794
 C,0,1.3375388366,-4.6439342891,-0.4203582217
 C,0,1.3002487303,-3.2299086639,-0.3430981022
 C,0,2.523999287,-2.5543189967,-0.6293775484
 C,0,3.9582397292,-0.7338215524,-0.9196003571
 C,0,5.0806512878,-1.1319658957,-0.0829623423
 C,0,4.3765541548,0.309933783,-1.7450161587
 C,0,7.2581183601,0.0071567127,0.3128552804
 C,0,8.2273977732,-0.9795297666,0.4753187573
 C,0,9.3284578975,-0.7210839299,1.2866383199
 C,0,9.4665211554,0.5182770243,1.9079280149
 C,0,8.4930399724,1.5007740542,1.7330441639
 C,0,7.3745850068,1.2452784261,0.9464180567
 C,0,6.5937569585,1.3186138856,-2.2680465213
 C,0,3.6474073757,0.975517405,-2.8528300712
 H,0,1.9998998355,2.9583344512,-0.3862569563
 H,0,1.8469193761,5.4128026247,-0.267335806
 H,0,-0.33203437,6.5284727829,0.1998327774
 H,0,-2.3456200256,5.1437916099,0.5756569406
 H,0,-3.4327033729,3.2027004948,0.7374135994
 H,0,-6.5703901058,-2.0127600958,-0.8024727989
 H,0,-8.5692483704,-2.510215144,-2.1894971984
 H,0,-10.3331899468,-0.7896421367,-2.4862584306
 H,0,-10.1125498929,1.41792002,-1.3744542543
 H,0,-8.1402173669,1.8885722437,0.0697615133
 H,0,-7.0909821949,-0.6530786037,2.9778780057
 H,0,-6.0136413891,-2.0757674584,2.869448644
 H,0,-7.2993228445,-1.8527418278,1.6717125376
 H,0,-4.1299642295,-0.7777800752,3.8380295397
 H,0,-3.5580212886,-2.037314393,2.7282337797
 H,0,-2.6231394252,-0.5449223749,2.9497220396
 H,0,-2.0452075944,-2.8906986171,0.2756244738
 H,0,-1.9270357754,-5.3478291994,0.1019211009
 H,0,0.2473244921,-6.4851687746,-0.3311501009
 H,0,2.290059436,-5.1234524053,-0.6277965432
 H,0,3.4049333197,-3.1872734299,-0.7372393897
 H,0,8.1133349662,-1.9325242713,-0.0299660407
 H,0,10.0854691438,-1.4871124068,1.4222723543
 H,0,10.3330100019,0.7195099288,2.5302914248
```

H,0,8.5953256961,2.4646747587,2.2216550641
H,0,6.5959057846,1.9929810701,0.8268375116
H,0,7.3257357306,1.8247847731,-1.6398770617
H,0,6.044102369,2.0646882733,-2.8388002456
H,0,7.1033255184,0.6284837417,-2.9468399147
H,0,3.5888123776,2.0570382456,-2.701217965
H,0,4.1419576089,0.7894288345,-3.8112796566
H,0,2.6329030529,0.5781119561,-2.9214657103

Sum of electronic and zero-point Energies= -5297.921921
Sum of electronic and thermal Energies= -5297.877235
Sum of electronic and thermal Enthalpies= -5297.876291
Sum of electronic and thermal Free Energies= -5298.008693

$[Cu_2(L^1)_2]^{2+}$ (S =0)

Cu,0,1.4195199533,0.2074005371,0.4676004528
O,0,-0.0453249422,-1.2500936133,0.09419324
O,0,5.3933630987,-2.0168236891,-0.5601063591
N,0,2.8119486655,-1.0498934954,0.7767979851
N,0,6.2855995523,-0.1740961204,0.5460055426
N,0,5.7618032971,0.8547103563,1.308240526
C,0,0.14496599,-2.5382084924,0.1796140967
C,0,-0.9510446999,-3.4257776468,0.1089346092
C,0,-0.7608906506,-4.7903696515,0.1155820694
C,0,0.5319851594,-5.3349533686,0.2315206892
C,0,1.6127223782,-4.4903923714,0.3497913423
C,0,1.4666729245,-3.0813334601,0.3467996776
C,0,2.6690095987,-2.3406704043,0.5649334137
C,0,4.0828591812,-0.5304584755,0.8618097837
C,0,5.265097002,-1.0560228785,0.1906563856
C,0,4.4599225233,0.6222990003,1.5491047497
C,0,7.4807952504,-0.0010618882,-0.2031390724
C,0,7.6987006693,1.1681381762,-0.9337151857
C,0,8.873109358,1.2996753026,-1.6678602741
C,0,9.8032008377,0.2618647718,-1.696435502
C,0,9.5641955005,-0.9089001633,-0.9798152511
C,0,8.406382172,-1.0421076308,-0.2192543807
C,0,6.6481491834,1.6389353305,2.1491496809
C,0,3.6731359559,1.4553042408,2.4916564028
Cu,0,-1.4442334887,-0.1092010813,-0.5194139331
O,0,-0.0336368778,1.3363265995,-0.1026034254
O,0,-5.2752754069,1.8899953032,0.7912462636
N,0,-2.8236351685,1.1405293429,-0.8565696301
N,0,-6.1739798903,0.0494342836,-0.3083982389
N,0,-5.7004905125,-0.8591775563,-1.2338070029
C,0,-0.1968958188,2.6130989375,-0.2799369576
C,0,0.9203020214,3.478211522,-0.3115952296
C,0,0.7480864712,4.8420779046,-0.3573664156
C,0,-0.5433753563,5.410266431,-0.4226694271
C,0,-1.6447460383,4.590515764,-0.4601339696
C,0,-1.5172684131,3.1774603602,-0.4245578537
C,0,-2.7103833857,2.4356153664,-0.6083359151
C,0,-4.0486253998,0.5524000258,-0.8370295918
C,0,-5.183873775,0.9682565729,-0.0084327578
C,0,-4.4475596859,-0.5759510199,-1.5796816405
C,0,-7.4319315559,-0.0955505252,0.3438886634
C,0,-8.5051125678,0.6859687435,-0.0786922996
C,0,-9.7280806725,0.5648513274,0.5743808492
C,0,-9.8692672282,-0.3335269713,1.6302670577
C,0,-8.7883360216,-1.1103749302,2.04498469
C,0,-7.5583786743,-0.9901822237,1.4064631948
C,0,-6.5863755143,-1.8610951002,-1.7850940011
C,0,-3.7002529907,-1.3107391144,-2.6298240431
H,0,-1.9455785688,-2.9979354764,0.0230390832
H,0,-1.6193939926,-5.4503860863,0.035057534
H,0,0.673013347,-6.4101325244,0.2432360784
H,0,2.6111113328,-4.9036229803,0.4618276221
H,0,3.5776993067,-2.9417179277,0.587133871
H,0,6.954329603,1.9590915234,-0.9295991675
H,0,9.0530118389,2.2104570568,-2.2304967929
H,0,10.7139580424,0.3660457688,-2.2780677471
H,0,10.2869564598,-1.7185990893,-1.0003175628

H,0,8.2145319231,-1.9396083387,0.3584848666
H,0,6.9908685267,1.0449575749,3.0020857807
H,0,6.1015551649,2.5132241515,2.4986131416
H,0,7.5047808781,1.9719772241,1.5648660697
H,0,4.0875115021,1.3955632987,3.5031831368
H,0,3.6620201183,2.5058302945,2.1871831324
H,0,2.6415469349,1.0975084132,2.5377053051
H,0,1.9095205651,3.0338849838,-0.2540044741
H,0,1.6186389648,5.4907811854,-0.3440193538
H,0,-0.6605077752,6.4874027873,-0.465163666
H,0,-2.6398350298,5.0173867065,-0.5428410702
H,0,-3.6341620957,3.0132494181,-0.6029949511
H,0,-8.3748073199,1.376495644,-0.9057604645
H,0,-10.5704691467,1.1703804525,0.2557623316
H,0,-10.8260410264,-0.4275240554,2.1347677133
H,0,-8.8999341527,-1.8055375955,2.8709079233
H,0,-6.7020475484,-1.5767556807,1.7251216464
H,0,-6.9687405828,-2.4986636663,-0.9860493884
H,0,-6.0192651579,-2.4648433956,-2.4896129224
H,0,-7.4193410585,-1.3754556945,-2.2993443882
H,0,-3.4881552838,-2.3405404042,-2.3279827071
H,0,-4.263087802,-1.3340344976,-3.5671329483
H,0,-2.753229976,-0.8032763984,-2.8261056405

Sum of electronic and zero-point Energies= -5297.899853
Sum of electronic and thermal Energies= -5297.856056
Sum of electronic and thermal Enthalpies= -5297.855112
Sum of electronic and thermal Free Energies= -5297.982221

$[Cu_2(L^1)_2(\eta^2\text{-}O_2)]^{2+}$ (S =1)

Cu,0,-1.6234046948,-0.622344217,-1.5084273499
O,0,-0.2755744125,-1.9864681926,-1.4310581709
O,0,-4.0173778846,-1.2360847786,1.3569197552
N,0,-3.0601902759,-1.7806157925,-1.4546901571
N,0,-5.0848979174,0.5428938488,0.2999139572
N,0,-5.2087095156,0.9407087135,-1.0257246238
C,0,-0.5222217482,-3.2504930205,-1.4428898693
C,0,0.4984664778,-4.1654224528,-1.8060347878
C,0,0.3244897188,-5.5101805283,-1.5886658605
C,0,-0.8832497617,-6.0372816362,-1.0602861461
C,0,-1.9246198157,-5.1966724632,-0.7835961515
C,0,-1.8015387758,-3.796101721,-1.0213554421
C,0,-2.9467421813,-3.008296528,-0.9390821538
C,0,-3.8512217854,-0.7966189044,-1.0313791522
C,0,-4.294829193,-0.5833186086,0.3737016016
C,0,-4.517264608,0.1850983913,-1.8471293006
C,0,-5.7319822576,1.2193593056,1.3763849915
C,0,-5.1035921009,2.3174027118,1.9620947282
C,0,-5.7296162046,2.9587786234,3.0256337285
C,0,-6.9583971724,2.495954392,3.4940354821
C,0,-7.5708873089,1.3916912699,2.9038212004
C,0,-6.9593500822,0.7443782516,1.8350569913
C,0,-6.0612460504,2.0680460791,-1.3505428065
C,0,-4.5146210327,0.3051366678,-3.3223967061
Cu,0,1.4030726941,-0.1156134078,-1.7149698958
O,0,-0.3530326974,0.7891976006,-1.6532650126
O,0,4.3966002389,2.2657723562,1.0127056138
N,0,2.0538110563,0.6065496771,-0.0101744704
N,0,5.371277458,0.1694483078,1.3115737648
N,0,5.0111223212,-1.1405885863,1.015534068
C,0,-0.5083396003,1.9728067688,-1.0329383761
C,0,-1.5641219742,2.8067080797,-1.4200716619
C,0,-1.7844467658,4.0242894153,-0.7924243493
C,0,-0.9431834476,4.4507393006,0.2385089191
C,0,0.1219228629,3.6500299558,0.6093153167
C,0,0.3756640904,2.4095432355,-0.0114148246
C,0,1.5453084737,1.7066486083,0.4616166142
C,0,3.2650107021,0.1639229949,0.5231540576
C,0,4.3337242239,1.0394640089,0.9710121231
C,0,3.708660322,-1.1335701333,0.6075195603
C,0,6.7378634374,0.5412994615,1.3172879921
C,0,7.1419196233,1.5934967263,2.1400810838
C,0,8.4762092704,1.9877204471,2.1354513483
C,0,9.4069225544,1.325367673,1.337214611
C,0,8.9949740875,0.2702829368,0.5258086073

C,0,7.6591868133,-0.1187429591,0.5010831224
C,0,5.5387424672,-2.1772485411,1.8940340136
C,0,2.9596739036,-2.3973601585,0.4002919415
O,0,2.779253204,-1.0966234217,-2.7506450774
O,0,1.7617811809,-0.9223646161,-3.5151967537
H,0,1.4325288266,-3.767841881,-2.1862281786
H,0,1.1389048219,-6.1905049082,-1.8197243596
H,0,-0.98262812,-7.105917132,-0.9077001661
H,0,-2.8735194878,-5.5829711213,-0.4246146291
H,0,-3.8604640479,-3.4459918008,-0.5379465959
H,0,-4.1421880645,2.6558292836,1.5877934482
H,0,-5.254820064,3.8161779924,3.4912352794
H,0,-7.4408451278,2.9981856982,4.3268353297
H,0,-8.5255845751,1.033040896,3.274388943
H,0,-7.4190536094,-0.117006834,1.3611030414
H,0,-7.0620889871,1.8825210797,-0.9579164713
H,0,-6.095558809,2.1676630529,-2.4323040021
H,0,-5.6472378329,2.9737414171,-0.903290844
H,0,-5.5248391521,0.1564719704,-3.7156679455
H,0,-4.1584448307,1.286130088,-3.6483397949
H,0,-3.8661760997,-0.4626087108,-3.7461443643
H,0,-2.2014987769,2.4855253906,-2.2377487842
H,0,-2.611674342,4.6489033269,-1.1161440244
H,0,-1.1130019254,5.4008992315,0.7330706217
H,0,0.7947181987,3.9778086596,1.3971090161
H,0,2.0643064363,2.184607295,1.2921933946
H,0,6.4133596722,2.0934223086,2.7673701245
H,0,8.7906011275,2.8098932946,2.7712850194
H,0,10.4489321303,1.6300054698,1.3474800089
H,0,9.7122696815,-0.2472545944,-0.1040146656
H,0,7.3260781349,-0.920002075,-0.1513298439
H,0,6.6216857249,-2.0747291893,1.9577325024
H,0,5.3127513542,-3.1476712488,1.4532762289
H,0,5.1030893316,-2.1095557614,2.8967061232
H,0,3.4704902136,-3.0528260524,-0.3107806807
H,0,2.8451489192,-2.9431254907,1.3429696171
H,0,1.9575613617,-2.1799447958,0.0280505582

Sum of electronic and zero-point Energies= -5448.065590
Sum of electronic and thermal Energies= -5448.018391
Sum of electronic and thermal Enthalpies= -5448.017447
Sum of electronic and thermal Free Energies= -5448.152403

$[Cu_2(L^1)_2(\eta^2\text{-}O_2)]^{2+}$ (S =0)

Cu,0,-1.5230309563,-0.452365967,-1.3579004066
O,0,-0.2432188563,-1.8532903935,-1.0307005145
O,0,-4.3923272796,-1.3300765227,1.381470704
N,0,-3.0192778965,-1.5693499918,-1.2865177649
N,0,-5.4297016665,0.4671701733,0.326304717
N,0,-5.3776802919,0.9869058178,-0.9590596204
C,0,-0.5052758709,-3.099694929,-1.1636124077
C,0,0.5216148764,-4.010087511,-1.5340230075
C,0,0.3075557272,-5.358447019,-1.4099034941
C,0,-0.9441171809,-5.8844030701,-0.9850703628
C,0,-1.9872553578,-5.0416668456,-0.7156311919
C,0,-1.8242314835,-3.6348781762,-0.8606230685
C,0,-2.9545318051,-2.8213545907,-0.814651481
C,0,-3.9340273739,-0.6771939248,-0.9151184341
C,0,-4.5782129621,-0.6115726023,0.4206050335
C,0,-4.5228290079,0.3469802992,-1.7275119253
C,0,-6.2724396787,0.9984771837,1.3473468934
C,0,-5.8031964173,2.0470619676,2.1370057112
C,0,-6.6208725783,2.5447029766,3.1461166403
C,0,-7.8820309037,1.9902970613,3.3592664019
C,0,-8.3352267588,0.9369060413,2.5668866518
C,0,-7.529917698,0.4329070943,1.5506847889
C,0,-6.2527271138,2.0854590275,-1.3177850082
C,0,-4.3284640209,0.6068058816,-3.1725539517
Cu,0,1.5213756682,-0.0745118756,-1.6331183258
O,0,-0.139650622,0.8740165632,-1.5996661272
O,0,4.7273844711,2.2585711041,0.6930012616
N,0,2.2646978513,0.6641693578,-0.02360566
N,0,5.6067661416,0.153722321,1.1815602117
N,0,5.1601932405,-1.1565103117,1.0522764721
C,0,-0.2313858079,2.0978540003,-1.0414243595

C,0,-1.2682271911,2.9432469536,-1.4461716904
C,0,-1.4210632665,4.2021216796,-0.8822386357
C,0,-0.5352707098,4.6533355016,0.0993110882
C,0,0.5062005095,3.8330608213,0.492424405
C,0,0.6912248622,2.5521150361,-0.0667438052
C,0,1.8255908444,1.8078083247,0.4144572935
C,0,3.4702043596,0.1846926925,0.4920908143
C,0,4.6041105153,1.0403927603,0.7896592782
C,0,3.8423442424,-1.1203540356,0.703891563
C,0,6.9910140536,0.4436492169,1.0984200309
C,0,7.4869052737,1.5410070727,1.8030657646
C,0,8.8390844302,1.8550437007,1.7097721147
C,0,9.6958096186,1.0693276235,0.9411832897
C,0,9.1919024469,-0.0293514721,0.2480723847
C,0,7.8370901777,-0.3404890745,0.3114232759
C,0,5.6839056756,-2.1263897308,2.0056995876
C,0,3.0168518734,-2.3524798447,0.6776026549
O,0,2.751508513,-1.1433239272,-2.4430031852
O,0,1.6804930681,-1.0078802977,-3.2256021879
H,0,1.4815219633,-3.6010354533,-1.8294968217
H,0,1.1170410219,-6.0467798124,-1.6338456057
H,0,-1.0742934803,-6.9580341336,-0.9083197063
H,0,-2.9626335177,-5.4320805932,-0.4422915735
H,0,-3.8946758435,-3.2608728674,-0.4842626743
H,0,-4.8143266247,2.4585100897,1.9601637008
H,0,-6.2704233299,3.3616482655,3.7683545331
H,0,-8.5150434844,2.3802905268,4.150304096
H,0,-9.3160841945,0.5059489315,2.7390232797
H,0,-7.8632694956,-0.3876026282,0.923247358
H,0,-7.2918481498,1.7670128031,-1.2151329691
H,0,-6.0464022276,2.3620759267,-2.3484889628
H,0,-6.0557139011,2.9316109346,-0.6575041359
H,0,-5.2575697933,0.4157097,-3.7182729914
H,0,-4.0246310729,1.6397481341,-3.3612134875
H,0,-3.561109231,-0.0615549246,-3.5653090147
H,0,-1.9370956053,2.6015748087,-2.2286449961
H,0,-2.2325647011,4.839913681,-1.2191269215
H,0,-0.6549942666,5.6365915083,0.5406679476
H,0,1.2114065103,4.1743712099,1.245062377
H,0,2.3847047996,2.2761394064,1.2238490543
H,0,6.8148441836,2.1372937901,2.4091091296
H,0,9.2256970864,2.7118739741,2.2532730099
H,0,10.752300389,1.3122984072,0.8824155486
H,0,9.8517021971,-0.6425369034,-0.3582340896
H,0,7.4321340037,-1.17673591,-0.2502445227
H,0,6.7725982548,-2.0831905627,1.9986910837
H,0,5.3786286675,-3.1214780523,1.6842200055
H,0,5.3139000022,-1.9284294657,3.0173415729
H,0,3.4567692431,-3.111901344,0.0255104103
H,0,2.9233719364,-2.7787545253,1.6821323325
H,0,2.0122209757,-2.1201610619,0.3237606167

Sum of electronic and zero-point Energies= -5448.041354
Sum of electronic and thermal Energies= -5447.994650
Sum of electronic and thermal Enthalpies= -5447.993705
Sum of electronic and thermal Free Energies= -5448.126709

$[Cu_2(L^1)(L^2)]^+$ (S =1)

Cu,0,2.2454026568,1.6890812348,-0.060068512
O,0,3.2017426206,3.0535700654,0.8089473929
O,0,3.971619337,-2.0716526787,1.2609433058
N,0,3.681280148,0.4958799969,-0.3111800162
N,0,2.6994655632,-2.9459086761,-0.4921948934
N,0,2.280591443,-2.4697696448,-1.7292823068
C,0,4.4836307239,3.0292129865,1.0412190294
C,0,5.0941780951,4.1993657709,1.5535640538
C,0,6.4300333872,4.2149094408,1.8938296419
C,0,7.2421612864,3.0764349677,1.7271478302
C,0,6.6843780669,1.9333196938,1.2068066728
C,0,5.3163902535,1.8791094845,0.8375257557
C,0,4.8516167968,0.6740818036,0.2476636291
C,0,3.2336351001,-0.7693870222,-0.6532893845
C,0,3.3751832675,-1.9393071554,0.1981586432
C,0,2.5545654006,-1.1451301181,-1.7992100197
C,0,2.9402523789,-4.3303905602,-0.3041068969

C,0,2.7103827161,-4.8790719725,0.957300646
C,0,2.9738992456,-6.2285790494,1.1700371412
C,0,3.4387438434,-7.0296566738,0.1288187552
C,0,3.6570480183,-6.4730356545,-1.1298318199
C,0,3.4229750229,-5.1191910012,-1.3501310951
C,0,1.0743458154,-3.0552824454,-2.3048826382
C,0,2.1340342901,-0.3121741175,-2.9537019213
Cu,0,-0.6213933631,0.3450604564,-0.0479607764
O,0,0.31910696,1.9777950253,-0.2475472369
O,0,-5.4619869706,1.4275639766,-0.4063114142
N,0,-2.4162027887,1.0119351682,-0.2707339239
N,0,-5.4788337387,-0.8197005911,0.1957562428
N,0,-4.5173077497,-1.7502200114,0.5742349353
C,0,-0.2431272028,3.1253463783,-0.6733826495
C,0,0.5819991611,4.226623477,-0.92546877
C,0,0.0551230063,5.4342288692,-1.3593224773
C,0,-1.3205039698,5.5811497126,-1.5509915134
C,0,-2.1469288626,4.5038280083,-1.296500494
C,0,-1.645371438,3.2590408469,-0.8581405665
C,0,-2.6393350877,2.2399573402,-0.6291614776
C,0,-3.4417579316,0.1007397724,-0.0640040207
C,0,-4.8635016359,0.3841585339,-0.1459574521
C,0,-3.292564171,-1.2092832705,0.3366852685
C,0,-6.7961077845,-0.9083910132,0.7118098143
C,0,-7.8546689335,-0.471439679,-0.0844147379
C,0,-9.1512031848,-0.5244102362,0.4178297754
C,0,-9.3941741473,-1.0316053931,1.6928415248
C,0,-8.3305087585,-1.4738539479,2.4769342435
C,0,-7.0261887936,-1.402304481,1.9975989805
C,0,-4.8242585478,-3.1558013106,0.3425338489
C,0,-2.0416217656,-2.0291427521,0.5205253178
O,0,-0.8882157707,-1.4272476118,0.0534941639
H,0,4.4666261003,5.073456054,1.694235593
H,0,6.8610097141,5.125125726,2.3019602973
H,0,8.2912809285,3.1055231461,2.0002824125
H,0,7.2930088732,1.0450746722,1.0581068876
H,0,5.542756564,-0.1694415702,0.2320851825
H,0,2.3336755088,-4.2498392172,1.7555760457
H,0,2.8010616479,-6.6571927055,2.1525140208
H,0,3.6305814229,-8.0847991821,0.2976331923
H,0,4.0253337682,-7.0898388796,-1.9439092894
H,0,3.6202354472,-4.6720769409,-2.3197305405
H,0,1.1674895701,-4.1406354373,-2.3079793967
H,0,0.9900042604,-2.7135632904,-3.3360868112
H,0,0.1966344829,-2.7464979336,-1.7258129281
H,0,2.4283936449,-0.7805238951,-3.8968971096
H,0,1.0488262159,-0.165359876,-2.9739733157
H,0,2.6135416524,0.6665318274,-2.8931851161
H,0,1.6515131586,4.1268052398,-0.7586315248
H,0,0.7255488472,6.2677917581,-1.5460684828
H,0,-1.7353697145,6.524546878,-1.8889250061
H,0,-3.2202897432,4.6014148506,-1.4343235673
H,0,-3.6815788346,2.5329954417,-0.7684761763
H,0,-7.655489122,-0.0938414081,-1.0806917974
H,0,-9.976209448,-0.179862958,-0.1982762128
H,0,-10.4093382144,-1.0826813313,2.0743081027
H,0,-8.5117201636,-1.8648986082,3.4735082194
H,0,-6.1895470668,-1.7184019849,2.6132767106
H,0,-5.8268334288,-3.3642664148,0.714077544
H,0,-4.1212110461,-3.7631201457,0.9118286432
H,0,-4.7672231017,-3.4067906499,-0.721785708
H,0,-2.1868181614,-2.9858301533,-0.0069800757
H,0,-1.9756157703,-2.2755589539,1.5953106084

Sum of electronic and zero-point Energies= -5372.632671
Sum of electronic and thermal Energies= -5372.588592
Sum of electronic and thermal Enthalpies= -5372.587648
Sum of electronic and thermal Free Energies= -5372.716310

$[Cu_2(L^1)(L^2)]^+$ (S =0)

Cu,0,2.0258162674,1.8617715949,-0.0609444945
O,0,3.2368624374,3.191364986,0.568690063
O,0,3.4327886653,-2.1669304865,1.418256516
N,0,3.2203256442,0.4020769672,-0.1925748719
N,0,2.1918322882,-3.0291903849,-0.3604281764

N,0,1.7920050414,-2.5404507439,-1.5941815719
C,0,4.4834757699,2.9704197745,0.8150957003
C,0,5.3343971364,4.0737746429,1.0947305917
C,0,6.6381759465,3.8792988597,1.4852517269
C,0,7.1936337697,2.5832046119,1.5743055903
C,0,6.4168119091,1.4990786804,1.2524179666
C,0,5.0627161823,1.6524797165,0.8501400807
C,0,4.4011511145,0.4906502132,0.3923542994
C,0,2.7336392783,-0.8488044442,-0.5005573409
C,0,2.8539300473,-2.0226143521,0.3469625957
C,0,2.049229157,-1.2185959694,-1.6486978041
C,0,2.4499042671,-4.4131988837,-0.1863992236
C,0,2.1771402193,-4.9875265845,1.0544863258
C,0,2.4548293186,-6.3361770633,1.2549435912
C,0,2.9755026304,-7.1104138381,0.2199219531
C,0,3.2360992564,-6.5281854336,-1.0190046828
C,0,2.9888857672,-5.1745413817,-1.2252486532
C,0,0.6359601077,-3.1449409502,-2.2355374459
C,0,1.5926202413,-0.3701698831,-2.7723255224
Cu,0,-0.3138424738,1.000583739,-0.0240826198
O,0,0.3263256342,2.7040517885,-0.0949860022
O,0,-5.2614844431,1.3189462028,-0.534304815
N,0,-2.2001305922,1.4122574147,-0.2207793892
N,0,-4.934238437,-0.8935870667,0.1186368748
N,0,-3.8529483081,-1.6427744295,0.5734976456
C,0,-0.3215972442,3.7759596728,-0.5697866596
C,0,0.4023014576,4.9433797324,-0.8193984807
C,0,-0.246039012,6.0839148192,-1.2720957948
C,0,-1.6275112629,6.0831808389,-1.4835124443
C,0,-2.3473851999,4.9284137872,-1.2382017389
C,0,-1.7256579214,3.7478536382,-0.7816533767
C,0,-2.5802606143,2.6027364932,-0.57252595
C,0,-3.0756149544,0.3580856036,-0.0421229473
C,0,-4.5157808565,0.3943639055,-0.2140537103
C,0,-2.7285997348,-0.8980066086,0.4038392745
C,0,-6.2483544145,-1.2049297672,0.550412535
C,0,-7.3108501958,-0.9658247225,-0.3208971693
C,0,-8.6094368348,-1.2361794544,0.0993699381
C,0,-8.8455885682,-1.763818914,1.3673138587
C,0,-7.7761485093,-2.0077275691,2.2267371227
C,0,-6.4746255035,-1.7172949464,1.8296200082
C,0,-3.9070146516,-3.0820824785,0.3422996292
C,0,-1.3536262243,-1.4233573331,0.7377891863
O,0,-0.3297562252,-0.8044094874,0.0333484138
H,0,4.9008927504,5.0669520089,1.0393016153
H,0,7.2529189681,4.740930443,1.7307296654
H,0,8.2266896419,2.4515933052,1.8769363684
H,0,6.8351097069,0.4965298172,1.2849640929
H,0,4.9628220598,-0.4401855604,0.4727924374
H,0,1.7560019061,-4.3786115927,1.8465064913
H,0,2.2489570623,-6.7853445134,2.2216867809
H,0,3.1778208202,-8.1652347098,0.3780761819
H,0,3.6476340804,-7.1244192226,-1.8276322434
H,0,3.2175553775,-4.7073369325,-2.1784120955
H,0,0.7069541918,-4.2290717787,-2.1642625376
H,0,0.6367050244,-2.8640360795,-3.288302643
H,0,-0.2800796177,-2.7885198945,-1.7535387693
H,0,1.8097351055,-0.8365598898,-3.7368969647
H,0,0.5107410444,-0.2019008755,-2.7136972467
H,0,2.0979161002,0.5963756973,-2.7375277176
H,0,1.4730782852,4.9323746681,-0.6407432084
H,0,0.3331330804,6.983106611,-1.4598251148
H,0,-2.1310272867,6.9766779578,-1.8363330509
H,0,-3.4215767344,4.9140179134,-1.4003480056
H,0,-3.6511575316,2.7510872733,-0.7352304491
H,0,-7.1141119654,-0.5703316671,-1.3107388459
H,0,-9.4387041048,-1.04567651,-0.5750906183
H,0,-9.8599808339,-1.9847454829,1.6849077626
H,0,-7.9531716023,-2.4134815718,3.2181538221
H,0,-5.6387571453,-1.8778194187,2.5037621391
H,0,-4.8915133525,-3.447055282,0.6322013896
H,0,-3.1689057514,-3.56775091,0.9792141308
H,0,-3.7203428818,-3.323077858,-0.7091582174
H,0,-1.3267755849,-2.5003925089,0.5188606549
H,0,-1.2301281856,-1.3295079424,1.8309235941

Sum of electronic and zero-point Energies=   -5372.604800

Sum of electronic and thermal Energies= -5372.560704
Sum of electronic and thermal Enthalpies= -5372.559760
Sum of electronic and thermal Free Energies= -5372.687411

$[Cu_2(L^1)_2(OOH)]^+$ (S =1/2)

Cu,0,2.2230680876,-2.5409183938,-0.344225339
O,0,3.1255682819,-3.7372478827,-1.3865335225
O,0,3.1318868382,1.3738835311,-1.8102118043
N,0,3.5981081363,-1.1660203073,-0.2773662998
N,0,2.4769862559,2.18507141,0.28275364
N,0,2.5820127318,1.734242742,1.5999445731
C,0,4.3090548534,-3.5803652218,-1.9186296428
C,0,4.8574188011,-4.6439035394,-2.6685762902
C,0,6.0896279569,-4.52168983,-3.2789204339
C,0,6.8433293666,-3.3391909289,-3.1740960577
C,0,6.3345452871,-2.2908310348,-2.4426816138
C,0,5.0781898469,-2.3816531489,-1.7949735082
C,0,4.6534457031,-1.2498700714,-1.0412186966
C,0,3.2336092604,0.0772492231,0.2403376983
C,0,2.9595155427,1.2221712631,-0.6057682426
C,0,2.9800113569,0.4192557875,1.5397531923
C,0,2.2900259782,3.5449741325,-0.0144916245
C,0,1.6345137871,3.8777089404,-1.2121191199
C,0,1.397832488,5.2200359421,-1.5134222098
C,0,1.7918628724,6.2220047701,-0.6320477522
C,0,2.4541589935,5.8796154817,0.5461539604
C,0,2.7139067829,4.5492602746,0.8590152873
C,0,1.4903095753,2.099718957,2.5024222419
C,0,3.076985459,-0.4143838891,2.7626729019
Cu,0,-0.1215968265,-0.3369271519,-0.387501777
O,0,0.6570383459,-1.8868711269,0.5226259713
O,0,-4.7475832282,-1.0285613102,1.0180279181
N,0,-1.8415241353,-0.22733085,0.7933842116
N,0,-5.1102358546,0.9519676017,-0.139040891
N,0,-4.3109748375,1.9244849302,-0.7249543716
C,0,0.2118484256,-2.398194714,1.678544881
C,0,0.96527826,-3.4067523529,2.3017490423
C,0,0.5812262677,-3.9792285172,3.5031849168
C,0,-0.5965183998,-3.5686710455,4.1307743207
C,0,-1.3618840645,-2.5924681457,3.5231294369
C,0,-0.995666934,-1.976003196,2.3056878375
C,0,-1.96436841,-1.0122670649,1.8175143043
C,0,-2.954408733,0.505997617,0.3957650144
C,0,-4.3288358362,0.0103349771,0.5170840722
C,0,-3.0151769342,1.6633632555,-0.3373929571
C,0,-6.4045055636,0.7032782168,-0.6550379594
C,0,-7.3878750066,0.2106722735,0.2042329407
C,0,-8.6569958248,-0.0581291404,-0.2981963543
C,0,-8.9537952663,0.1833269768,-1.6382866901
C,0,-7.9674298732,0.6842800404,-2.485162522
C,0,-6.6865378994,0.9354237012,-2.0031194006
C,0,-4.8453812785,3.2857774656,-0.6623699259
C,0,-2.0107502588,2.6993746345,-0.7201968684
O,0,-0.264499396,1.246485032,-1.4892542444
O,0,-0.6682802221,2.2299880117,-0.4752345246
H,0,4.2733881759,-5.5543223249,-2.7566960623
H,0,6.4796882638,-5.3573243048,-3.853648081
H,0,7.8085186176,-3.2566863088,-3.6616622849
H,0,6.8992812597,-1.3670657765,-2.345254013
H,0,5.2949810962,-0.3680970699,-1.0948794048
H,0,1.4044625456,3.0916565941,-1.9293745787
H,0,0.9024842784,5.4735970341,-2.4456031318
H,0,1.5971271937,7.2636735129,-0.8652282371
H,0,2.7825137135,6.6565005699,1.2298516675
H,0,3.2556483679,4.2888134828,1.7623425275
H,0,1.3744460911,3.1824254546,2.5219366269
H,0,1.7585746179,1.7696154861,3.5054768989
H,0,0.5468354391,1.6327448081,2.1968504044
H,0,3.6310465905,0.1089769681,3.5469375699
H,0,2.0874029576,-0.6682507304,3.1562211983
H,0,3.5978013365,-1.344371196,2.5301999467
H,0,1.8847408071,-3.742079053,1.8238978916
H,0,1.2023507397,-4.7512183298,3.9475378819
H,0,-0.9114687002,-4.0127825258,5.0688062018
H,0,-2.2908520885,-2.2751439914,3.9900720573
H,0,-2.8887677949,-0.9857262915,2.3961820509

H,0,-7.1514740152,0.037396768,1.2473122202
H,0,-9.4214827108,-0.4466620943,0.3678659243
H,0,-9.9496573512,-0.0179002346,-2.0209495049
H,0,-8.1882402979,0.8698328169,-3.5319697735
H,0,-5.9050355233,1.2987485955,-2.6631099209
H,0,-5.8596997933,3.2807399742,-1.0602041524
H,0,-4.2429781313,3.9326754371,-1.3009934214
H,0,-4.8539811433,3.6677555848,0.3642102224
H,0,-2.085592126,2.9579162398,-1.7796142398
H,0,-2.1032955888,3.6017097488,-0.1050294064
H,0,-0.0190075871,2.9769828305,-0.613612796

Sum of electronic and zero-point Energies= -5448.240947
Sum of electronic and thermal Energies= -5448.195620
Sum of electronic and thermal Enthalpies= -5448.194676
Sum of electronic and thermal Free Energies= -5448.323264

$[Cu_2(L^1)(L^2)(\mu\text{-OH})]^+$ (S =1/2)

Cu,0,-0.2335965734,0.460439006,-1.8101714885
O,0,0.2976929063,2.0283074152,-0.9300207378
O,0,2.8105587943,-2.8265117315,-0.6935936892
N,0,1.5791768926,-0.3148718575,-1.8784297793
N,0,2.343048001,-3.7115448317,-2.8028583725
N,0,1.9212046573,-3.1880138608,-4.023422335
C,0,1.4389079405,2.2597312889,-0.3456525693
C,0,1.5946923643,3.4629981543,0.3840924201
C,0,2.7727896454,3.7544361271,1.041077095
C,0,3.8665697302,2.8707546118,1.0038479644
C,0,3.7468993356,1.6997705644,0.2900489964
C,0,2.5536298742,1.367754192,-0.3954809049
C,0,2.5525955829,0.155953781,-1.1466381401
C,0,1.7893703346,-1.5534005044,-2.4990333889
C,0,2.3607228811,-2.7076321361,-1.8313874823
C,0,1.5193658566,-1.894542949,-3.7966287486
C,0,3.1939926608,-4.8411008377,-2.7832984126
C,0,3.1830382026,-5.6696485998,-1.6594053812
C,0,4.0302139849,-6.7722556285,-1.6160312525
C,0,4.8665434193,-7.0658614875,-2.6915689341
C,0,4.8640644595,-6.2385537164,-3.8125127275
C,0,4.0397941175,-5.1182836053,-3.8601288785
C,0,1.1118230343,-4.0785904399,-4.8493924417
C,0,0.8956924122,-1.0862044853,-4.873652446
Cu,0,-3.0237584198,-0.608360411,-2.0420260297
O,0,-2.1960975113,1.1774350237,-1.9752124001
O,0,-7.6955122564,0.9263074137,-0.7588480276
N,0,-4.8283176499,0.2017476366,-1.6966929552
N,0,-7.7421110547,-1.3376652692,-0.3021256098
N,0,-6.8489638125,-2.3777603884,-0.4240762947
C,0,-2.7356696845,2.3070581902,-2.3234428338
C,0,-1.9284002036,3.4059966643,-2.6949628275
C,0,-2.5006104173,4.6052124932,-3.0516097497
C,0,-3.9043288016,4.7818094577,-3.0650639558
C,0,-4.7123080001,3.7350482423,-2.7103179483
C,0,-4.1685455239,2.4716947813,-2.3383566664
C,0,-5.0954135016,1.4715754632,-1.9850452925
C,0,-5.8068692516,-0.5832196311,-1.1939285018
C,0,-7.1534157028,-0.1709184793,-0.7516061887
C,0,-5.6976056843,-1.9699735753,-0.9448324982
C,0,-9.0539789798,-1.4875839366,0.2326027532
C,0,-10.118359882,-1.7269007976,-0.6353078141
C,0,-11.4006084734,-1.8534878707,-0.1103105574
C,0,-11.6065862138,-1.7396534724,1.2635977494
C,0,-10.5347872401,-1.4958779828,2.1208208136
C,0,-9.2482758371,-1.3658782082,1.6076045883
C,0,-7.2039338562,-3.6929437567,0.0664216114
C,0,-4.4859299797,-2.8433574154,-1.1387281798
O,0,-3.6287948187,-2.3762079164,-2.1005396938
O,0,-1.2031090861,-1.0446567837,-2.4965586612
H,0,0.7497791907,4.14402963,0.4162838334
H,0,2.8531381553,4.6846871427,1.5974876576
H,0,4.7872676303,3.1109640053,1.5246157041
H,0,4.5805857088,1.0033323278,0.2386235691
H,0,3.4768513875,-0.4235184107,-1.1147553663
H,0,2.5213056933,-5.4403733393,-0.8326354809

H,0,4.0250583422,-7.4129091418,-0.7391698236
H,0,5.5165291458,-7.9347884274,-2.6563541948
H,0,5.5166467316,-6.4552801841,-4.6530105946
H,0,4.055869116,-4.4529077822,-4.7176317735
H,0,1.6627411525,-5.0015421759,-5.0303969907
H,0,0.935973288,-3.590415782,-5.8076333456
H,0,0.154560733,-4.309085208,-4.3683084752
H,0,1.4275943175,-1.2163112484,-5.8198314527
H,0,-0.1525990351,-1.3661816858,-5.015974911
H,0,0.9241288999,-0.0298006362,-4.6014134475
H,0,-0.8525827727,3.277013041,-2.6613853409
H,0,-1.857956967,5.4362792682,-3.3280592548
H,0,-4.3301445473,5.7367047311,-3.3524942186
H,0,-5.7926243608,3.8487423283,-2.7121495684
H,0,-6.1406435371,1.776444654,-1.9440440403
H,0,-9.936554632,-1.8096620346,-1.7021611448
H,0,-12.2381113635,-2.0397474075,-0.7748516474
H,0,-12.6090628157,-1.8389203663,1.6685241964
H,0,-10.6995983517,-1.4034154702,3.1894713057
H,0,-8.4016104702,-1.1684521053,2.2575846453
H,0,-7.2007420501,-3.6950399737,1.1590329178
H,0,-6.4706122675,-4.4053289755,-0.303631154
H,0,-8.1954527566,-3.9583230773,-0.3017196833
H,0,-4.8332645583,-3.8550087292,-1.409199228
H,0,-0.929566374,-1.9209341315,-2.2081707495
H,0,-4.0197013044,-2.9479187762,-0.138355138

Sum of electronic and zero-point Energies= -5448.372793
Sum of electronic and thermal Energies= -5448.326726
Sum of electronic and thermal Enthalpies= -5448.325782
Sum of electronic and thermal Free Energies= -5448.459723

$[Cu_2(\mu\text{-}O)(L^2)(L^{3\prime})]^+$ (S =1)

Cu,0,-0.7626772647,0.2223492804,-1.2574980475
Cu,0,2.3427292921,1.174750931,-0.3467844226
O,0,0.4019300532,1.6894605541,-0.5465354724
O,0,-5.1882773944,1.6797795353,0.8353060436
O,0,-1.7441681081,-1.0738278475,-2.1656892211
O,0,3.5205895345,2.3691703494,0.7309664019
O,0,0.9723957013,-0.2967875701,-2.4191326801
O,0,0.2781457128,-1.2663879062,0.2061048835
N,0,-2.4053804436,1.0408409503,-0.4164121677
N,0,-5.5514134116,-0.5300572675,0.2703610852
N,0,-4.8171307763,-1.513000142,-0.3487438715
N,0,3.7466780654,0.0230553062,-0.9380612325
N,0,2.3776190662,-2.2892245235,-0.0015764987
N,0,3.4258393641,-2.3440425877,-0.9814336435
C,0,-0.0046686107,2.9096028619,-0.2894818305
C,0,0.9407489033,3.9523076555,-0.1808149152
C,0,0.5497167314,5.2454320233,0.0852099896
C,0,-0.8092146303,5.5815412265,0.272253549
C,0,-1.7500206993,4.5910078622,0.1938024926
C,0,-1.3949842405,3.2394302687,-0.091112661
C,0,-2.4664898718,2.3258180157,-0.0951925528
C,0,-3.5109069041,0.2727992025,-0.2830470624
C,0,-4.7994456005,0.6304674773,0.3415797602
C,0,-3.6108698403,-1.0757697398,-0.6889962054
C,0,-6.90224637,-0.702961947,0.6898074296
C,0,-7.1610753413,-1.0444750714,2.0159980637
C,0,-8.4818031603,-1.1906170392,2.4286092375
C,0,-9.5218657011,-0.9969909911,1.521203777
C,0,-9.2502492119,-0.6513663409,0.1982674859
C,0,-7.9341543225,-0.4976974757,-0.2252415575
C,0,-5.3825811661,-2.8373979811,-0.5072223119
C,0,-2.5448408263,-1.8780709603,-1.3892741032
C,0,4.782687444,2.168783938,0.903546972
C,0,5.518338338,3.0853812081,1.7119939437
C,0,6.8626115199,2.9284508581,1.9579648151
C,0,7.583700286,1.843116894,1.4174258107
C,0,6.9149702696,0.9380706651,0.6300721074
C,0,5.5300264131,1.0651345774,0.3437858839
C,0,4.9699107175,0.0605350687,-0.4941020892
C,0,3.2777778886,-1.0890690145,-1.7479060459
C,0,1.776895094,-0.8038623515,-1.6378390194

C,0,1.3609816611,-1.4761489143,-0.3501618572
C,0,3.8582769086,-1.1198347481,-3.1414987094
C,0,2.5603397689,-2.9874605882,1.2132586299
C,0,1.4703469645,-3.2519354833,2.0501032946
C,0,1.6858946284,-3.927128561,3.2466475501
C,0,2.9636624284,-4.3471777192,3.6094818358
C,0,4.0389098955,-4.0851658433,2.7633712417
C,0,3.846555321,-3.4082122281,1.5646061798
C,0,3.2747561589,-3.5763459649,-1.7619293852
H,0,1.99246291,3.7056249732,-0.2936217051
H,0,1.3067420047,6.0214231821,0.1528447416
H,0,-1.0969657533,6.6056551873,0.4817358007
H,0,-2.8010565896,4.8194178498,0.3453603987
H,0,-3.4386052592,2.7209077661,0.1977534828
H,0,-6.3365871614,-1.1891552469,2.7068004488
H,0,-8.6973293889,-1.4554147234,3.4587202452
H,0,-10.550815475,-1.1131673627,1.8475530261
H,0,-10.0628369564,-0.4963418713,-0.5041155712
H,0,-7.7025119,-0.2190929505,-1.2486375327
H,0,-5.6180098793,-3.2490872629,0.4762316931
H,0,-6.2905877447,-2.7784446388,-1.1099085494
H,0,-4.6480432394,-3.4678765779,-1.0005924575
H,0,-3.0336503362,-2.6362006558,-2.021136042
H,0,-1.9888487675,-2.4344406328,-0.6109569066
H,0,4.9658713687,3.919400588,2.13505134
H,0,7.3770030787,3.6542109279,2.5832923506
H,0,8.6429936019,1.7278692228,1.6209787335
H,0,7.4491397608,0.0927460298,0.2010414159
H,0,5.6417457034,-0.7514842364,-0.7903818534
H,0,4.9263838307,-1.3500649842,-3.1094290384
H,0,3.3530076022,-1.8495486675,-3.7766984701
H,0,3.7293656334,-0.1300332741,-3.5839420505
H,0,0.4765987141,-2.9291769432,1.7679966929
H,0,0.8404009746,-4.1302618484,3.8968810857
H,0,3.1197031136,-4.8777789955,4.5435597906
H,0,5.0395800183,-4.4069720213,3.0352747148
H,0,4.6779240547,-3.1937225536,0.903209654
H,0,2.3393194001,-3.6156631989,-2.3374701206
H,0,4.1278227303,-3.6691929091,-2.434543767
H,0,3.2978137162,-4.419304074,-1.0689924501

Sum of electronic and zero-point Energies= -5447.744451
Sum of electronic and thermal Energies= -5447.699440
Sum of electronic and thermal Enthalpies= -5447.698496
Sum of electronic and thermal Free Energies= -5447.828449

$[Cu_2(\mu\text{-}O)(L^2)(L^{3'})]^+$ (S =0)

Cu,0,-0.7365340262,0.4926207938,-1.5437321728
Cu,0,2.200247954,1.1635789865,-0.2480947867
O,0,0.3121926136,1.7490907867,-0.5425727579
O,0,-4.5795576749,1.4634887553,1.3182652788
O,0,-1.7314462621,-0.6639196018,-2.5856816369
O,0,3.2270307723,2.3086325395,0.9745836559
O,0,0.9951880601,-0.0239804704,-2.502950535
O,0,0.0208333798,-1.1990584604,-0.0588936506
N,0,-2.3689669867,1.2344800506,-0.7723470449
N,0,-5.0269200198,-0.7074984865,0.5965023837
N,0,-4.5259326549,-1.5301575737,-0.4045753802
N,0,3.6359432272,0.0597772208,-0.7851179205
N,0,2.111902528,-2.2575652936,-0.136165606
N,0,3.2445483585,-2.2824775916,-1.0144162522
C,0,-0.0182347244,3.0373896987,-0.5916015216
C,0,0.9702599903,4.0267794897,-0.7091734189
C,0,0.6258305013,5.3656232961,-0.6557908016
C,0,-0.7117343856,5.767567264,-0.5101540276
C,0,-1.6986698335,4.8102045014,-0.417707933
C,0,-1.3801314796,3.4358950736,-0.4799209091
C,0,-2.4426429602,2.4928305939,-0.4265460917
C,0,-3.3149202614,0.3294213702,-0.4244508976
C,0,-4.3221371301,0.4917196562,0.6185130363
C,0,-3.4783278528,-0.9346592382,-0.9814339217
C,0,-6.3443956115,-0.8766676197,1.1000145501
C,0,-6.547617412,-0.7652414078,2.4737901934
C,0,-7.8383729419,-0.8874836206,2.9792909763
C,0,-8.9071322762,-1.1436812343,2.1228640991

C,0,-8.689930698,-1.2617569567,0.751090592
C,0,-7.4089999707,-1.1136337445,0.2290728852
C,0,-4.7334222392,-2.9651256682,-0.3280729989
C,0,-2.5262459341,-1.57596105,-1.9391919037
C,0,4.469166198,2.0963750781,1.2582659256
C,0,5.1153025704,2.9741781138,2.176472232
C,0,6.428840647,2.8049789981,2.5481354012
C,0,7.2060567009,1.7468206405,2.0319533393
C,0,6.6253964073,0.8807604942,1.1391513044
C,0,5.2745104959,1.0208617542,0.7223998833
C,0,4.8097991936,0.0649592292,-0.2215610059
C,0,3.2074846941,-0.9810357002,-1.7026173514
C,0,1.7150676349,-0.6119926259,-1.6788003006
C,0,1.1552973639,-1.3824089685,-0.5090750593
C,0,3.8971659564,-0.9423805384,-3.0445911702
C,0,2.1468696247,-3.0615845898,1.0261519923
C,0,0.9675515909,-3.3672073022,1.7141787717
C,0,1.0402365729,-4.1431223404,2.8660719278
C,0,2.2638183543,-4.6232384156,3.3273762553
C,0,3.4294920714,-4.3197237475,2.6272933024
C,0,3.3804997082,-3.5414807229,1.476723817
C,0,3.1473168956,-3.4621780939,-1.8803440018
H,0,2.0097259853,3.7219912851,-0.7860640818
H,0,1.4084252043,6.1152124682,-0.7241348384
H,0,-0.9647959692,6.8214899821,-0.4757100024
H,0,-2.7403691985,5.099589333,-0.3145841395
H,0,-3.4210765055,2.8409014055,-0.0900918051
H,0,-5.7029231122,-0.5842503153,3.1294630998
H,0,-8.0050654004,-0.7954198664,4.0479499854
H,0,-9.9102263061,-1.250952253,2.5239233034
H,0,-9.5213354608,-1.4551930058,0.0805243617
H,0,-7.2339968618,-1.1737857614,-0.8410999358
H,0,-4.1034000972,-3.4031485915,0.4518068996
H,0,-5.7819279273,-3.1707313396,-0.1177406129
H,0,-4.4804468433,-3.3956402295,-1.2972017961
H,0,-3.1113177371,-2.1104247084,-2.7086707979
H,0,-1.9551290115,-2.34817299,-1.3923459932
H,0,4.5195039454,3.7870858232,2.5809449342
H,0,6.8742061052,3.500120044,3.2555895935
H,0,8.2401313705,1.6227854938,2.3350954014
H,0,7.2041212559,0.0579885151,0.7248372473
H,0,5.5094467025,-0.7285587197,-0.5013308825
H,0,4.9487686269,-1.2230933232,-2.9446932657
H,0,3.4153679606,-1.6042244755,-3.766363047
H,0,3.8452554228,0.0795958077,-3.4247966572
H,0,0.0155616309,-2.9993943237,1.3541613945
H,0,0.1255409942,-4.3782867544,3.4016370447
H,0,2.3082672854,-5.2326260813,4.2245999091
H,0,4.3890655278,-4.6874471933,2.977597083
H,0,4.283015685,-3.2930099911,0.9302897555
H,0,2.2690153338,-3.4466564742,-2.5399522917
H,0,4.0583899124,-3.5322823128,-2.4749914689
H,0,3.0932247522,-4.3451747693,-1.2413291411

Sum of electronic and zero-point Energies= -5447.728387
Sum of electronic and thermal Energies= -5447.684017
Sum of electronic and thermal Enthalpies= -5447.683073
Sum of electronic and thermal Free Energies= -5447.809041

$[Cu_2(L^2)(L^3)]$ (S =1)

Cu,0,-0.7000816167,0.4760741328,-0.9104808298
Cu,0,2.215517794,1.2255046211,-0.8337484969
O,0,0.4084480621,2.0027835379,-0.3072294196
O,0,-5.1804436412,1.5820405192,1.1772486708
O,0,-1.5417268204,-0.937891456,-1.8940493972
O,0,3.465944511,2.4141895171,-0.0859461982
O,0,1.0193038124,0.0834610586,-1.8231520864
O,0,0.7210266478,-2.0575090672,-2.5445438648
O,0,0.3476723608,-1.3450188813,0.5207336988
N,0,-2.3234725772,1.1058133273,0.0305295574
N,0,-5.510298544,-0.5694649273,0.3699720076
N,0,-4.790383314,-1.4633885494,-0.4149313886
N,0,3.5032055673,-0.1964697362,-1.1745379253
N,0,2.3189280912,-2.4884666123,0.0664684062
N,0,3.2641337835,-2.569759593,-0.9994775044

C,0,0.0092438115,3.0873916406,0.3414825384
C,0,0.9151796465,4.1345891862,0.5845845704
C,0,0.5173493951,5.282681841,1.2496681392
C,0,-0.7990350532,5.4344377614,1.7015052185
C,0,-1.697921518,4.4115557114,1.4754023854
C,0,-1.3310014601,3.2270997148,0.7975719873
C,0,-2.378872536,2.2522613481,0.6475433418
C,0,-3.4512870143,0.2843193273,0.0227567711
C,0,-4.7494015802,0.5760845393,0.611039416
C,0,-3.5270969819,-0.9621492693,-0.5522004851
C,0,-6.9246926498,-0.5827213259,0.3294635093
C,0,-7.6332606307,-0.1576504929,1.4545140409
C,0,-9.0240553609,-0.1461652735,1.4203203887
C,0,-9.7078667855,-0.5772078432,0.2849963406
C,0,-8.9920991198,-1.0084719727,-0.8298445116
C,0,-7.6005784579,-1.0018503082,-0.819041961
C,0,-5.0203560749,-2.8790526326,-0.1431339331
C,0,-2.4401096969,-1.7501341428,-1.2204231566
C,0,4.7287921701,2.1701906894,0.1369672024
C,0,5.5062839127,3.1877700067,0.7432500268
C,0,6.8460383086,3.0064360995,1.019270064
C,0,7.4968060576,1.799234072,0.7097790014
C,0,6.7686313879,0.7913250852,0.1185913012
C,0,5.3948183465,0.9430001902,-0.1833139481
C,0,4.7419602244,-0.1662202769,-0.8082378801
C,0,2.9522665215,-1.3948604406,-1.8362503612
C,0,1.4232464631,-1.227577656,-1.6927895678
C,0,1.2577080923,-1.698384991,-0.2283471854
C,0,3.4446257228,-1.5025342974,-3.2618616294
C,0,2.6726394235,-3.0353363209,1.318926117
C,0,1.6954414092,-3.256935862,2.2965851376
C,0,2.0691219053,-3.7923163489,3.5247748576
C,0,3.3971932962,-4.1218823221,3.7873975109
C,0,4.3601178034,-3.9087412905,2.8040186508
C,0,4.0071023337,-3.3685778564,1.5717379412
C,0,3.1562496214,-3.877034573,-1.6557392399
H,0,-0.2312114188,-1.7623981407,-2.4033276253
H,0,1.9400413473,4.0057598938,0.252108661
H,0,1.2433444647,6.0730731668,1.4211420175
H,0,-1.1068374118,6.3350090332,2.2223548501
H,0,-2.7242663573,4.505628527,1.8216989595
H,0,-3.3311873066,2.5168493607,1.1098362642
H,0,-7.0930214922,0.1625813109,2.3374341926
H,0,-9.5751843894,0.1894576761,2.2937401891
H,0,-10.7934743604,-0.5774917223,0.2693281941
H,0,-9.5162840485,-1.3405088491,-1.7210020706
H,0,-7.0366968525,-1.30828164,-1.694660974
H,0,-6.086133369,-3.0910174497,-0.2267285105
H,0,-4.4954300145,-3.4661183258,-0.8960246552
H,0,-4.6665883774,-3.1538443092,0.8562082121
H,0,-2.910246927,-2.4497545824,-1.9291939911
H,0,-1.9493775919,-2.3711524034,-0.4468258472
H,0,5.0061748089,4.1203631488,0.9862749066
H,0,7.4045496525,3.8138190644,1.4858679828
H,0,8.5499988093,1.6661215146,0.9326755555
H,0,7.2470526504,-0.1525633324,-0.1326983857
H,0,5.3499055377,-1.0596462898,-0.9785013375
H,0,4.520625218,-1.6974716053,-3.2905335419
H,0,2.9132341757,-2.2875633776,-3.8008736168
H,0,3.2518411316,-0.5507961968,-3.7624788464
H,0,0.6634998526,-3.0005640818,2.0953555872
H,0,1.3072104757,-3.9582363745,4.280866594
H,0,3.6776797963,-4.5442227388,4.7474324419
H,0,5.3991472059,-4.1626265128,2.9926716289
H,0,4.7525242578,-3.1968173111,0.8037818929
H,0,2.1751096684,-4.0445977231,-2.1142284387
H,0,3.9405875111,-3.9556778863,-2.4097471724
H,0,3.3424233036,-4.6439544512,-0.9004779459

Sum of electronic and zero-point Energies= -5523.728057
Sum of electronic and thermal Energies= -5523.683728
Sum of electronic and thermal Enthalpies= -5523.682783
Sum of electronic and thermal Free Energies= -5523.808225

$[Cu_2(L^2)(L^3)]$ (S =0)

Cu,0,13.0466021708,15.1325824229,7.6267137501
Cu,0,12.5923378047,12.1451912689,6.7719249329
O,0,13.0482068967,14.013572878,5.9874370277
O,0,15.3825687385,19.2718105934,6.0098323841
O,0,12.6582884889,15.9682038695,9.2909026535
O,0,12.8304961086,10.8830065019,5.3829178452
O,0,12.3190467389,13.4397756061,8.1853032895
O,0,11.9891623645,13.7249078165,10.4345895035
O,0,14.9326384101,13.6858396803,9.2996681832
N,0,13.905797468,16.6429193492,6.7418678557
N,0,15.3880935675,19.5342096177,8.3173338524
N,0,14.8006176993,18.8842461853,9.3964679242
N,0,12.4716289159,10.8915246548,8.2508177592
N,0,14.3456848787,11.6814997977,10.3174919375
N,0,13.1608622268,10.9253757179,10.5520464748
C,0,13.2167035712,14.4424237895,4.7434317556
C,0,12.9232119005,13.5862301673,3.6673550751
C,0,13.0940508922,14.0053906003,2.3585353507
C,0,13.5616214017,15.2927145806,2.0672036763
C,0,13.8599939828,16.1421121824,3.1133409644
C,0,13.6957600279,15.753117548,4.461496065
C,0,14.0546402167,16.7296910573,5.4509212964
C,0,14.3767731741,17.6663716872,7.561498972
C,0,15.0934362387,18.8580128339,7.1335520058
C,0,14.2585985524,17.7220440342,8.9308019705
C,0,15.6497287354,20.9236358588,8.3892518816
C,0,16.7161044262,21.4442669791,7.6547247658
C,0,16.970848737,22.8112990175,7.6989443632
C,0,16.1868054786,23.6517959765,8.487068092
C,0,15.1301164038,23.1211451473,9.2240482811
C,0,14.8478002543,21.7596211831,9.1696165056
C,0,15.5342394414,18.9350293543,10.6567868735
C,0,13.689153608,16.6958669454,9.8643886986
C,0,12.9533416729,9.6009493857,5.5816154936
C,0,13.1803538546,8.7764536851,4.4485368348
C,0,13.3237543219,7.4092706836,4.5587402691
C,0,13.2547555812,6.7701598626,5.8090167602
C,0,13.0378443549,7.5405074379,6.9292774497
C,0,12.8797298793,8.9452179196,6.8571571271
C,0,12.6544862457,9.6221122783,8.1016900802
C,0,12.194715509,11.4632365296,9.5858234809
C,0,12.5836253689,12.9545955887,9.4551467333
C,0,14.1087944516,12.86270914,9.6807007011
C,0,10.7477218322,11.229291988,9.961709979
C,0,15.5899613811,11.0791269433,10.598057032
C,0,16.7557731311,11.851958202,10.6698288629
C,0,17.9705686233,11.2311928401,10.9417236295
C,0,18.0410114228,9.8563225775,11.1557712485
C,0,16.874994189,9.0973226414,11.0933139125
C,0,15.6515418841,9.6985891432,10.8172787647
C,0,12.7880937176,11.0155521663,11.9676479939
H,0,12.2104931661,14.6652064342,10.1630336567
H,0,12.5856571513,12.5800339152,3.8953741942
H,0,12.8608285233,13.3179579846,1.5498248227
H,0,13.6923387166,15.6155554925,1.039839303
H,0,14.2298860477,17.1438933096,2.9107675483
H,0,14.5086960734,17.647621679,5.0714599695
H,0,17.3286048784,20.7802370461,7.0562420614
H,0,17.7970752458,23.2179041751,7.1234796415
H,0,16.398627941,24.7158884821,8.5270431965
H,0,14.5105227626,23.7697397162,9.8360275005
H,0,14.0078386897,21.3438414535,9.7175532687
H,0,15.732692111,19.9752733813,10.9138426766
H,0,14.9092049589,18.5036795399,11.4381829391
H,0,16.4783688292,18.3845054262,10.5889222685
H,0,13.3046813267,17.219153948,10.7545363168
H,0,14.5165339428,16.0489450935,10.209375853
H,0,13.2362423279,9.2686547153,3.4822144716
H,0,13.4944169588,6.8200341959,3.6612453601
H,0,13.3712286933,5.6945880619,5.8885602337
H,0,12.9808189091,7.0706284041,7.9087079366
H,0,12.6495070059,8.9943691616,8.9983063946
H,0,10.556484903,10.1628871193,10.1114543506
H,0,10.4782635968,11.7850561643,10.8601695912
H,0,10.1210014297,11.5802461525,9.1385525679
H,0,16.7038123648,12.9193905751,10.5010734099
H,0,18.8710638377,11.8365803762,10.9918143211

H,0,18.9936056317,9.3825866416,11.3722658847
H,0,16.9117576478,8.02456536,11.259419027
H,0,14.7425528263,9.1104676776,10.7638778744
H,0,12.5501272729,12.0386846016,12.2808987994
H,0,11.9345553252,10.3612318331,12.1490866537
H,0,13.6272109625,10.6405849674,12.557807587

Sum of electronic and zero-point Energies= -5523.674746
Sum of electronic and thermal Energies= -5523.630126
Sum of electronic and thermal Enthalpies= -5523.629182
Sum of electronic and thermal Free Energies= -5523.755312